# EU ACADEMY OF SCIENCES
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# The President of EUAS

Professor E.G. Ladopoulos

# & The Board Governors of EUAS

# Contents

**11** **Is 4-D Real Time Expert Seismology the most Convenient Petroleum Exploration Method for the Major Petroleum Companies ?**
**by Prof. Evangelos Ladopoulos, President & CEO of EUAS**

**17** **Standard Model Reformation in Fundamental Subatomic Physics.**
**by Prof. Bo Lehnert, Member EUAS**

**23** **Laser-Based Advanced Manufacturing and Nano-photonics.**
**by Prof. Lin Li, Member EUAS**

**27** **Colorectal Carcinogenesis & the Biology of GI Cancer Cell Invasion & Metastasis.**
**by Prof. Robert Daniel Beauchamp, Member EUAS**

**31** **Mathematical Models in Flood Management Mitigation and Control : A Brief Overwiew.**
**by Prof. Daniele De Wrachien, Member EUAS**

**36** **New Findings Using Spaceborne Remote Sensing for Condition Monitoring of Soils, Vegetation and Glaciers.**
**by Prof. Manfred F. Buchroithner, Member EUAS**

**41** **Research Activities within Structural Safety, Monitoring and Control.**
**by Prof. Hong-Nan Li, Member EUAS**

**44** **Electrochemical Applications for Clean Energy Generation / Storage and Corrosion Control.**
**by Prof. Jingli Luo, Member EUAS**

**48** **Innovative Computing Methods in Cloud Computing, Big Data and Bioinformatics Applications.**
**by Prof. Yi Pan, Member EUAS**

**52** **Synthesis and Processing of Nanomaterials for Energy Storage and Structural Applications.**
**by Prof. Leon L. Shaw, Member EUAS**

**56 Unusual Photophysical Phenomenon the Aggregation-Induced Emission (AIE) & the Exploration of High-Tech Applications of AIE Luminogens (AIEgens).**
**by Prof. Ben Zhong Tang, Member EUAS**

**60 Stochastic Optimal Control Problems with Fixed Terminal Time & First Exit Time.**
**by Prof. Kok Lay Teo, Member EUAS**

**64 Acid Catalysis & Asymmetric Catalysis for C- C Bond Formation by Chiral Lewis and Brønsted Acids.**
**by Prof. Hisashi Yamamoto, Member EUAS**

**67 Double Wall & Jet Array Cooling - Turbine Blade Heat Transfer & Flow Dynamics.**
**by Prof. Phil Ligrani, Member EUAS**

**73 New Investigations in Flat Panel Technolgies.**
**by Prof. Vladimir Chigrinov, Member EUAS**

**77 Investigations in Atmospheric Propagation & Microwave Biophysics.**
**by Prof. André Vander Vorst, Member EUAS**

**82 Progress on the Next Generation of Subsea Production System.**
**by Prof. Menglan Duan, Member EUAS**

**86 Recent Trends in Biomedical Materials and Clinical Biochemistry.**
**by Prof. Pankaj Vadgama, Member EUAS**

**92 New Contributions in Aletrnative Energy.**
**by Prof. Arthur Ragauskas, Member EUAS**

**97 Resilience of Structures and Infrastructure under Extreme Transient Loads.**
**by Prof. Adnan Ibrahimbegovic, Member EUAS**

**101 Distributed Resilient Secondary Control of DC Microgrids against Unbounded Attacks.**
**by Prof. Frank Lewis, Member EUAS**

**104 New Contributions in Inorganic Materials Chemistry.**
**by Prof. Glen Deacon, Member EUAS**

**107 Big Picture of Relativistic Molecular Quantum Mechanics.**
**by Prof. Wenjian Liu, Member EUAS**

**112 Functionalized Cellulose Nanocrystals for Advanced Material Applications.**
**by Prof. Qinglin Wu, Member EUAS**

**118 New Trends at the Institute of Nanotechnology (INT) of the Karlsruhe Institute of Technology (KIT).**
**by Prof. Herbert Gleiter, Member EUAS**

**122 Experiments on Continuous Unbonded Post-Tensioned Beams.**
**by Prof. Thomas Kang, Member EUAS**

**125 Epigenetics Drug Discovery for Cancer.**
**by Prof. William Nelson, Member EUAS**

**129 Fatigue and Fracture Mechanisms of Metallic Materials.**
**by Prof. Zhe Feng Zhang, Member EUAS**

**134 Mechano - Electrochemical Effect of Pipeline Corrosion.**
**by Prof. Y. Frank Cheng, Member EUAS**

**138 Optoelectronic Materials and Applications.**
**by Prof. Henry Radamson, Member EUAS**

**142 Bata Quay Wall Design and Ground Characterization.**
**by Prof. Pedro Pinto, Member EUAS**

**146 Materials Science, Novel Materials for Environmental Responsive Applications.**
**by Prof. Shu Yin, Member EUAS**

**150 Climate Change & Variability, Climate Forecasting & Hydrometeorology.**
**by Prof. Chris Folland, Member EUAS**

**156 Lithium Ion Battery Fire Dynamics & Prevention - Research on Hydrogen Safety.**
**by Prof. Jinhua Sun, Member EUAS**

**160 The "Nanomachine", NhaA Na+/H+ Antiporter.**
**by Prof. Etana Padan, Member EUAS**

**163 Hydrodynamics of Fluidization & Heat Transfer: Supercomputer Modeling.**
**by Prof. Dimitri Gidaspow, Member EUAS**

**166 Novel Synthesis and Property of Inorganic 1D/2D Nanomaterials and Their In-situ TEM Study.**
**by Prof. Yoshio Bando, Member EUAS**

**169 Toward Data Science Computing Model: Interactive Granular Computing (IGrC).**
**by Prof. Andrzej Skowron, Member EUAS**

**173 Progress in Nanomagnetism.**
**by Prof. Hartmut Zabel, Member EUAS**

**177 Disorder and Interface Dominated Architected Metastable Materials.**
**by Prof. Jürgen Eckert, Member EUAS**

**181 Artificial Intelligence & Robotic Solutions for Complex Applications.**
**by Prof. Andrew Goldenberg, Member EUAS**

**184 Aerosol Sciences and Nanoparticle Technology to Biophysics.**
**by Prof. Wolfgang Kreyling, Member EUAS**

**187 Application of Neutron Radiography to Study Water Movement in Porous Materials.**
**by Prof. Folker H. Wittmann, Member EUAS**

**192 Spray-on Piezoelectric Transducer Technology.**
**by Prof. Bernhard R. Tittmann, Member EUAS**

**197 Mechanical and Physiological Role of Bone Microdamage / Bone Quality.**
**by Prof. David B. Burr, Member EUAS**

**202 Recent Contributions of Thermodynamics & Kinetics of Nanomaterials.**
**by Prof. Qing Jiang, Member EUAS**

**205 Atomic Layer Deposition of Emerging 2D Semiconductors, HfS2 and ZrS2, for Optoelectronics.**
**by Prof. Markku Leskelä, Member EUAS**

**211 Contributions in Numerical Methods for Singularly Perturbed and Degenerate PDEs and PDE constrained Optimisation Problems in Classic and Financial Engineering.**
**by Prof. Song Wang, Member EUAS**

**215 Sleep Scheduling in Energy Harvesting Wireless Body Area Networks.**
**by Prof. Amiya Nayak, Member EUAS**

**221 Possibility for Controlling Global Warming by Launching Nanoparticles into the Stratosphere.**
**by Prof. Shigenao Maruyama, Member EUAS**

**225 In-Phase and Anti-Phase Synchronization in a Laser Frequency Comb.**
**by Prof. Erich Gornik, Member EUAS**

**227 Two-Drug Combinations as First-Step Antihypertensive Treatment.**
**by Prof. Giuseppe Mancia, Member EUAS**

**232 Advances in Water Microbiology, Water Quality and Public Health Safety.**
**by Prof. Joan Rose, Member EUAS**

**237 Drug-drug Interaction Extraction based on Transfer Weight Matrix and Memory Network.**
**by Prof. Fuji Ren, Member EUAS**

**240** **Mechanics of Compliant Materials.**
**by Prof. Alan D. Freed, Member EUAS**

**244** **A Sputtered Nanocrystalline Coating For High Temperature Applications On The Nickel-base Single Crystal Superalloy René 5.**
**by Prof. Fuhui Wang, Member EUAS**

**249** **Viruses in the Brain...? Any Connections to Parkinson's and other Neurodegenerative Diseases?**
**by Prof. Alain L. Fymat, Member EUAS**

**253** **Supercritical Hydrothermal Reactions for Material Synthesis.**
**by Prof. Tadafumi Adschiri, Member EUAS**

**258** **Vehicle Scanning Method for Bridges.**
**by Prof. Yeong-Bin Yang, Member EUAS**

**262** **University Education in Crisis. Transdisciplinary Approaches in the Arts, Humanities and Sciences.**
**by Prof. Marcel Van de Voorde, Member EUAS**

**268** **PST TiAl Single Crystals - High-Strength Low-Alloy Steels.**
**by Prof. Guang Chen, Member EUAS**

**272** **Conversion of Mg-Li Bimetallic Alloys to Magnesium Alkoxide and Magnesium Oxide Ceramic Nanowires.**
**by Prof. Gleb Yushin, Member EUAS**

**276** **Optimizing Analysis of Spectral Data.**
**by Prof. David Aspnes, Member EUAS**

**279** **Oral Peptide Delivery using Intestinal Permeation Enhancers and Nanoparticles.**
**by Prof. David J. Brayden, Member EUAS**

**284** **Recent Developments in Ion-Solid Interactions.**
**by Prof. William J. Weber, Member EUAS**

**287** **Innovative Energy Research at University of Stavanger.**
**by Prof. Mohsen Assadi, Member EUAS**

**292** **Mechanistic-Empirical Analysis of Geogrid-Stabilized Layered Systems.**
**by Prof. Jie Han, Member EUAS**

**297** **Data Science with Integration of Methodology and Application Domain.**
**by Prof. Fionn Murtagh, Member EUAS**

**302** **Photon Generation by Electron Transfer Reactions at Electrodes and Development of Sensors.**
**by Prof. Kalathur Santhanam, Member EUAS**

**306** **Global Potential Energy Surface for HO2+ Using the CHIPR Method.**
**by Prof. António Varandas, Member EUAS**

**312** **New Contributions of Robotics for Societal Services.**
**by Prof. Aarne Halme, Member EUAS**

**317** **Electrochemical Surface and Interface Science of Applied Electrochemical Systems.**
**by Prof. Roland De Marco, Member EUAS**

**321** **Constitutive Model of Material Behavior.**
**by Prof. Viktor P. Astakhov, Member EUAS**

**324** **Structuring and Functionalization of Materials in Green Energies and Biosensing Systems.**
**by Prof. Changming Li, Member EUAS**

**329** **New Aspects of Advanced Materials for Energy Storage & Conversion.**
**by Prof. Zongping Shao, Member EUAS**

**333** **Sluggish Kinetics of the Oxygen Reduction Reaction (ORR) & the Oxygen Evolution Reaction (OER).**
**by Prof. Shaojun Guo, Member EUAS**

**336** **Ferritin - Conjugated Lectins for Cell Surface Carbohydrate Structures.**
**by Prof. Garth L. Nicolson, Member EUAS**

**343** **Science and Technology of a Multifunctional Oxide and Nanocarbon Thin Films and Application to Development and Commercialization of a New Generation of Multifunctional Industrial, High-Tech and Implantable Medical Devices.**
**by Prof. Orlando Auciello, Member EUAS**

**349** **Stability and Barrier Systems of Municipal Waste Deposits.**
**by Prof. Heinz Brandl, Member EUAS**

**352** **Nanostructured Electrode Materials for Energy Applications.**
**by Prof. Haitao Huang, Member EUAS**

**356** **Material Model to Capture the Damage Effects in a Football Player's Brain.**
**by Prof. Mark F. Horstemeyer, Member EUAS**

**359** **Transforming Liquefied Natural Gas (LNG) Plant Construction Productivity through Mobile Computing Technologies.**
**by Prof. Xiangyu Wang, Member EUAS**

**363** **Vascular Dysfunction in Cardiovascular (CV) Disease.**
**by Prof. Thomas F. Lüscher, Member EUAS**

**366** **Improvements in Watershed Science.**
**by Prof. Jeffrey J. McDonnell, Member EUAS**

**370** **Publication Ethics in the Open-Access Era.**
**by Prof. George Perry, Member EUAS**

**375** **Global Change Impact on Deep-Sea Ecosystems.**
**by Prof. Roberto Danovaro, Member EUAS**

**381** **A Method for Design of High Strength Concrete Composition Considering Curing Temperature and Duration.**
**by Prof. Yuri Ribakov, Member EUAS**

**384** **New Aspects by using Remotely Sensed Spatiotemporal Information to tackle Emerging Environmental Problems.**
**by Prof. Soe W. Myint, Member EUAS**

**390** **Activities in Materials Science and Engineering.**
**by Prof. Derek O. Northwood, Member EUAS**

## 397 Non-invasive Load Monitoring of Induction Motor Drives using Magnetic Flux Sensors.

**by Prof. Wenping Cao, Member EUAS**

# Is 4-D Real Time Expert Seismology the most Convenient Petroleum Exploration Method for the Major Petroleum Companies ?

## by Evangelos Ladopoulos, President & CEO of EUAS

Short Biography

*Prof. Dr. Civil Engineer, Mechanical (Aerospace) Engineer & Petroleum Engineer, D.Sc.*
*Included in the list of 2000 Outstanding Scientists of 20th Century by Cambridge Bio Centre.*
*Included in the list of 2000 Outstanding Scientists of 21st Century by Cambridge Bio Centre.*
*Included in the list of 100 Top Scientists of 2007 by Cambridge Bio Centre.*
*Over 400 publications in high quality scientific journals and 5 books.*
*Project Manager for over 500 Projects in Civil Engineering, Mechanical Engineering, Aerospace Engineering and Petroleum Engineering.*
*Chairman and Professor by Interpaper Research Organization.*
*Visiting Professor at Universities in Europe and USA.*
*Editor-in-Chief of many SCI Engineering Journals.*
*High Index by Google Scholar.*
*President & CEO of the EU Academy of Sciences.*
*Member by several Academies in USA.*

*"Non-linear Real-Time Expert Seismology"* is proposed for the designation of the exact location of the on-shore and off-shore oil and gas reserves all over the world. Such sophisticated method, is applied by using a non-linear 3-D elastic waves real - time expert system and so the on-shore and off-shore petroleum reservoir can be easily determined. Also, the exact location of the oil reserves may be designated in the special areas where anticlines occur. The above very modern petroleum exploration method is working under Real Time Logic for searching the on-shore and off-shore oil & gas reserves developed on the continental crust and on deeper water ranging from 300 to 3000 m, or even deeper. Besides, the modern technology of petroleum reserves exploration can be used at any depth of seas and oceans worldwide and for any depth in the subsurface of existing petroleum reservoir. On the other hand, very recent theoretical and experimental evidence demonstrates the possibility that hydrocarbons may have formed in the depths of the earth, according to the theory of abiotic hydrocarbon generation. If this is true, then the proposed groundbreaking method can be used for the exploration of oil reservoir in very deep depths, like 20,000 to 30,000 m. Thus, 3-D seismic information allows petroleum engineers and scientists to see a more reliable view of the underground area. By the current research it will be shown that 4-D seismic imaging is more convenient than 3-D imaging, as it incorporates many 3-D seismic surveys over the same reserves at specified intervals of time. So, by studying multiple time-lapsed 3-D surveys, or three-dimensional subsurface images, portrays the changes in the reservoir over time. As every very deep drilling costs more than 100 mill EURO, then the major petroleum companies should have many

financial losses for dry drillings. By the proposed sophisticated study the exact location of every big petroleum reserves can be exactly designated.

## 1. Petroleum Generation by the Abiotic Theory

The energy demand for petroleum will increase up to 2030 by 50-60%, as it is increasing worldwide yearly at a pace of 1.5 to 2.0%. Besides, the total estimated hydrocarbon worldwide in place stands today approximately at 1.5 trillion barrels, and with current petroleum consumption at 90 million barrels per day, the hydrocarbons in place are predicted to last for the next 40 years. Thus, there is an absolute need by the major petroleum companies worldwide to increase their stock by finding new petroleum reservoir. For this reason major petroleum companies should be looking into other alternatives, like to drill to ever deeper horizons and in the relatively unexplored ocean depths.

As it is well known, oceans cover about 70% of the earth's surface and most of the waters are at more than 2000 m deep. So, major petroleum companies and scientific oil organizations should be prepared for tapping into the relatively unknown areas with potential for large discoveries. In order to answer to the question how deep the major companies should drill to find petroleum and gas, then the current depth records should be stated. Up to today, the deepest hole ever created by humans lies beneath the tower enclosing Kola's drill, in Russia. A number of boreholes split from the central branch, but the deepest is designated "SG-3," a hole about nine inches wide which snakes over 12.262 kilometers (7.5 miles) into the Earth's crust. The drill spent twenty-four years chewing its way to that depth, until its progress was finally halted in 1994, about 2.7 kilometers (1.7 miles) short of its 15,000-meter goal. The KOLA peninsula borehole, drilled in 1984, reached the crystalline basement, and gases like, He. H2, N2, CO2, methane and other hydrocarbons flowed at a depth of 9101 m. Hence, it was a very big surprise to the petroleum engineers, that they didn't find the expected transition from granite to basalt at 3-6 kilometers beneath the surface. Additionally, data had long shown that seismic waves travel significantly faster below that depth, and geologists and petroleum engineers had believed that this was due to a "basement" of basalt. Instead, the difference was discovered to be a change in the rock brought on by intense heat and pressure, or metamorphic rock.

Furthermore, deepest gas wells have been in Anadarko basin, Oklahoma, USA. There were two wells, drilled in the 1970s. Well GHK/Lone Star Bertha Rogers #1-27, for which drilling started in 1974 and stopped at 9,583 m when it struck molten sulfur. The second deepest U.S. well was the Lone Star/GHK #1-28 E.R. Baden well (total depth 9,162 m), for which drilling started in 1970 and ended in 1972. Also, deepest petroleum producing subsea well is in the Perdido field, located 200 miles south of Freeport Texas operated by Shell. This is the deepest drilling and production facility in the world, placed in 2382 m of water, operated by Shell in the Gulf of Mexico. Full development plan calls for a total of 35 wells. Another very deep producing offshore well is in the Tahiti field in the Gulf of Mexico, in a depth of more than 8138 m, a record for the Gulf, according to Chevron.

On the other hand, the existence of very big petroleum reserves in very deep depths of the earth's subsurface can be proved by the abiotic theory of hydrocarbon generation. According to the theory of abiotic (or abiogenic) origin of petroleum, the hydrocarbons have been formed in the depths of earth by reduction of CO2 and H2 gases in the presence of metal catalysts. So, the consequences of this theory, could be extraordinary, as earth's mantle becomes the inexhaustible provider of the cheapest energy source on earth, by today's standards, and shattering not only the oil-depletion myth but also pointing out to oil-rich regions in places devoid as prolific as before, because of belief of biogenic origin.

Consequently, the abiotic theory of the genesis of petroleum states that under high pressures (less than 5000 bar) and high temperatures (between 500 and 1500 $C^{o}$) methane could be formed from reduced carbon resulted from calcite. The process has been supported theoretically, via thermodynamic analysis, and experimentally. Besides, methane can be formed from volatile rich fluids resulting from partial melting of rocks within earth's interior. Thermodynamics indicate that at 1300 K, CO2 and CO should be the predominant carbon rich gases, while at lower temperatures CH4 should be predominant. Strong support for this hypothesis is the fact that methane and

hydrocarbons are abundant in the outer solar system. There is therefore reported evidence of abiotic formation of complex organics from methane in Saturn's satellite Titan's atmosphere, although it is stated that there may be no connection to primitive earth, because at the low surface temperature of Titan (at 46 K) all water is turned into ice.

In addition, the finding of very deep gas reservoirs, down to almost 10,000 m, with extremely high success rates of more than 55%, has also been reported as evidence of abiotic generation of hydrocarbons. So, the major petroleum companies should be rethinking about oil and gas exploration strategies in view of the substantial evidence about abiotic hydrocarbon origin. On the contrary, it was analyzed theoretically, via thermodynamic computations, the possibilities for hydrocarbon generation at high pressures and temperatures and showed that it is possible. By using therefore the abiogenic theory of hydrocarbon generation it can be concluded that Earth's hydrocarbon budget is much larger than it is currently thought.

As the recent theoretical and experimental evidence demonstrates the possibility that petroleum may have formed in the depths of the earth, then major petroleum companies must be ready to face the new challenges of drilling even deeper, to the basement rock, where very huge oil and gas fields may await to be discovered. Thus, modern technologies will have a major impact in the future. Through the technological progress to be achieved in the future exploration, then major reductions in costs can be very much expected. It is believed that the expected progress of enhanced oil recovery methods will reduce their future technical cost substantially. It is therefore absolutely sure that drilling depths will be increasing in the future and the industry should be geared up and ready for meeting the many challenges. According to the current research the drillings in the near future could reach the 20,000 m, or even the 30,000 m in the subsurface of earth.

On the contrary, since 1920 and for over a century the basic and prevalent theory on petroleum reserves exploration, was *"Reflection Seismology"* and *"Refraction Seismology"*. According to the above methods the basic idea is to collect reflections of elastic (seismic) waves and then through various mathematical operations, by using Snell's law and Zoeppritz equations or the Kirchhoff equations to convert them to maps of the earth's structure. Hence, the methods of *"Reflection Seismology"* and *"Refraction Seismology"* for almost a century, have been used with several improvements for petroleum resources exploration.

By the present research for the on-shore and off-shore petroleum reservoir exploration the new theory of *"Non-linear Real-Time Expert Seismology"* is further improved, as was recently proposed by E.G.Ladopoulos. Besides, the above theory results as an extension of the non-linear methods for fluid mechanics as proposed by E.G.Ladopoulos. Hence, *"Non-linear Real-Time Expert Seismology"* is a very "*innovative*" and "*groundbreaking*" method on oil and gas reserves exploration. According to the above modern method a non-linear 3-D elastic waves real - time expert system is proposed for the exploration of oil and gas resources all over the world, including the off-shore petroleum reservoir, of the seas and oceans worldwide. This modern generic technology will work under Real Time Logic] for searching off-shore fuel reserves developed on the continental crust and on deeper water ranging from 300 to 3000 m, or even much more. Furthermore, the new exploration method will be the best device for searching the on-shore and off-shore hydrocarbon resources in very deep depths, even approaching 20,000 m or 30,000 m. So, by using a new and very sophisticated model, then the exact location of petroleum reserves may be designated in the special areas where geological anticlines occur.

Thus, there are many basic benefits for the new theory of "*Non-linear Real-Time Expert Seismology*" in comparison to the existing theories of *"Reflection Seismology"* and *"Refraction Seismology"*, which makes the new method to be the most convenient method for petroleum exploration. Some of them are the following:

A) The new method *"Non-linear Real-Time Expert Seismology"* is based on the special form of the geological anticlines, normal faults, reverse faults or deformations caused by intrusion of the bottom of the sea, in order to decide which areas of the bottom have the most possibilities to include hydrocarbon reserves. This is effected by using the proposed modern technology.

On the contrary, the existing theory is only based to the best chance and do not include any theoretical and sophisticated model. Thus, currently big oil companies by using the existing

methods of *"Reflection Seismology"* and *"Refraction Seismology"* must do a lot of expensive test drillings in big areas of seas, if they want to have a chance to find oil and gas reserves. As every deep drilling cost at least 100 mill. EURO, then every dry drilling would cost a lot of money to petroleum companies.
B) The new proposed technology of elastic (sound) waves is based on the difference of the speed of the sound waves which are travelling through solid, liquid, or gas. In a solid the elastic waves are moving faster than in a liquid and the air, and in a liquid faster than in the air. On the other hand, existing theories are based on the applications of Snell's law and Zoeppritz equations or the Kirchhoff equations, which are not giving good results, as these which we are expecting by the new method.
C) The new method *"Non-linear Real-Time Expert Seismology"* is based on a Real-time Expert System working under Real Time Logic, that gives results in real time, which means every second. Existing theories do not include real time logic.

From the above described analysis, it is clear the evidence of the applicability of the new technology of "*Non-linear Real-Time Expert Seismology*". Also its novelty, as it is based mostly on a theoretical and very sophisticated Real-time Expert model and not to practical tools like the existing methods. Thus, the new method will be the best technology for searching the very deep waters (2000 to 3000 m, or even more) and the very deep depths of the basement rock of earth (20,000 to 30,000 m).

In addition, through the new technology exact 3-D images are produced of the underground topography of the area. Besides, 4-D imaging can be taken on a given area multiple times over an extended period of time. Thus, through the current research the 4-D seismic imaging is proposed, which incorporates many 3-D seismic surveys over the same reservoir at specified intervals of time. Studying multiple time-lapsed 3-D surveys, or three-dimensional subsurface images, portrays the changes in the reservoir over time. Four-Dimensional seismic can determine changes in flow, temperature, pressure and saturation. By scanning a reservoir over a given period of time, the flow of the hydrocarbons within can be traced and better understood. For example, as hydrocarbons are depleted from a field, the pressure and composition of the fluids may change. Furthermore, geologists are interested in understanding how the reservoir reacts to gas injection or water flooding. So, 4-D seismic can help to locate untapped pockets of oil or gas within the reservoir. Typically, 4-D seismic data is processed by subtracting the data from one survey from the data of another. The amount of change in the reservoir is defined by the difference between the two. If no change has occurred over the time period, the result will be zero.

## 2. Is Four-dimensional Non-linear Real-time Expert Seismology the most Convenient Petroleum Exploration Method ?

In general, off-shore operations consist of 90% of all data collected worldwide for petroleum reserves exploration. The depth of the drillings are usually up to 6000 m, but as discussed in the previous section in order to find big petroleum and gas reserves they must be extended to 10,000 m or even from 20,000 m to 30,000 m. Additionally, by studying geological surveys all over the world indicate that petroleum reserves do not necessarily end at the edge of the continental shelf. Hence, there is a serious expectation that main resources will be found in areas of thick sedimentary sequences developed on the continental crust. According to the new exploration method oil reservoir should occur in areas of geological anticlines. Also, there are good possibilities for finding off-shore petroleum and gas reserves in deeper waters, too, ranging up to 2500 m to 3000 m, or even more and in very deep drillings ranging from 20,000 to 30,000 m.

Setting the stage for all studies of reservoir performance is the physical nature of the reservoir itself, its location, structure, lithology, internal geometry and extent. There are four basic conditions that must be satisfied in order a geological part to form a suitable reservoir, for example for the accumulation of petroleum and gas. These are porosity, permeability, seal and closure. By porosity is defined the pore space in the rock - space in which the oil and gas may collect. Permeability is the attribute of the rock that permits the passage of fluid through it. In general, it is a measure of the

degree interconnectedness, of the pore space, but some reservoir (e.g. in the massive limestone deposits, or in igneous intrusions) depends for fluid flow on a network of fractures within the rock.

Moreover, by seal is denoted the "cap" of the reservoir and prevents the petroleum from leaking away. Closure is a measure of the vertical extent of the sealed trap or, in the case of hydrocarbon accumulation bounded below by a moving body of water, of the "height" of the sealed trap where that height is measured along a line perpendicular to the oil - water contact.

Three general categories of resources can be mentioned for off-shore reserves: structural traps, stratigraphic traps and combination traps. Sometimes there was no trap along the path of the water / hydrocarbon mixture as it moved through the formation on its journey from the source beds. In some cases those traps that were present were insufficient in volume to hold all of the hydrocarbons in the percolating stream and sometimes the seal of the trap was not perfect. In each of these circumstances, some of the petroleum moved eventually into near-surface locations where most of the light ends evaporated over the years, leaving behind a heavy tarlike residue, so thick that it would no longer flow at ambient temperatures.

In addition, elastic waves are sound waves, usually three-dimensional which may be transmitted through matter in any phase - solid, liquid, or gas. Thus, in general any body vibrating in air gives rise to such waves, as it alternately compresses and rarefies the air adjacent to its surfaces. Also, a body vibrating in a liquid, or in contact with a solid, likewise generates similar longitudinal waves. It is obvious that the frequency of the waves is the same as the frequency of the vibrating body that produces them. Hence, there are two types of elastic waves produced: a) P-waves, which are primary or “compressional” waves, and b) S-waves, or shear waves.

On the contrary, wavelength of the wave is the distance between two successive maxima (or between any two successive points in the same phase) and is denoted by $l$. Since the waveform, traveling with constant velocity $u$, advances a distance of one wavelength in a time interval of one period, then follows that the velocity of sound waves $u$ is given by the following relation:

$$u = l\, v \tag{2.1}$$

in which $v$ denotes the frequency.

Thus, it is clear, that the velocity $u$ differs when the sound waves are traveling through solid, liquid, or gas. In a solid the elastic waves are moving faster than in a liquid and the air, and in a liquid faster than in the air. If searching for example for off-shore petroleum resources over the sea, by transmitting sound waves, then there will be a difference in the velocity of the waves in the sea, the solid bottom and in a potential reservoir.

In order the new technology to be better explained, consider the example of Figure 1. In the above example consider that in the bottom of the sea there is a potential petroleum reservoir. In this case, the speed of the elastic waves in the air ($u_{air}$), will be different from the speed in the water ($u_{water}$), and different from the speed in the solid bottom ($u_{solid}$) and different from the speed in the potential reservoir ($u_{oil}$), while the frequency of the elastic waves remaining the same when transmitted through every different matter.

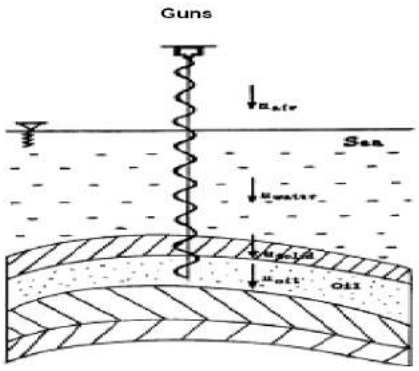


**Fig. 1** Elastic Waves Method for the Exploration of Oil Reserves.

Consequently, by the current research a real - time non-linear 3-D plane - polarized elastic waves expert system is proposed in order to explore the on-shore and off-shore petroleum reserves, according to the new theory of *"Non-linear Real-Time Expert Seismology"*, in contrast to the old theory of *"Reflection Seismology"*. This modern and innovative Sound Waves Technology will work under Real Time Logic for searching off-shore petroleum reserves developed on the continental crust and on deeper waters ranging from 300 m to 3000 m, or even deeper and for very deep depths in the subsurface of earth up to 20,000 m or even to 30,000 m (Figure 2). So, according to the theory of abiotic generation of hydrocarbon resources there are many deeper water prospects around the seas and oceans all over the world, but because of the paucity of the available information it is not possible at present to quantify the amounts that may be recoverable from them.

Thus, the proposed real - time elastic waves expert system will be the best device for the exploration of the continental margin areas and the very deep waters ranging of more than 2500 ÷3000 m, too. Moreover, through the very sophisticated method of "*Non-linear Real-Time Expert Seismology*", will be effected the exploration of a significant part of on-shore and off-shore oil and gas reserves even in drilling depths of 20,000 m to 30,000 m, very fast and by a low cost.

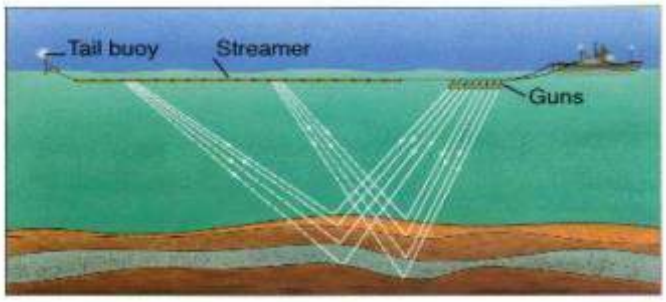


**Fig. 2** Non-linear Real-time Expert Seismology.

According to the proposed theory of *"Non-linear Real-Time Expert Seismology"* the average velocity of the sound waves is calculated by providing important information about the composition of the solids through of which passed the sound waves. For example the velocity of the sound waves through the air is 331 m/sec, through liquid 1500 m/sec and through sedimentary rock 2000 to 5000 m/sec. Moreover, according to the law of Reflection the angle of reflection equals the angle of incidence (Figure 3). Then according to the new method the arrival times of the seismic waves are analyzed. After the sensor measures the precise arrival time of the wave, then the velocity of the wave can be calculated by using a sophisticated method.

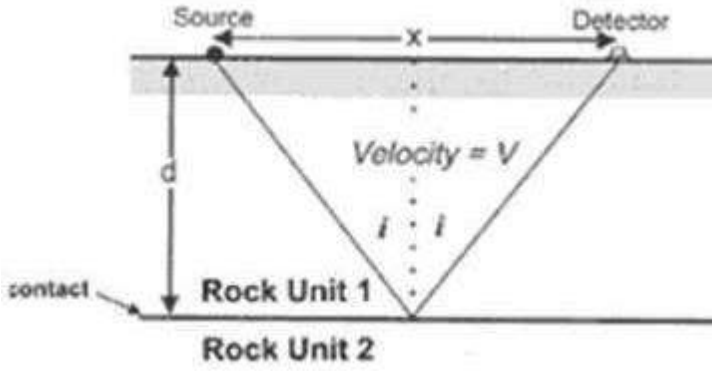


**Fig. 3** Law of Reflection.

So, the *"Non-linear Real-Time Expert Seismology"* is really the most convenient method for petroleum exploration by the major petroleum companies.

# Standard Model Reformation in Fundamental Subatomic Physics

## by Bo Lehnert, Member EUAS

Short Biography

*Born in Stockholm, Sweden, on March 30 in 1926.*
*Doctoral degree at Royal Institute of Technology, Stockholm 1955. Full Professor, Personal Chair of Swedish Atomic Research Council in 1968. Head of Plasma Physics Division of European Physical Society 1969-1972. Member of International Fusion Research Council of the International Atomic Energy Agency, Vienna, in 1970–1991.*
*Fellow of Institute of Mathematics and its Applications, London, 1973, member of Royal Swedish Academy of Sciences 1974, of Royal Swedish Academy of Engineering Sciences 1975, of the Electromagnetics Academy, Cambridge, Mass. USA, 1980. Original contributions in international journals on magnetohydrodynamics, plasma physics, thermonuclear fusion, revised quantum electrodynamics and subatomic physics, with five books in these fields.*
*Recipient of Edlund Prize of Royal Swedish Academy of Sciences, of Celsius Gold Medal of the Science Society in Uppsala, and of the Medal of His Majesty the King of Sweden.*

**Abstract**

To extend the research beyond the conditions of conventional atomic physics, a study of the internal properties of elementary particles becomes necessary, in terms of subatomic physics. The Standard Model of elementary particles, with its associated concept of a vacuum state of empty space, leads to strongly restricted results in subatomic physics. Examples are given by vanishing rest masses and an associated spinless state of the photon. In a revised quantum electrodynamic theory by the author, new results have been deduced which cannot be obtained from the Standard Model. These are due to a vacuum state populated by Zero Point Energy and a corresponding nonzero electric charge density. This leads to a screwshaped photon configuration with rest mass, spin and possibilities of needle radiation, to a deduced value of the elementary charge of the electron, muon and tauon being close to its experimental value, to a deduced mass being nearly equal to 125 GeV of the Higgs particle detected at CERN, and to the discovery of large intrinsic charges of both polarities within the volume of a particle. In their turn, these charges give rise to effects of the same magnitude as that of the strong force, and can account for the binding energy of 8 MeV of the neutron and proton. This makes a unification possible of electrodynamics with the strong nuclear force.

### 1. Introduction

In conventional electromagnetic theory of atomic physics, particles of given charge and mass form the basis of corresponding macroscopic field equations. The particles are embedded in a vacuum of empty space. This theory is well established, and is not considered in this investigation.

To extend research *beyond* the conditions of atomic physics, and to study the interior of elementary particles, a different situation has to be handled. This concerns the microscopic structures and behaviour of the original sources of the same particles, in terms of *subatomic* physics.

In a vacuum of empty space, however, the lack of sources for charge and mass severely restrict the corresponding solutions of the field equations. As shown in recent investigations by the author, these restrictions can be removed in the case of a vacuum state which includes the concept of Zero Point Energy (ZPE).

The fundamental properties of elementary particles have earlier been discussed by the author in terms of subatomic physics, as given by a revised quantum electrodynamic theory [1,2]. These properties will here be reconsidered with special emphasis on the concepts of rest mass, spin, elementary electric charge, intrinsic electric charges, needle radiation, the strong force, the binding energy of neutrons and protons, the Higgs mass, and the relation between relativity and quantum mechanics.

The shortcomings of conventional theory, based on a vacuum state of empty space, will first be elucidated in Section 2. This is followed in Section 3 by a description of the revised subatomic field equations of a vacuum state populated by Zero Point Energy. In its turn, this leads to new subatomic properties of the elementary particles, as being discussed in Section 4.

## 2. Shortcomings of Conventional Theory

In conventional electromagnetic theory and such applications as plasma physics, particles of *given* electric charge and mass form the basis of corresponding macroscopic field equations. The latter are then related to a vacuum state of empty space. This theory is well established and will not be further discussed here.

A different situation arises, however, when attempts are made to treat the *interior* of elementary particles in terms of subatomic theory. In this section some important examples are given on what happens if the vacuum concept of empty space is being retained. It implies that the electric charge density represented by the local value div **E** of the electric field strength **E** *vanishes* identically.

The first example concerns the conventional equations being applied to a model of the propagating photon, treated with div **E** = 0 by means of the Hertz vector, as given by Stratton[3]. According to Chapter 9 of [1], these equations have solutions in plane, cylindrical, and spherical geometry which all lead to a vanishing total angular momentum (spin). In particular for cylindrical geometry the local spin contributions $s_{z1}$ and $s_{z2}$ of the TM and TE wave types become

$$s_{z1} = s_{z2} \propto K^2 n[J_n(Kr)]^2 (\sin 2n\varphi) \tag{1}$$

where:

$$K^2 = (\omega/c)^2 - k^2 \tag{2}$$

for a wave form $f(r)\exp[i(-\omega t+kz+n\varphi)]$ in a cylindrical frame $(r,\varphi,z)$ with $J_n(Kr)$ as a Bessel function. The total integrated contribution to the spin then vanishes for all $K$ and $n$. Consequently, conventional theory does not become reconcilable with a physically relevant photon model which should possess spin according to experiments.

The second example concerns the steady state with both div **E** = 0 and $\partial/\partial t = 0$. Then the charge density $\varepsilon_0$ div **E** and curl **B** of the magnetic field **B** will vanish. This implies that there are no local sources of the electromagnetic field. As also being pointed out in Section 6.1 of [1], this is in agreement with Quigg[4] who states that the symmetry of the conventional field equations does not permit masses for quarks and leptons. Consequently, the existence of particle-like states rests on a nonzero div **E** and an associated broken symmetry between **E** and **B**.

A third point concerns the conventional description of the photon in terms of plane waves. This is not only in contradiction with a nonzero spin, but also with the experimentally proved needle-like behavior, as described in Chapter 4.1 of [1]. Both these circumstances influence the way in which the concept of special relativity has to be transferred from a plane-wave model to a multidimensional model, such as that of cylindrical geometry later treated in this paper. Needless to say, this does not affect the general lines of

thought of special relativity by Einstein.

## 3. Revised Subatomic Field Equations

The shortcomings of conventional theory impose restrictions on a treatment of subatomic physics. A way out of this dilemma is provided by the following sections. The present treatment thus includes terms with a nonzero div **E** which are not present in a conventional analysis, and where div **E** acts somewhat like a hidden variable.

### 3.1 The Zero Point Energy

In a study of the quantum mechanical energy levels of the harmonic oscillator, M. Planck found that there is a nonzero ground level, the Zero Point Energy (ZPE), as further described in a review by Schiff[5]. The related electromagnetic vacuum fluctuations were investigated by Casimir[6] who predicted that two metal plates separated by a small spacing will attract each other, due to the fact that only small wavelengths can exist within the spacing. Such a net differential force was first demonstrated experimentally by Lamoreaux[7]. Part of the fluctuations also carry electric charge, as pointed out by Abbott[8]. Consequently, the vacuum is not merely a state of empty space, but includes photon-like modes being each of frequency $v$ and energy $hv/2$ and which result in a real macroscopic pressure. Even if these fluctuations occur at the lowest ZPE level, their spatial inhomogeneity can produce a pressure gradient. Since the Casimir force is due to a comparatively small differential pressure, the total ZPE can become much larger. More detailed discussions are presented elsewhere [9,10,11].

The basis of the present subatomic field equations is thus formed by the concepts of ZPE and the Casimir force, in combination with special relativity.

### 3.2 The Extended Equations

With the basic concepts of the previous subsection, a revised quantum electrodynamic theory (RQED) is now established [1]. Thereby the new inclusion of terms with a nonzero div **E** becomes sources of electric charge and matter, in accordance with the incorporated effects of the ZPE. It thus leads to a four-dimensional representation

$$LA_\mu = \left(\frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \nabla^2\right) A_\mu = \mu_0 J_\mu \tag{3}$$

of the Lorentz invariant field equations with $\mu$ = 1,2,3,4. Here $A_\mu$ = (**A**, $i\phi/c$) where **A** is the magnetic vector potential, $\phi$ the electrostatic potential, $c^2 = 1/\mu_0\varepsilon_0$ where $c \cong 2.998 \times 10^8$ m/s denotes the velocity constant of light determined by the magnetic permeability $\mu_0$ and the dielectric constant $\varepsilon_0$, and $J_\mu = (\mathbf{j}, ic\bar{\rho})$ where **j** stands for the electric current density and $\bar{\rho} = \varepsilon_0 \,\mathrm{div}\,\mathbf{E}$ for the electric charge density. Since $J_\mu$ is relativistically invariant, it has to satisfy the condition

$$\mathbf{j}^2 - c^2\,\bar{\rho}^{-2} = const. \tag{4}$$

where the constant must vanish because $J_\mu$ disappears when there are no sources of charge and current density. This leads to the final form

$$J_\mu = \bar{\rho}\ (\mathbf{C}, ic) \tag{5}$$

where

$$\mathbf{C}^2 = c^2 \tag{6}$$

and **C** is a *velocity vector* with the modulus $c$.

In a three-dimensional representation the new extended *subatomic* field equations of the *vacuum* state become

$$c^2 \mathrm{curl}\,\mathbf{B} = (\mathrm{div}\,\mathbf{E})\mathbf{C} + \frac{\partial \mathbf{B}}{\partial t} \tag{7}$$

$$\text{curl } \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} \tag{8}$$

where

$$\mathbf{B} = \text{curl } \mathbf{A}, \qquad \text{div } \mathbf{B} = 0 \tag{9}$$

$$\mathbf{E} = -\nabla\phi - \frac{\partial \mathbf{A}}{\partial t}, \qquad \text{div } \mathbf{E} = \bar{\rho}/\varepsilon_0 \tag{10}$$

As compared to conventional theory, these include the additional contributions from div **E** due to ZPE in Equations (7) and (10), with the vector **C** of Equation (6) replacing the velocity constant *c*. This replacement is associated with the extension of the plane-wave representation of special relativity to a two-dimensional one, such as that of cylindrical geometry with an *incorporated* spin concept.

## 4. Resulting New Subatomic Properties

A number of new results have been obtained from Equations (3)–(10) which cannot be deduced in terms of the Standard Model. Corresponding particle models of steady axisymmetric states thus arise from a related generating function. As shown in Chapter 6 of [1], a radially convergent such function leads to vanishing net electric charge $q_0$ and magnetic moment $M_0$, whereas a divergent one results in net values of $q_0$ and $M_0$ under certain circumstances. In this section a number of examples[2] will be reconsidered.

### 4.1 Photon Model with Spin and Rest Mass

The solution for cylindrical waves in a frame $(r,\varphi,z)$, with the velocity vector $\mathbf{C} = c(0,\cos\alpha,\sin\alpha)$, $\cos\alpha \ll 1$, and a constant angle $\alpha$, leads to a *screw-shaped* configuration which includes spin and an associated very small but nonzero rest mass, as shown in Chapter 11 of [1]. The phase and group velocities become slightly smaller than *c*, the field geometry is *helical* with nonzero *axial* field components, and it becomes *limited* in space.

For a generating function with a convergent radial part there is an effective photon radius

$$\hat{r} = \frac{\varepsilon\lambda_0}{2\pi(\cos\alpha)} \tag{11}$$

with a main wavelength $\lambda_0$ of a corresponding wave packet, and a parameter $\varepsilon = 1$. As an illustration, $\cos\alpha \leq 10^{-4}$ and $\lambda_0 = 3 \times 10^{-6}$ m yields a photon rest mass $m_0 \leq 10^{-40}$ kg. The phase and group velocities then only deviate by a factor less than $5 \times 10^{-9}$ from the velocity constant *c*. The spin thus exists at the expense of a very small reduction of the momentum which is related to the axial propagation.

There is also a photon mode originating from a generating function with a divergent radial part. A revised renormalization procedure is applied to this mode, to obtain finite values for the parameters of a wave packet as shown in Chapter 11.3.5 of [1] and in [12]. The effective radius of Equation (11) is then obtained for $0 < \varepsilon \ll 1$. With $\varepsilon \leq \cos\alpha \leq 10^{-4}$ and $\lambda_0 = 3\times10^{-6}$ m we then have $\hat{r} < 5\times10^{-7}$ m. This represents a form of *needle radiation*.

### 4.2 The Elementary Charge

The main features of steady axisymmetric states can be deduced from the time-independent field equations of a separable generating function

$$F(r,\theta) = G_0 G(\rho,\theta) \qquad G = R(\rho)\cdot T(\theta) \tag{12}$$

in a spherical frame $(r,\theta,\varphi)$, where all relevant quantities are independent of the angle $\varphi$ and $\rho = r/r_0$, with $r_0$, as a characteristic radial dimension. To arrive at a particle with net electric charge and magnetic moment, a divergent radial part

$$R = \rho^{-\gamma} e^{-\rho} \qquad \gamma > 0 \tag{13}$$

is chosen, in combination with a polar part *T* of top-bottom symmetry.

The divergence problem of infinite self-energy which arises in the resulting *point-chargelike* geometry, can be tackled by a process of *renormalization*. The conventional way of proceeding is described by

Ryder[13] among others, implying that the divergent behaviour is outbalanced by adding extra *ad hoc* counter terms to the Lagrangian. In the present approach an alternative way is chosen, where the "infinity" of the divergent system is out balanced by the "zero" of a *counter-factor*[14]. Such a factor is already inherent in the present theory and has not to be imposed, as shown in Chapter 7.3 of [1].

Corresponding deductions have been performed on the electron, muon, and tauon, leading to the following results:

- There is a net electric charge $q_0 = Q_0 f_p$ where $Q_0 = (\varepsilon_0 ch)^{1/2} \simeq 8.86 \times 10^{-19}$ C and $f_p$ is a dimensionless profile factor. $Q_0$ is related to the fine-structure constant, and it can be taken as an example where relativity is linked with quantum mechanics through the present theory.
- A variational analysis on the factor $f_p$ finally results in a *minimum elementary charge* $q_0$=1.60 × $10^{-19}$ C within an uncertainty a few percent as compared to the experimental value of $e$ [1,15,16].
- The product of the rest mass $m_0$ and the magnetic moment $M_0$ becomes

$$m_0 M_0 = (ch/4\pi)\left[1 + \left(e^2/4\pi\varepsilon_0 ch\right)\right] = 8.46 \times 10^{-34}\,\mathrm{kg \cdot A \cdot m^2} \tag{14}$$

  This agrees with experimental data for $m_0 M_0$ of the electron, muon and tauon within the limit of a few percent.

The obtained characteristic charge $Q_0$ and the deduced minimum value of $q_0$ being close to the experimental value of the elementary charge $e$, thus suggests that the latter should be considered as a deduced quantity, and not as a fundamental and independent parameter.

### 4.3 The Z Boson and the Higgs Particle

The treatment of the vacuum as an empty space leads to a number of shortcomings, such as to a missing rest mass of elementary particles. This point was made clear by P. W. Higgs and F. Englert among others. The theory by Higgs[17] is based on a *spontaneous nonlinear* mechanism of *symmetry breaking* of an empty vacuum state, by which an unstable boson of unspecified but large rest mass is being formed. This particle has zero net electric charge and zero spin. In its turn, the same particle is considered to decay into a set of all other lighter and massive elementary particles. An open point concerns the theoretically undetermined value of the rest mass.

A particle was later discovered at the projects ATLAS[18] and CMS[19] of CERN, being unstable, having vanishing net electric charge and spin, and with a rest mass of 125 GeV. This discovery was understood to be a confirmation of the heavy particle due to the theory by Higgs.

An alternative and different way of explaining the results by CERN has been presented by the author[20,21,22], as being characterized by *intrinsic linear broken symmetry*. It starts with a model of the Z boson determined from a convergent axially symmetric generating function. From superposition of the solutions of two such Z boson models with antiparallel spin directions, a composite model can be formed. With a mass of 91 GeV for each of the original Bosons, the composite particle obtains characteristical data given by lacking electric charge, magnetic field, and spin. It is purely electrostatic and highly unstable, and has a minimum mass close to 125 GeV. This appears to be in good agreement with the results by CERN. The composite particle solution is also consistent with the point made by Quigg[4] that the Higgs is perhaps not a truly fundamental particle, but is built out of as yet unobserved constituents.

### 4.4 Intrinsic Charges and the Strong Force

The local nonzero behaviour of div **E** does not only generate a net integrated electric elementary charge $e$, but also intrinsic integrated electric charges $\pm Q_i$ of both polarities within various parts of the volume of an elementary particle[1,2,23]. This can be demonstrated by a model of an individual quark being deduced from a convergent generating function, in a frame of spherical coordinates $(r,\theta,\varphi)$ being independent of $\varphi$. We further consider a tentative model of the neutron, given by three individual quarks which are mutually bound to each other, to form a triangular configuration[24]. In a first simplified treatment equal models are used for these quarks.

The following points concern the model of an individual quark:

- In the triangular configuration each quark is assumed to have a mass of 5.57 × $10^{-28}$ kg being a third of the neutron mass.
- Integration of the local electric charge density over various parts of the quark volume results in large positive and negative intrinsic charges $\pm Q_i$ where $Q_i/e \cong 19.9$. Thus $Q_i$ becomes an order of magnitude larger than the elementary charge.

  Concerning the interaction between two quarks, the following points should be observed:
- The source terms of the present theory lead to a volume force density

$$\mathbf{f} = \bar{\rho}\,\mathbf{E}_i \qquad \mathbf{E}_i = \mathbf{E} + \mathbf{C} \times \mathbf{B} \tag{15}$$

Here part of the electric contribution **E** is outbalanced by the magnetic contribution **C**×**B**. Therefore the total field $\mathbf{E}_i$ only becomes noticeable within the innermost part of the quark volume. The result $(Q_i/e)^2 = 396$ implies that the interaction due to $\mathbf{E}_i$ would become more than two orders of magnitude larger than that arising between two elementary charges. But in the real situation the added influence of **C**×**B** partly outbalances that of **E**.

- The total interaction between two quarks in the triangular configuration thus is of *short-range* character, and becomes about *two orders* of magnitude larger than that between two elementary charges.
- The mutual quark force and its corresponding work can be determined in terms of the distance between the quark centra. It is obtained from the force due to the local intrinsic charge density of quark number I, in combination with the reversed total field $\mathbf{E}_i$ generated by quark number II.
- When gradually shrinking the distance between the quark centra, a corresponding work of the mutual forces and their associated potential distributions is being traversed. This results in an outer potential barrier, followed by an intermediate well, and thus ending at an additional barrier. The mutual quark interaction thus becomes *stable* and *attractive*.
- An application to the neutron then leads to a well depth of about 7.7 MeV, being rather close to the binding energy of 8 MeV obtained from experiments reported by Bethe[24]. Since the additional net charges of the proton are comparable to the elementary charge, a similar result should also hold for the proton.
- In the triangular quark model an outer radius of about $3\times10^{-15}$ m and a core radius of about $10^{-15}$ m are obtained. These values are comparable with a nuclear radius of $1.5 \times 10^{-15}$ m given by experiments.

These deduced data are impaired by some uncertainties. Nevertheless the general outcome could still hold. The obtained short-range character and the order of magnitude of the attractive and stable interaction thus gives a clear indication that it should become possible to *unify* the fundamental phenomena of electromagnetics and the strong nuclear force.

### 4.5 Special Relativity versus Quantum Mechanics

In quantum mechanics an instantaneous behaviour of entangled states can take place through long-range interaction. A vacuum state of empty space leads on the other hand to a limited relativistic velocity propagation in subatomic physics. When div **E** = 0, Equations (7)–(10) thus result in a conventional transverse electromagnetic EM wave, with the velocity *c*. This is not reconcilable with instantaneous long-range interaction.

A possible way out of this dilemma[25] may be provided by the transition to a vacuum state with ZPE and div **E** ≠ 0. Equations (7)–(10) then lead to two wave types. The first is an EMS nontransverse electromagnetic space-charge wave with curl **E** ≠ 0 and a limited relativistic propagation determined by the velocity constant *c*. The second type is an S wave of purely longitudinal electric space-charge character with curl **E** = 0. This wave depends only on the dielectric constant $\varepsilon_0$, has *no* relation to relativity, and is not limited in its velocity of propagation, as defined by the vector **C** in Equation (7).

The EMS and S concepts are here proposed to be combined into a system which satisfies the requirements of long-range interaction. Thus, two spatially limited EMS particle models being at a long mutual distance become linked by an S mode which is not limited in its speed of transition. This would imply that relativity and quantum mechanics do not necessarily have to be in conflict. But it remains so far as an open question which requires more investigation. There are the remaining questions whether the S mode becomes a physical reality, and how the matching of the axial electric field components of the EMS and S modes can be realized in detail.

## 5. Conclusions

From the present revised subatomic field equations, new results have been obtained in terms of the Zero Point Energy. These results cannot be deduced from the conventional Standard Model. They concern the spin, rest mass and needle radiation of the photon, a deduction of the value of the elementary electric charge, and of the mass of the CERN particle. The latter deduction is not related to the theory by Higgs. The present theory has further debouched into the discovery of intrinsic electric charges and related forces acting within

corresponding particle models. These forces give rise to a potential well depth being rather close to the binding energy of the neutron and proton. This provides a possibility of unifying electrodynamics and the strong nuclear force.

It is improbable that all these different obtained results should merely by chance happen to agree with experimentally confirmed facts.

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# Laser-Based Advanced Manufacturing and Nano-photonics

## by Lin Li, Member EUAS

Short Biography

*Professor Li obtained a BSc degree in Control Engineering from Dalian University of Technology (China) in 1982 and a PhD degree in Laser Engineering from Imperial College London in 1989. He worked at University Liverpool (UK) between 1988-1994 as a Research Associate and Research Fellow in laser materials processing and became a Lecturer in manufacturing at UMIST (University of Manchester Institute of Science and Technology), UK and promoted to a full Professor in Laser Engineering in 2000.*

*Professor Lin Li is an elected Fellow of Royal Academy of Engineering (UK), International Academy of Production Engineering, International Academy of Photonics and Laser Engineering, Laser Institute of America, and Institute of Engineering and Technology. He has been the Director of Laser Processing Research Centre since 2000, and Associate Dean for Business Engagement and Innovation in the Faculty of Science and Engineering at The University of Manchester, UK since 2015.*

*He has served as the President of Laser Institute of America (2016), President of International Academy of Photonics and Laser Engineering (2013-2015), and President of Association of Industrial Laser Users (AILU – 2017-2019).*

*Professor Li is the author and co-author of over 600 scientific publications of which over 370 are in peer-reviewed journals related to the science, technology and applications of laser based manufacturing and photonics. Professor Li is an inventor of the microsphere lens super-resolution optical microscope that has broken the optical diffraction limit, widely reported by press and media including BBC and New York Times. The technology has been commercialised. He is a pioneer of industrial laser cleaning of metallic alloys that have been successfully used in the aerospace and automotive industries for welding preparations. He is also an inventor of laser powder bed fusion based multiple material additive manufacturing (3D printing) technology.*

*He received Arthur Charles Main Award from the Institute of Mechanical Engineers in 2001 for work in laser based nuclear decommissioning technology. He received the Sir Frank Whittle Medal from the Royal Academy of Engineering (UK) in 2013 for innovative manufacturing that has led to economic impacts. In 2014 he received Wolfson Research Merit Award from the Royal Society for his research on laser nano-fabrication and nano-imaging, and received Researcher of the Year medal from The University of Manchester in 2014.*

## Selected Publications

1. ***Z.B.Wang, W.Guo, L.Li, B.Luk'yanchuk, A,Khan, Z.Liu, Z.Chen and M.H.Hong, "Optical virtual imaging at 50 nm lateral resolution with a white-light***

***nanoscope", Nature Communications, Vol. 2, Issue 218, 2011, DOI:10.1038/ncomms1211***

Optical microscope is inherently limited in resolution by optical diffraction limit to half of the optical wavelength. For visible light of 400-700 nm wavelengths, this theoretical imaging resolution is 200 nm. This research demonstrated a new imaging method utilising transparent microsphere lenses placed in the virtual imaging plane of standard optical microscope allowing the direct optical imaging resolution to reach 50 nm. This work has led to a new field of study in optics and commercialisation for optical nanoscopy.

2. **L.Li, W.Guo, Y.Z.Yan, S.J.Lee, T.Wang, "Label-free super-resolution imaging of adenovirus by submerged microsphere optical nanoscopy"** ***Light: Science and Applications,*** **Vol. 2, 2013, E60, doi:10.1038/lsa.2013.60**

   Most viruses have sizes below the standard optical microscope imaging resolution limit of 200 nm. This research demonstrated a method of optical imaging using submerged microsphere lens to allow the direct observation of denovirus of 75 nm in size, breaking the theoretical optical diffraction limit of optical microscopes. The associated scientific mechanism is described. This technology has been commercialized.

3. ***Y.Z.Yan, L.Li, C.Feng, W.Guo, S.Lee, M.H.Hong, "Microsphere-coupled scanning laser confocal nanoscope for sub-diffraction-limited imaging at 25 nm lateral resolution in the visible spectrum", ACS Nano, Vol .8 Issue 2, 2014. pp.1809-1816. DOI: 10.1021/nn406201q.***

   By combining microsphere lenses with a confocal microscope, direct optical imaging resolution has been demonstrated to reach 25 nm well beyond the theoretical optical diffraction limit of 200 nm for visible light. The fundamental scientific principles were proposed.

4. **M.W. Turner, P.L.Crouse and L.Li, "Comparative interaction mechanisms for different laser systems with selected materials on titanium alloys",** ***Applied Surface Science*****, Vol. 253 (19), 2007, 7992-7997.**

   This is one of the earliest studies on laser cleaning of titanium alloys for welding process preparation. The research has identified the basic mechanisms and a suitable approach to cleaning of titanium alloys without causing damages to the material. This technology has led to the world's first successful application of laser cleaning in the aerospace industry for aero-engine production.

5. ***A.W. AlShaer, L. Li and A.Mistry, "The effect of short pulse laser surface cleaning on porosity formation and reduction in laser welding of aluminium alloy for automotive component manufacture" Optics and Laser Technology, Vol.64. 2014. pp.162-171***.

   This scientific study identified the basic characteristics of the effect of laser cleaning on the subsequent laser welding performance and has demonstrated the effectiveness of laser cleaning in reducing or eliminating porosities in laser welding of aluminum alloy. This study has paved way for the successful deployment of laser cleaning in a large automotive company for car production.

6. ***C.Wei, L.Li, X.J.Zhang, Y.H.Chueh, "3D printing of multiple metallic materials via modified selective laser melting" CIRP Annals- Manufacturing Technology, Vol. 67, Issue 1, 2018, pp. 245-248, DOI: 10.1016/j.cirp.2018.04.096***

   Additive manufacturing is an emerging manufacturing technology that components of complex geometry to be manufactured without the need for a die or mould. Additive manufacturing of metallic materials is currently limited to single material. It is desirable to be able to tailor material properties at different locations of a component. This research set a new milestone in additive manufacturing to show that multiple metallic material additive manufacturing is possible with combined powder-bed fusion and point-by-point ultrasonic powder deposition and powder removal.

7. ***Y.Huang, L.Zeng, C. Liu, D.Zeng, Z.Liu, X. Liu, X.Zhong, W.Guo and L.Li, "Laser direct writing of heteroatom (N&S) doped graphene from a polybenzimidazole (PBI) ink donor on polyethylene terephthalate (PET) polymer and glass substrates", SMALL, Vol. 14, issue 44, Nov. 2018. Article number: 1803143.***

   Graphene is a 2D material that has superior electrical and thermal conductivities. Deposition of patterned graphene on a substrate is desirable for a wide range of applications including sensors and batteries. This research demonstrates a new method of depositing patterned and doped graphene by a laser photo-chemical process changing an organic ink into graphene on a substrate. This also allows the tuning the energy gap of graphene.

# Colorectal Carcinogenesis & the Biology of GI Cancer Cell Invasion & Metastasis

## by Robert Daniel Beauchamp, Member EUAS

Short Biography

*I serve as the John Clinton Foshee Distinguished Professor of Surgery after having served as Chairman of the Section of Surgical Sciences and Surgeon-in-Chief of Vanderbilt University Medical Center for 17 years, from July 2001 through June 2018. As of July 1, 2018, I was appointed as Vice President for Vanderbilt-Ingram Cancer Center Network Affairs, planning strategic growth of our cancer center. I hold a joint appointment as Professor in the Department of Cell and Developmental Biology. My service also includes functioning as Deputy Director of the Vanderbilt-Ingram Cancer Center and as co-leader of the GI Cancer Program for the Cancer Center. Our research efforts have largely involved colorectal carcinogenesis, the biology of GI cancer cell invasion and metastasis, and in the identification of novel molecular biomarkers and therapeutic targets in colorectal and other alimentary tract malignancies. I also have a longstanding interest and experience in the field of TGF-beta superfamily signaling and its roles in the GI tract and in GI carcinogenesis, particularly in the colon. My laboratory uses molecular genetics and 3-D cell culture and organoid culture of small intestinal epithelium and colon as approaches to examine mechanistic questions in epithelial cell biology. Our laboratory uses a variety of mouse models, including xenografts and genetically modified mouse models. We also use de-identified human intestinal tissues and tumor tissues in our research under approved protocols. Extending from a post-doctoral fellowship in the laboratory of Dr. Hal Moses, my research focus has included understanding the roles of transforming growth factors in the GI tract and in GI malignancies, along with epithelial to mesenchymal transition. Over the past 25 years, I have trained and mentored a diverse group of 26 postdoctoral fellows and have served as primary mentor for 6 graduate students who have completed their Ph.D. work in my laboratory. In addition, I have co-mentored at least 6 other doctoral students, mentored at least eight junior faculty members in their research career development, and have supervised and mentored numerous college undergraduate students and medical students for summer research rotations or year-long medical scholars projects or honors thesis work.*

***Positions & Honors***

***Positions & Employment***

| | |
|---|---|
| *1987-1988* | *Research Instructor of Cell Biology, Vanderbilt University, Nashville, TN* |
| *1988-1989* | *Research Assistant Prof of Cell Biology and Assistant Professor of Surgery (non-tenure track), Vanderbilt University, Nashville, TN* |
| *1989-1993* | *Assistant Professor, Departments of Surgery and Human Biological Chemistry & Genetics (tenure track), UTMB, Galveston, TX* |
| *1993-1994* | *Associate Professor with tenure, Departments of Surgery and Human Biological Chemistry and Genetics, UTMB, Galveston, TX* |
| *1994-1997* | *Associate Professor with tenure, Depart. of Surgery (Division of Surgical Oncology) and Cell and Developmental Biology, Vanderbilt University School of Medicine, Nashville, TN* |
| *1995-1999* | *Deputy Associate Director for Clinical Programs, The Vanderbilt Cancer Center* |
| *1997-2001* | *Professor of Surgery, The John Sawyers Prof. of Surgery, Director, Division of Surgical Oncology, Vanderbilt University* |
| *1997-present* | *Professor, Department of Cell and Developmental Biology, Vanderbilt University* |
| *1999-2011* | *Associate Director for Clinical Programs, Vanderbilt-Ingram Cancer Center* |
| *2001-2018* | *J.C. Foshee Distinguished Prof. and Chairman, Section of Surgical Sciences, Vanderbilt University, Surgeon-in-Chief, Vanderbilt University Hospital* |
| *2018-present* | *J.C. Foshee Distinguished Professor of Surgery* |
| *2011-2018* | *Deputy Director, Vanderbilt-Ingram Cancer Center, Nashville, TN* |
| *2014-present* | *Co-Director, GI Oncology Program, Vanderbilt-Ingram Cancer Center* |

*2018-present* *Vice President for Cancer Center Network Affairs, Vanderbilt University Med Ctr*

***Other Experience and Professional Memberships***

*1990-present* *Member, American Gastroenterological Association*
*1990-present* *Fellow: American College of Surgeons*
*1991-present* *Member: American Association for Cancer Research*
*1992-present* *Member: Society of University Surgeons, past Councilman at large, past President.*
*1993-present* *Member: American Society for Cell Biology*
*1993-present* *Member: Society for Surgery of the Alimentary Tract*
*1994-present* *Member: American Society of Clinical Oncology*
*1994-present* *Member: Society of Surgical Oncology*
*1995-present* *Member: Eastern Cooperative Oncology Group*
*1996-2003* *Editorial Board Member: Journal of Surgical Research*
*1997-1012* *Fellow: American Surgical Association, program committee member, Chair 2012*
*1997-2005* *Editorial Board Member: Surgery*
*1998-present* *Associate Editor: Sabiston Textbook of Surgery, Editions 16-20*
*1999-2003* *Editorial Board Member: Annals of Surgical Oncology*
*2001-2006* *Member: Surgical Research and Education Committee, American College of Surgeons*
*2001-present* *Member: American Society for Clinical Investigation*
*2003* *NIH SPORES in Pancreatic Cancer Peer Review Study Section*
*2003-2007* *NIH Gastrointestinal Cell and Molecular Biology (GCMB) Study Section, regular member*
*2003-present* *Editorial Board Member: Journal of the American College of Surgeons*
*2007-2010* *American Gastroenterology Association Institute, Research Awards Panel*
*2007-present* *Editorial Board Member: American Journal of Surgery*
*2010-2011* *Member: Pancreatic Cancer Action Network-AACR Innovative Grants Scientific Review Committee*
*2010-2012* *NIH College of CSR Reviewer*
*2016-present* *Gastroenterology, Advisory Board member*

***Honors***

*1981* *Elected to Alpha Omega Alpha*
*1982* *The Herman R. Barnett Memorial Award for Academic Achievement in Surgery and Anesthesiology- UTMB Galveston*
*1982* *Gold Headed Cane Award, Honorable Mention-UTMB Galveston*
*1982* *UTMB Medical School, Graduated Highest Honors*
*1983* *Outstanding Surgical PGY-1 House Officer*
*1987* *Physician Scientist Award, NCI, K11*
*1997* *First recipient of the John Sawyers Endowed Professorship, Vanderbilt University*
*2001* *Elected to the American Society for Clinical Investigation*
*2009* *The Frank Boehm Award for Excellence in Teaching Continuing Medical Education*
*2009-2012* *Vanderbilt University Faculty Senate, elected*
*2012* *Elected to the National Academy of Medicine (previously IOM)*
*2013* *Elected Fellow of the American Association for the Advancement of Science*
*2015* *The Flance-Karl Award for Scientific Achievement from the American Surgical Assoc.*
*2015* *Ashbel Smith Distinguished Alumnus Award, UTMB Galveston*
*2016* *The Rodman E. Sheen and Thomas G. Sheen Award*

## Contributions to Science

1. We identified inhibition of cyclin D1 expression and G1 cell cycle arrest as an important effect of TGFβ on intestinal epithelial cells. We further showed that intestinal adenomas from Min/+ mice expressed decreased levels of TGFβ type II receptor, along with increased levels of cyclin D1 and Cdk4. Human adenomas from FAP patients also exhibited increased levels of cyclin D1 and Cdk4. We subsequently demonstrated that forced expression of cyclin D1 in the liver caused hepatic adenomas and hepatocellular carcinoma in transgenic mice.

a. Ko TC, Sheng H-M, Reisman D, Thompson EA, **Beauchamp RD**. Transforming growth factor-β 1 inhibits cyclin D1 expression of intestinal epithelial cells. *Oncogene* 1995, 10:177-184.

b. Ko TC, Yu W, Sakai T, Sheng H, Shao J, **Beauchamp RD**, Thompson EA. TGF-β1 effects on proliferation of rat intestinal epithelial cells are due to inhibition of cyclin D1 expression. *Oncogene* 1998, 16:3445-3454.
c. Zhang T, Nanney LB, Peeler MO, Williams CS, Lamps L, Heppner KJ, DuBois RN, **Beauchamp RD**. Decreased TGF-β Type II receptor expression in intestinal adenomas from Min/+ Mice is associated with increased cyclin D1 and Cdk4 expression. *Cancer Research* 1997, 57:1638-1643.
d. Deane NG, Parker MA, Aramandla R, Diehl L, Lee WJ, Washington MK, Nanney LB, Shyr,Y., and **Beauchamp RD**. Hepatocellular Carcinoma Results from Chronic Cyclin D1 Overexpression in Transgenic Mice. *Cancer Research* 2001, 61 (14):5389-5395.

2. Our work elucidated the role of COX2 and its regulation, in part by TGFβ, in intestinal neoplasia, particularly in cells with activated RAS. COX-2 was shown to be an important potential therapeutic target for both chemoprevention of colorectal cancers and possibly therapeutic for established cancers. Our laboratory helped to identify important mechanisms involved in upregulation of COX-2 expression in colorectal cancer.

a. Sheng H, Shao J, Kirkland SC, Isakson P, Coffey RJ, Morrow J, **Beauchamp RD**, DuBois RN. Inhibition of human colon cancer cell growth by selective inhibition of cyclooxygenase-2. *The Journal of Clinical Investigation* 1997, 99:2254-2259.
b. Sheng H, Williams CS, Shao J, Liang P, DuBois RN, **Beauchamp RD**. Induction of cyclooxygenase-2 by activated Ha-ras oncogene in Rat-1 fibroblasts and the role of mitogen-activated protein kinase pathway. *The Journal of Biological Chemistry* 1998, 273:22120-22127.
c. Sheng H, Shao J, Dixon DA, Williams CS, Prescott SM, DuBois RN, **Beauchamp RD**. TGF-β1 enhances Ha-Ras-induced expression of cyclooxygenase-2 in intestinal epithelial cells via stabilization of mRNA. *Journal of Biological Chemistry* 2000, 275 (9):6628-6635.
d. Dixon D, Balch G, Kedersha N, Anderson P, Zimmerman G, **Beauchamp RD**, Prescott SM. Regulation of Cyclooxygenase-2 Expression by the translational Silencer TIA-1. *Journal of Experimental Medicine* 2003, Vol 198 (3):475-81. PMID: 12885872

3. In collaboration with colleagues in the departments of Biostatistics and Biomedical Informatics, we have conducted studies to identify molecular subtypes of primary human colorectal cancers in order to identify prognostic, and eventually predictive, molecular biomarkers to guide therapeutic decisions. This work also has the goal improving our understanding of the complex biology underpinning the genomic alterations in colorectal cancers.

a. Smith JJ, Deane NG, Wu F, Merchant NB, Zhang B, Jiang A, Lu P, Johnson JC, Schmidt C, Bailey CE, Eschrich S, Kis C, Levy S, Washington MK, Heslin MJ, Coffey RJ, Yeatman TJ, Shyr Y, **Beauchamp RD**. Experimentally Derived Metastasis Gene Expression Profile Predicts Recurrence and Death in Patients with Colon Cancer. *Gastroenterology.* 2010 Mar, 138(3):958-68. Epub 2009 Nov 13. PMID: 19914252. PMCID: PMC3388775
b. Oh SC, Park YY, Park ES, Lim JY, Kim SM, Kim SB, Kim J, Kim SC, Chu IS, Smith JJ, **Beauchamp RD**, Yeatman TJ, Kopetz S, Lee JS. Prognostic Gene Expression Signature Associated with Two Molecularly distinct subtypes of Colorectal Cancer. *Gut.* 2012 Sep; 61(9):1291-8. Epub 2011 Oct 13. PMID: 21997556. PMCID: PMC3419333.
c. Tripathi MK, Deane NG, Zhu J, An H, Mima S, Wang X, Padmanabhan S, Shi Z, Prodduturi N, Ciombor KK, Chen X, Washington MK, Zhang B, **Beauchamp RD**. Nuclear Factor of Activated T-cell Activity is Associated with Metastatic Capacity in Colon Cancer. *Cancer Res.* 2014 Dec1;74(23):6947-57. doi: 10.1158/0008-5472. CAN-14-1592. Epub: 2014 Oct 15. PMID: 25320007. PMCID: PMC4252979
d. Zhu J, Deane NG, Lewis KB, Padmanabhan C, Washington MK, Ciombor KK, Timmers C, Goldberg RM, **Beauchamp RD**, Chen X. Evaluation of frozen tissue-derived prognostic gene expression signatures in FFPE colorectal cancer samples. *Sci Rep.* 2016 Sep 14;6:33273. doi: 10.1038/srep33273. PMID: 27623752

4. Much of our work over the past decade has been focused on understanding EMT and its roles in cancer cell invasion and metastasis. As part of that investigation, we have explored the dysregulation of epithelial cell junctional proteins such as E-cadherin and adherens junction components such as β-catenin in colorectal cancers. This work has also led to improved understanding of Wnt signaling in colorectal cancer.

a. Dhawan P, Singh AB, Deane NG, No Y, Shiou SR, Schmidt C, Neff JG, Washington MK, **Beauchamp RD**. Claudin-1 regulates cellular transformation and metastatic behavior in colon cancer. *J Clinical Investigation* 2005, 115:1765-1176. PMID: 15965503
b. Singh AB, Sharma A, Smith JJ, Krishnan M, Chen X, Eschrich S, Washington MK, Yeatman TJ, **Beauchamp RD**, Dhawan P. Claudin-1 Up-regulates the Repressor ZEB-1 to Inhibit E-Cadherin Expression in Colon Cancer Cells. *Gastroenterology*. 2011 Dec;141(6): 2140-53. Epub 2011 Aug 28. PMID: 21878201. PMCID: PMC3395068
c. Hanson AJ, Wallace HA, Freeman TJ, **Beauchamp RD**, Lee LA, Lee E. XIAP monoubiquitylates Groucho/TLE to promote canonical Wnt signaling. *Mol Cell*. 2012 Mar 9:45(5):619-628. Epub 2012 Feb 1. PMID: 22304967. PMCID: PMC3299836
d. Sato-Diaz K, Benchabane H, Tiwari A, Tien A, Li B, Thompson JJ, Hyde AS, Sawyer LM, Jodoin JN, Santos E, Lee LA, Coffey RJ, **Beauchamp RD**, Williams CS, Kenworthy AK, Robbins DJ, Ahmed Y, Lee E. APC inhibits ligand-independent Wnt signaling by the clathrin endocytic pathway. Dev Cell 2018 Mar 12; 44:566-581, e8, PMID:29537782; PMC5884143

5. Our work has contributed to a better understanding of the complex roles of TGFβ family signaling, particularly via the canonical SMAD4 pathway, in normal intestinal epithelial homeostasis and how this signaling is altered in colorectal carcinomas and other cancers. We demonstrated that RAS oncogene activation markedly alters responses to TGFβ signaling from tumor suppression to tumor promoting effects. Our work has also elucidated the importance of TGFβ signaling in tumor immunosurveillance and more recently, the role of this pathway on regulation of epithelial cell inflammatory responses and carcinogenesis.

a. Torre-Amione G, **Beauchamp RD**, Koeppen H, Park BH, Schreiber H, Moses HL, Rowley DA. A highly immunogenic tumor transfected with a murine transforming growth factor type $\beta_1$ cDNA escapes immune surveillance. *Proc Natl Acad of Sci USA*, 1990 Feb; 87(4):1486-1490.
b. Shiou SR, Singh AB, Moorthy K, Datta PK, Washington MK, **Beauchamp RD**, Dhawan P. Smad4 Regulates Claudin-1 Expression in a Transforming Growth Factor-β – Independent Manner in Colon Cancer Cells. *Cancer Res.* 2007 Feb 15, 67(4):1571-1579. PMID: 17308096.
c. Freeman TJ, Smith JJ, Chen X, Washington MK, Roland JT, Means AL, Eschrich SA, Yeatman TJ, Deane NG, **Beauchamp RD**. Smad4-Mediated Signaling Inhibits Intestinal Neoplasia by Inhibiting Expression of β-Catenin. *Gastroenterology*. 2012 Mar;142(3):562-571.e2. Epub 2011 Nov 22. PMID: 22115830. PMCID: PMC3343368
d. Means AL, Freeman TJ, Zhu J, Woodbury LG, Marincola-Smith P, Wu C, Meyer AR, Weaver CJ, Padmanabhan C, An H, Zi J, Wessinger BC, Chaturvedi R, Brown TD, Deane NG, Coffey RJ, Wilson KT, Smith JJ, Sawyers CL, Goldenring JR, Novitskiy SV, Washington MK, Shi C, Beauchamp RD. Epithelial Smad4 deletion upregulates inflammation and promotes inflammation-associated cancer. Cellular and Molecular Gastroenterology and Hepatology 2018. Published online **2018** May 24. doi: 10.1016/j.jcmgh.**2018**.05.006. PMCID: PMC6083016

# Mathematical Models in Flood Management Mitigation and Control : A Brief Overwiew

**by Daniele De Wrachien, Member EUAS**

Short Biography

*Daniele De Wrachien is currently Retired Professor of Agricultural Hydraulics at the Department of Agricultural and Environmental Sciences of the State University of Milan and Member of the Board of Director of the Wessex Institute of Technology ( WIT ), Southampton, UK. He graduated from the State University of Milan as geologist and obtained his PhD in Advanced Engineering Geology. He performed his duties as ,Director of the Institute of Agricultural Hydraulics (2000-2006 ,Director of Computer Centre of the Faculty of Agriculture,(1992-95), Tutor of MPhil and PhD students of the Faculty of Agriculture External Examiner to MPhil and PhD students, Visiting Professor at the Wessex Institute of Technology (WIT). Daniele received the following Honours and Awards : Award for Truthful Support and Help in Organizing and Improving Scientific Level of the Symposia "Actual Tasks on Agricultural Engineering", Croatian Agricultural Engineering Society , Award in Recognition of Services to the European Society of Agricultural Engineers, Award for outstanding contribution to Engineering Sciences ,WIT ,Award for the Best Performing Working Body ,International Commission on Irrigation and Drainage.*

*Daniele is Author of over 150 scientific publications: papers, key-note lectures, books and technical reports and Member of the Editorial Board of the following International Journals :International Journal of Agricultural and Biological Engineering, 2009 : Journal of Agricultural Sciences ( Editor-in-Chief ) ,2010 , Journal of Irrigation&Drainage Systems Engineering (Executive Editor), 2010-,International Journal of Computational Methods and Experimental Measurements, 2010- ,Journal of Smart Grid and Renewable Energy, 2010 - Journal of Safety and Security Engineering ,2011- , International Journal of Advanced Renewable Energy Research , 2012-, American Journal of Experimental Agricultural ( Editor-in-Chief) 2013 –, Journal on Frontiers in Soil Science , 2013- , Journal of Agricultural Science and Application,2013- ., Irrigation and Drainage ( Associate Editor ), 1998- .*

*Daniele has been involved in the organization of more than sixty International Conferences , Congresses, Symposia and Workshop in Africa ,America , Asia , Australia and Europe ,performing the role of Chairman, Key-note Speaker and Member of the Scientific and Organizing Committees.*

*As President of the European Society of Agricultural Engineers ( 2002- 04 )Daniele established Agreements with national, regional and world-wide Organisations such as CIGR (International Commission of Agricultural Engineering) ,ESA (European Society of Agronomy) ,FAO (Food and Agriculture Organisation of the United Nations) ,*

*ICID (International Commission on Irrigation and Drainage) ,IUSS (International Union of Soil Sciences) , and others.*

*The scientific activity of Daniele deals with the following fields of interest: water resources management ,irrigation and drainage technology, performance assessment of sprinkler irrigation systems ,modelling of transport processes in porous media ,modelling and fluid-dynamics of debris and hyper-concentrated flows, flood control and mitigation measures, desertification and environmental impact of climate change, classical and quantum fluid-dynamical trajectories*

*Listed on :*

- *Who's Who in the World ,23rd,24th,25th Editions ,Marquis ( USA ) Editor ;*
- *Dictionary of International Biography ,33rd ,34th , International Biographical Centre (UK) Editor;*

- *2000 Outstanding Intellectuals of the 21st Century , Fifth Edition ;*
- *Great Minds of the 21st Century , 2006/2007 Edition , American Biographical Institute , USA*

**Abstract**

Floods are among the most damaging of natural hazards, and are likely to become more frequent, more relevant and more damaging in the future due to the increase in population, urbanization, land subsidence and, to a certain extent, the impact of climate change. One-third of the annual natural disasters and economic losses and more than half of the respective victims are flood related.

Knowledge and advanced scientific tools play a role of paramount importance in the strain of coping with flooding problems.In this context, flood modelling represents the basis for effective flood management mitigation and control.

The modelling approach aims to provide the best means for assessing and, subsequently, reducing the vulnerability of rural and urban prone areas.

Within this context the following paper provides a review and a general description of the main features and characteristics of the mathematical models currently used in flood management , mitigation and control , along with quantity and quality of experimental and field data to be used both as input and for model calibration .

Mathematical models are the best tools, nowadays available, for the design of efficient flood protection strategies and excellent supporters of decision-works.

**Mathematical Models**

Research work on flood dynamics has traditionally specialised in different mathematical models. They can roughly be categorized into stochastic and deterministic models.

Stochastic models are based on flood frequency analysis, defined as the means by which flood discharge magnitude is related to the probability of its being equalled or exceeded in any year or to its frequency of recurrence or return period.

Deterministic models are, generally, based on physical properties of elements that feature or influence the phenomenon under investigation, such as the catchment characteristics, the channel geometry, the rainfall-runoff process.

**Stochastic Models**

Estimation of floods corresponding to specified return periods is essential for the design of flood protection measures, assessment of regions at risk of flooding, and the pertinent management of flooded areas.

Due to climatic variability, which drives flood events, stochastic modelling has become widely applied to estimate the magnitude of flood corresponding to a specified risk [6, 7].

In particular, flood frequency analysis was developed, in the first instance, in response to the need for information for the safe and economical design of engineering structures, either for the conveyance of flood flows (bridges, culverts, diversion channels, reservoirs, spillways) or for the protection or mitigation from flooding of land and property (embankments and walls). Moreover, this procedure is currently used for planning purposes and the design of land-use categories based on flood zoning with respect to vulnerability.

Frequency analysis is most commonly applied to peak discharges, instantaneous or averaged over a specified duration. Analysis is carried out on an observed historic record of river flow with the aim of assessing future probabilities of exceedance. It is also usually assumed that there will be not temporal change in the underlying statistics due to climate variability or to land use changes.

A large number of probability distributions and methods of application have been used for interpolation or extrapolation.

The two main approaches to select the flood series for fitting a stochastic model to the observed floods are based on the series for maxima annual flows (MAF) or partial duration series of floods (PDF). The MAF series selects the maximum flood event for each year, while the PDF series consists of all flood peaks above a specified magnitude.

The MAF approach ignores the fact that the highest flows in some years can be lower than flood events in other years, and hence it excludes significant high flood events in the parameter estimation process. The PDF procedure, on the other hand, considers all significant flood events in its parameter estimation process and its size can extend far beyond the available years of recorded flows.

Recently, a new relation between the return period of the PDF and the MAF series was proposed , based on the assumption that flood events are independent [8]. The General Extreme Value (GEV) distributions, in addition to the Generalized Pareto (GP) distribution have been fitted and applied to analyse flood events.

**Deterministic Models**

Deterministic modelling (flood routing) can be defined as a mathematical procedure for predicting the changing magnitude, speed and shape of a flow wave as a function of time (i.e. the flow hydrograph) at one or more points along a watercourse. The watercourse may be a river, stream, reservoir, estuary, canal, discharge ditch, or storm sewer. The flow hydrograph can result from precipitation runoff, reservoir releases, landslides into reservoirs, or tides. Flood routing may be classified as hydrologic (lumped), or hydraulic (distributed), or hybrid.

*Hydraulic Models*

A good understanding of a complex flooding event can only be achieved by means of hydraulic models, because the flow rate, velocity, and depth vary in space along the watercourse and across a floodplain and/or a flood prone area. Estimation of these properties can be obtained by using the complete differential equations of 1D or 2D unsteady flow, known as the De Saint Venant (SV) or shallow water (SW) equations. Those equations allow the flow rate and water level to be computed as functions of space and time rather than time alone, as in the lumped flow routing methods. Distributed flow routing based on the complete SV or SW equations is known as hydrodynamic routing.

In some cases, the governing equations can be simplified to a 1D continuity equations and a uniform flow relationship, referred to as *kinematic wave routing*, which implies that the discharge can be computed as a simple function of depth alone. Uniform flow implies a balance between gravitational and frictional forces in the channel. This assumption can rarely be justified, especially on very flat slopes where effects of water surface cannot be ignored.

Selection of a flow routing model for a particular application is influenced by the relative importance placed on the following factors:

- the model's suitability to answer the user's questions;
- the model's accuracy;
- the type and availability of required data;
- the complexity of the mathematical formulation.

Distributed flow routing models are useful tools for determining floodplain depths, required heights of structures (bridges or levees), inundation maps for dam-break contingency planning, transient waves created in reservoirs by gate or turbine changes, landslide-produced waves in reservoirs and unsteady flow in storm sewer systems. The real flow process in each of these applications varies in all three space dimensions. However, normally the spatial variation of the flow characteristics can be approximated as varying in only one space dimension – the direction along the flow channel. Thus the 1D equations of unsteady flow are widely used.

*Hybrid models*

Until recently, hydraulic models were not reckoned a practical alternative for flood routing because they were considered not economically viable to obtain cross section data over the reaches involved in flood routing.

Recent investigations have revealed that hydraulic routing can be successfully used to determine discharge hydrographs in reaches where little channel geometry data are available, by approximating the model reach by a rectangular channel [10].

It was found that this "limited geometry" modelling approach – based on 1D SV equations – could accurately determine discharge hydrographs, making it an effective and suitable alternative to hydrologic flood routing. It was also found that this hybrid model offers the advantage of operationally combining the flood routing and the determination of flood levels [11]. In addition, the use of a hydraulic model opens up the potential for modelling more dynamic flood events such as ice jam release surges, which cannot be handled by traditional hydrological modelling approaches.

In practical applications, flood forecasting involves two steps.
First, a flood routing model (usually hydrologic) is used to obtain the flood peak by routing flood events between streamflow gauging stations. This flood wave must then be put into a hydraulic model based on detailed channel geometry in order to forecast flood events at key-sites.

A new deterministic approach uses unsteady flow hydraulic modelling for both flood routing and flood level determination. This hybrid model offers the advantage of operationally combining the flood routing and the determination of the flood level. Moreover, this procedure opens up the potential for modelling more dynamic flood events such as ice jam release surges, which cannot be handled by traditional hydrologic or hydraulic modelling approaches.

**Challenges and Developments**

Hydrological models play a role of paramount importance in the monitoring, forecasting and early warning process of flood events. To this end, it is a demanding task to precisely define the input data needed for flood modelling. Within this context, the most important question to be addressed when defining the quantity and quality of data to be used as input of a model is the purpose pursued. Modelling a flooding event in a specific area, caused by the failure of a dam, or by heavy rain, concern different data and ask for different approaches. In the event of dam failure, precise information on topography and soil characteristics are much more necessary than data on earlier flooding, while in flood forecasting over a broad area, data of historic flooding are essential [7, 8].

The exceptional conditions in which such extreme events occur do not generally permit a sufficient number of observations, for the same type of territory reality to work out the particular behavioural laws for that area. So references to different territorial situations for the same hazard typology are needed.

The ideal sequence that should be pursued in response to the challenge presented by the management and mitigation of floods by using hydrological models can be outlined as follows [12]:

- systematic collection of field data should be made to provide a large reliable database;
- effective mathematical models should be constantly developed, updated, tested and applied;
- hydrological and geological mapping techniques and identification of possible scenarios should be then set up;
- the best mitigation solutions should be designed and implemented on the basis of the knowledge gained in the planning phase;
- a program of systematic observations at the sites where risk has been mitigated should then be planned and carried out to detect any shortcomings and test the efficiency of the investigations and the models used.

Each of the above phases needs improvements and depends, on achieving them, on improvements in the other fields.

As an example, the application of existing models based on data collected in the field and the developments of the new ones would allow, on one hand, to better focus what to observe in the field and, on the other, improve mitigation methodologies and the models' reliability. In this way a sustainable development can be achieved.

**Concluding Remarks**

One-third of the annual natural disasters and economic losses and more than half of the respective victims are flood related. These hazards are likely to become more frequent and more relevant in the future, due to the effects of increase in population, urbanization, land subsidence and the impact of climate change.

A flood is a natural event of great complexity. The hydrological parameters of a flood (magnitude, frequency, celerity, volume, duration) reflect the stochastic behaviour of precipitation, interception, infiltration, evapotranspiration, soil moisture, overland and ground flows and river and channel hydraulics. Models not only help in understanding these phenomena, but are also essential for flood risk assessment of the current situation and for the assessment of the expected changes.

By using a model an attempt is made to replace trial and error-based measures. The modelling tool aims to provide the best approach to assess and reduce the vulnerability of rural and high-value urban flood-prone areas as well as industrial zones.

Mathematical models, combined with other measures aiming at solving water management problems, allow good opportunities to develop a set of measures suitable to reduce flood damages to an acceptable level. To this end, the model approach represents the best tool feasible to compare the effectiveness of the options against all the possible flood events, and to choose the best alternative. In this way a harmonious coexistence with floods can be achieved.

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# New Findings Using Spaceborne Remote Sensing for Condition Monitoring of Soils, Vegetation and Glaciers

## by Manfred F. Buchroithner EUAS

Short Biography

*Manfred Ferdinand Buchroithner (* 17-12-1950) studied Geology & Palaeontology at the University of Graz/Austria and both Remote Sensing and Cartography at ITC/Netherlands. He obtained his PhD in 1977 in Graz. In 1982 he went as Fulbright Scholar to the USA (Fort Worth/Texas, Boulder/Colorado and Stanford University/California). During the following years at the Institute for Cartography of the Austrian Academy of Sciences in Vienna and as Director of the Joanneum Research Institute of Digital Image Processing and Computer Graphics in Graz he spent several months of postdoctoral research at the Finnish National Research Center/VTT in Espoo near Helsinki and at the Jet Propulsion Laboratory/JPL of NASA in Pasadena. In 1985 he obtained his habilitation (venia legendi) for both General Geology and Remote Sensing. From 1992 to 2016 he was Full Professor, holding the Chair of Cartography at TU Dresden, Germany. He is member of several learned societies and obtained several scientific awards, i.a. the Friedrich Hopfner Medal (A) and the Denny Medal (UK).*

**Research Activities**

**Abdi, O., Kamkar, B., Shirvani, Z., Teixeira da Silva, J.A. & Buchroithner, M.F. (2018): Spatial-Statistical Analysis of Factors Determining Forest Fires: A Case Study from Golestan, Northeast Iran. Geomatics, Natural Hazards and Risk, 9, 1: 267 – 280. DOI: 10.1080/19475705.2016.1206629.**

Abstract

Intermittent fires in Northeast Iran in the autumn of 2010 resulted in the burning of some valuable forest habitats. The objective of this study was to apply geographic information systems (GIS) to determine to what degree three key factors (environmental, climatic, and anthropogenic) influence the severity rating of fires in these forests. The forest fire sites were surveyed and imported into GIS. The severity of burnt areas was considered in relation to the three factors. Statistical functions were used to calculate the effect of the factors at each fire site. Logistic and stepwise regressions were used to determine the fire severity rating related to each factor. The results indicate that as the number of cumulative days after the onset of fire increased, the burnt areas also increased at a rate of 303.5 ha/day (R2 = 0.95). Consequently, forest density, daily mean wind speed, daily mean temperature and distance to roads were highly correlated with the daily severity rating of forest fires, and only daily temperature and forest density affected the size of the burnt areas. Prediction maps show that about 24% of the forests have high fire durability, amounting to 7% of the fire-sensitive area. The findings from this case indicate that GIS can be effectively employed in fire management to assess damage, and possibly to prevent future fires, thus assisting in the preservation of valuable forest resources.

**Abdi, O., Shirvani, Z. & Buchroithner, M.F. (2018): Spatiotemporal Drought Evaluation of Hyrcanian Deciduous Forests and Semi-Steppe Rangelands Using Moderate Resolution Imaging Spectroradiometer Time Series in Northeast Iran. Land Degradation and Development, 2018, 29: 2525 – 2541. DOI: 10.1002/ldr.3025**.

Abstract
Advanced MODIS data have provided diverse products for assessing and monitoring natural vegetation affected by droughts. Between 2000 and 2016, we estimated monthly precipitation anomalies in the deciduous forests and semi-steppe rangelands of northeastern Iran using Kriging models, and analysed 16-day vegetation anomalies using vegetation greenness and water content indices—including the Enhanced Vegetation Index (EVI), the Normalized Difference Vegetation Index (NDVI) and, the Normalized Difference Water Index (NDWI). Vegetation anomalies showed high positive responses to inter-seasonal precipitation anomalies over the 17-year period, and low positive responses to monthly precipitation deficits during critical droughts. Forest and rangeland anomalies recorded higher Moran's coefficients based on the NDVI ($I$ = 0.253±0.102) and NDWI ($I$ = 0.284±0.087) with inter-seasonal precipitation anomalies, respectively. Throughout critical droughts, the NDWI anomalies showed higher coefficients with monthly precipitation deficits for both forests ($I$ = 0.0716±0.059) and rangelands ($I$ = 0.125±0.0615). Nevertheless, there were only significant differences between the Moran's coefficients of the three vegetation indices for rangelands ($F = 2.873$; $P < 0.05$). BiLISA maps indicated that sparse forests show higher spatial associations with drought conditions (High-high cluster), whereas dense forests experienced lower stresses by severe droughts (High-low outlier) during drought periods. Meanwhile, some severe vegetation stresses occurred at locations with low droughts (Low-high outlier), which indicate the impact of other significant climate-induced disturbances on vegetation anomalies.

**Abdi, O., Shirvani, Z. & Buchroithner, M.F. (2018): Visualization and Quantification of Significant Anthropogenic Drivers Influencing Rangeland Degradation Trends Using Landsat Imagery and GIS Spatial Dependence Models: A Case Study in Northeast Iran. Journal of Geographical Sciences, 28 (12): 1933 – 1952. DOI: 10.1007/s11442-018-1572-z.**

Abstract
Developing countries must consider the influence of anthropogenic dynamics on changes in rangeland habitats. This study explores happened degradation in 178 rangeland management plans for Northeast Iran in three main steps: (1) conducting a trend analysis of rangeland degradation and anthropogenic dynamics in 1986–2000 and 2000–2015, (2) visualizing the effects of anthropogenic drivers on rangeland degradation using bivariate local spatial autocorrelation (BiLISA), and (3) quantifying spatial dependence between anthropogenic driving forces and rangeland degradation using spatial regression approaches. The results show that 0.77% and 0.56% of rangelands are degraded annually during the first and second periods. The BiLISA results indicate that dry-farming, irrigated farming and construction areas were significant drivers in both periods and grazing intensity was a significant driver in the second period. The spatial lag (SL) model (wi=0.3943, Ei=1.4139) with two drivers of dry-farming and irrigated farming in the first period and the spatial error (SE) model (wi=0.4853, Ei=1.515) with livestock density, dry-

farming and irrigated farming in the second period showed robust performance in quantifying the driving forces of rangeland degradation. To conclude, the BiLISA maps and spatial models indicate a serious intensification of the anthropogenic impacts of ongoing conditions on the rangelands of northeast Iran in the future.

**Bayramov, E., Kada, M. & Buchroithner, M.F. (2018): Monitoring oil spill hotspots, contamination probability modelling and assessment of coastal impacts in the Caspian Sea using SENTINEL-1, LANDSAT-8, RADARSAT, ENVISAT and ERS satellite sensors. Journal of Operational Oceanography 11(4): 1 - 17. DOI: 10.1080/1755876X.2018.1438343.**

Abstract
Oil and gas development in the Caspian region is associated with pollution risks. This research aimed to better understand those risks by (1) using satellite data to characterise the spatial and temporal distribution of anthropogenic and naturally occurring oil slicks in the Azerbaijani portion of the Caspian Sea (2) performing stochastic modelling of the risk that the oil spills pose to water quality and shoreline ecosystems and (3) validating model predictions using satellite images. Over 411 satellite images acquired by SENTINEL-1, LANDSAT-8, RADARSAT, ENVISAT and ERS sensors between 1996 and 2017 were used for the semi-automatic detection and discrimination of oil spills and natural seepage slicks using object-based classification and visual interpretation. Anthropogenic oil pollution, natural seepage slicks and 'hotspots' or areas frequently covered by oil slicks were identified. Anthropogenic hotspots were observed at Oil Rocks Settlement, Chilov and Pirallahi Islands, three of the area's oldest oil platforms, with oil spill rates of up to 1264 m3 per day. The contamination probability of more than 50% was primarily located in the shoreline range of 464–508 km with the existence of high rank environmental and social sensitivities. The highest maximum accumulated emulsion mass (tonnes) was also observed in the shoreline range of 464–508 km with high contamination probability > 50% and with the existence of high rank environmental and social sensitivities. This research demonstrates how remote sensing data can be used to identify oil pollution hotspots and to quantitatively assess the risk to shoreline areas with high environmental value.

**Bayramov, E., Knee, K., Kada, M. & Buchroithner, M.F. (2018): Using Multiple Satellite Observations to Quantitatively Assess and Model Oil Pollution and Predict Risks and Consequences to Shoreline from Oil Platforms in the Caspian Sea. Human and Ecological Risk Assessment. An International Journal, 24, 6: 1501 – 1514.**

Abstract
A number of productive oil and gas fields are located in the Absheron Peninsula of Azerbaijan. It is well known that hydrocarbon fluid withdrawal activities cause ground deformation processes like subsidence and uplifts. The primary goal of the presented study was to quantitatively assess the ground deformation (subsidence and uplift) rates of oil and gas fields, determine natural and man-made influencing factors and predict deformation trends. Traditional ground surveying methods are important to accurately assess the subsidence and uplift rates, however, they are costly in terms of necessary equipment and human involvement. Nowadays, Persistent Scatterer Interferometry, an improved remote sensing tool, can be used for the recording of ground surface changes at millimeter scale.
The existence of ground deformation processes in the Absheron oil and gas fields was

observed for the period of 2015-2017 with the hotspots of highest subsidence rates in Bibi-heybat, Zigh, Balakhani-Sabunchi-Ramani and the hotspots of highest uplift rates in Garadagh, Kergez-Giziltepe-Shongar and Bibi-heibat oil and gas fields. The determined maximum displacement rates of subsidence and uplift processes were -26 mm/y and +23 mm/y, respectively. However trend, kernel and point density analysis of deformation velocity presented the natural patterns of uplift and subsidence tectonic processes from West to North-East and South-East. This allowed to determine that Bibi-heybat and Zigh oil and gas fields hold a higher probability of being affected by man-made oil and gas exploration activities, whereas the Balakhani-Sabunchi-Ramani oil field is affected by both natural and man-made processes.
Geographically Weighted Regression analysis revealed that well concentration and elevation factors provided 32% of explanation to subsidence processes of Bibi-heybat, Zigh and Balakhani-Sabunchi-Ramani oil fields.
Linearity ($R^2$) and Linear trend (OLS) also indicated temporal correlation of ground deformation processes for these three oil and gas fields with predicted monthly rate of ground deformations that ranges from -2.54 to 1.89 mm/month for subsidence and uplift processes, respectively.

**Ji, M., Liu, L. & Buchroithner, M.F. (2018): Identifying Collapsed Buildings Using Post-Earthquake Satellite Imagery and Convolutional Neural Networks: A Case Study of the 2010 Haiti Earthquake. Remote Sensing, 10 (11): 1689. DOI: 10.3390/rs10111689.**

Abstract
Earthquake is one of the most devastating natural disasters that threaten human life. It is vital to retrieve the building damage status for planning rescue and reconstruction after an earthquake. In cases when the number of completely collapsed buildings is far less than intact or less-affected buildings (e.g., the 2010 Haiti earthquake), it is difficult for the classifier to learn the minority class samples, due to the imbalance learning problem. In this study, the convolutional neural network (CNN) was utilized to identify collapsed buildings from postevent satellite imagery with the proposed workflow. Producer accuracy (PA), user accuracy (UA), overall accuracy (OA), and Kappa were used as evaluation metrics. To overcome the imbalance problem, random over-sampling, random under-sampling, and cost-sensitive methods were tested on selected test A and test B regions. The results demonstrated that the building collapsed information can be retrieved by using post-event imagery. SqueezeNet
performed well in classifying collapsed and non-collapsed buildings, and achieved an average OA of 78.6% for the two test regions. After balancing steps, the average Kappa value was improved from 41.6% to 44.8% with the cost-sensitive approach. Moreover, the cost-sensitive method showed a better performance on discriminating collapsed buildings, with a PA value of 51.2% for test A and 61.1% for test B. Therefore, a suitable balancing method should be considered when facing imbalance dataset to retrieve the distribution of collapsed buildings.

**Liu, L., Ji, M. & Buchroithner, M.F. (2018): Transfer Learning for Soil Spectroscopy Based on Convolutional Neural Networks and Its Application in Soil Clay Content Mapping Using Hyperspectral Imagery. Sensors, 18, 3169: 18 pp. DOI: 10.3390/s18093169.**

Abstract
Soil spectra are often measured in the laboratory, and there is an increasing number of large-scale soil spectral libraries establishing across the world. However, calibration models developed from soil libraries are difficult to apply to spectral data acquired from the field or space. Transfer learning has the potential to bridge the gap and make the calibration model transferrable from one sensor to another. The objective of this study is to explore the potential of transfer learning for soil spectroscopy and its performance on soil clay content estimation using hyperspectral data. First, a one-dimensional convolutional neural network (1D-CNN) is used on Land Use/Land Cover Area Frame Survey (LUCAS) mineral soils. To evaluate whether the pre-trained 1D-CNN model was transferrable, LUCAS organic soils were used to fine-tune and validate the model. The fine-tuned model achieved a good accuracy (coefficient of determination (R2) = 0.756, root-mean-square error (RMSE) = 7.07 and ratio of percent deviation (RPD) = 2.26) for the estimation of clay content. Spectral index, as suggested as a simple transferrable feature, was also explored on LUCAS data, but did not performed well on the estimation of clay content. Then, the pre-trained 1D-CNN model was further fine-tuned by field samples collect in the study area with spectra extracted from HyMap imagery, achieved an accuracy of R2 = 0.601, RMSE = 8.62 and RPD = 1.54. Finally, the soil clay map was generated with the fine-tuned 1D-CNN model and hyperspectral data.

**Sam, L., Bhardwaj, A., Kumar, R., Buchroithner, M.F. & Javier Martín-Torres, F. (2018): Heterogeneity in topographic control on velocities of Western Himalayan glaciers. Nature Scientific Reports 2018, 8: 12843, 16 pp. DOI: 10.1038/s41598-018-31310-y.**

Abstract
Studies of the seasonal and annual patterns of glacier velocities improve our understanding of the ice volume, topography, responses to climate change, and surge events of glaciers. Such studies are especially relevant and equally rare for the Himalayan glaciers, which supply many rivers that sustain some of the most heavily populated mountainous regions in the world. In particular, the control of the hypsometric distribution of geomorphometric parameters, such as slope, aspect, and curvature, on the dynamics of Himalayan glaciers have never been studied so far, at the river basin scale. Here, we present the degree to which topographic and hypsometric parameters affect the seasonal and annual average flow velocities of 112 glaciers in the Baspa River basin in the Western Indian Himalaya by analysing Global Land Ice Velocity Extraction from Landsat 8 (GoLIVE) datasets for the years 2013-2017. We observe, (i) significant heterogeneity in topographic controls on the velocities of these glaciers, (ii) elevation and the seasons play important roles in regulating the degree to which morphometric parameters (slope, aspect, and curvature) affect these velocities, (iii) a possible polythermal regime promoting both sliding and deformational forms of motion in a majority of these glaciers, and (iv) a detailed analysis of complex topographic controls within various elevation zones using a novel hypso-morphometric approach. These findings can help us to better model the dynamics of Himalayan glaciers and their responses to the future climatic scenarios. The inferences also suggest the need to incorporate dynamic topography in glacio-hydrological models in the wake of constant glacial evolutions.

# Research Activities within Structural Safety, Monitoring and Control

## by Hong-Nan Li, Member EUAS

Short Biography

*Dr. Hong-Nan Li was born on Aug. 29, 1957, in Shenyang City, China. He received his bachelor's degree from Shenyang Jianzhu University in 1982, his master's degree and PhD from the China Earthquake Administration in 1987 and 1990, respectively. He had conducted his postdoctoral research at Virginia Polytechnic Institute and State University from 1992-1994.He is the Distinguished Professor of School of Civil Engineering at Dalian University of Technology (DUT), China. He is the founding director of the Research Center for Structural Health Monitoring and Control at DUT.*

*He is a Fellow of American Society of Civil Engineers (ASCE). His research interests are primarily in safety and security of civil infrastructure systems, focusing on development of innovative and interdisciplinary science and technology for sensors, health monitoring, and damage assessment. He has successfully secured over Chinese $ 60 Million research grants in the capacity of PI from various government agencies (e.g., NSFC, Ministry of Education, Ministry of Science and Technology) over the past few years. He is the author/co-author of 7 books and 400 refereed journal papers including about 300 in top-tier international journals (includes SCHM, MSSP, SSS, ASCE ES, JSV, etc., H-Index: 36 (Web of Science). He is also an inventor or co-inventor of 45 invention patents and 5 computer software. He has delivered over 70 keynote and invited lecture at international conferences and universities in different countries.*

*He edited the first ever standard in the area of SHM in China "Design Standard for Structural Health Monitoring Systems (CECS 333: 2012)" and other 15 standards. His related achievements have been applied to the health monitoring of 60 major engineering projects, such as the Zhoushan Tower (The World's the Tallest Transmission Tower), Dalian gymnasium (The World's Largest Span Suspended Dome Structure), the long span suspension dome structure NB35-2 (Ultra Large Offshore Oil Platform), Shenyang Boguan bridge (Complicated Long-Span Arch Bridge), Dalian World Trade Center, etc. He received various prizes in recognition of his achievements in research, such as played a leading role in the 2015 National Technology Invention Award, 2010 & 2007 National Science and Technology Progress Awards, and more than 10 provincial Science & Technology awards in China.*

*With a long-term commitment to serving society, He is currently the Editor-in-Chief of Structural Monitoring and Maintenance, An international Journal, Associate Editor of Journal of Aerospace Engineering-ASCE and an editorial board member of more than 20 other journals. He also has held many extensive academic and professional leadership positions related to SHM: vice chair of the Advanced Materials and Structures committee & vice chair Dynamics and Controls Committee, American Society of Civil Engineers (ASCE); vice chair of China Panel, International Association for Structural Control and Monitoring (IASHM); council member of The International Society for Structural Health Monitoring of Intelligent Infrastructure (ISHMII), vice chair of the board for the Society of Structural Anti-Seismic, a branch of the Chinese Society of Vibration Engineering, etc.*

*He was elected Fellow of ASCE, and awarded "Outstanding Technical Contribution Award" by*

*ASCE Aerospace Division (2014). He was honored as Distinguished Professor in Cheung Kong Scholars Program by Ministry of Education of China, National Science Foundation for Distinguished Young Scholars of China (NSFC), National Young and Middle-aged Expert with Outstanding Contributions by Ministry of Human Resources and Social Security of China, State Department experts enjoying special government allowances by State Council of China, etc.*
*Dr. Li promoted the education of undergraduate students and graduate students in Civil Engineering. He has supervised more than 50 Ph.D. students and 60 Master students. Some thesis by his students were awarded provincial excellent theses.*

**Research Activities**

His research interests are primarily in the safety, monitoring and control of civil infrastructure systems, focusing on development of innovative and interdisciplinary science and technology for sensors, health monitoring, and damage assessment.

Conventional sensors and corresponding data acquisition system are usually infeasible to apply to large infrastructures for long-term monitoring, which make the advanced fiber optic sensor become one of the major focuses of the SHM research. Dr. Li has studied optical fiber sensing (OFS) technology for nearly 20 years and is a leading researcher in this field. He reveled the strain distribution along the fiber length of embedded OFSs, average strain transfer rate of OFS and critical adherence length, influence of the host material, and strain transferring mechanism for surface-bonded OFSs, and established a more suitable strain transferring for a multi-layered concentric model base on these findings. His group has developed various kinds of fiber optic sensors (FOS), such FBG strain sensor, FBG Temperature sensors, FBG displacement sensors, etc.

Optimal sensor placement (OSP) technique plays a key role in the SHM of large infrastructures. The issue of sensor placement attracts much attention from both academia and industry, especially due to the increased number of instrumented large structures for the SHM in the last decade.

Dr. Li and his students Dr. D.S. Li firstly discovered the connection between two influential methods, the EI and the MKE. The EI requires iteration computations, but the MKE not. In the iterations of EI, it redistributes the modal kinetic energy into the retaining DOFs and recomputed their MKE index for the reduced system using re-orthonormalized mode shapes. In this sense, the EI is an iterated version of MKE with re-orthonormalized mode shapes. Afterwards, Dr. Li proposed a new computation scheme of EI though the QR downdating. In the new scheme, the EI is computed with reduced modal matrix after a row is removed from the previous modal matrix and on the direct comparison of row norms of decomposed orthonormal matrix by the QR decomposition. Furthermore, the QR decomposition downdating steps based on the combination of the modified Gram-Schmidt and Householder transformations are implemented and further improve the EI computation efficiency considerably by eliminating the unnecessary costly QR decompositions in the EI iterations. This significant finding received the “Dominick J. DeMichele Scholarship Award” at the IMAC-XXVI Conference & Exposition on Structural Dynamics, Feb. 6, 2008, Orlando, USA.

There are many interesting intelligent algorithms to tackling sensor placement

problem, Dr. Li first adopted the Monkey algorithm (MA) in the field of sensor placement. Based on substantial improvements on the original MA, they presented a series of novel improved MAs for the sensor placement, including the simple monkey algorithm (SMA), asynchronous-climb monkey algorithm (AMA), distributed monkey algorithm (DMA), immune monkey algorithm (IMA), virus monkey algorithm (VMA), niching monkey algorithm (NMA), adaptive monkey algorithm (AMA), and collaborative-climb monkey algorithm (CMA). These improved MAs can be adopted to the various infrastructures that have different requirements. For example, the DMA outperforms the conventional algorithms both in terms of generating optimal solutions as well as faster convergence; the NMA can enhance the exploitation capability effectively. These developed method were designed as MATLAB Toolbox "optimal sensor placement strategy (OSPS)", which was published in "*Struct. Des. Tall Spec*., 2011, 20(7)" and is selected as "ESI Highly Cited Paper, Most cited articles contributing to the 2012 impact factor, Top-cited article from 2011 to 2013".

In the field of SHM, more and more kinds of sensors have been applied to sense a number of physical measurement such as the FBG for the strain and electric sensors for the acceleration, pressure, displacement, inclination and so on. A critical demand for a general-purpose data acquisition device to synchronously measure a great amount of polytypic sensors has been proposed to satisfy requirements of data processing, calculation and structure analysis in some SHM projects. Dr. Li developed a polytypic and synchronous data acquisition device system to measure the FBG sensors and electric signals, including voltage, current and digital I/O, which have covered most types of electric sensors. This breakthrough device is featured with three characteristics: a) A high-power, low-noise swept laser source for the FBG demodulation; b) A synchronous data acquisition mechanism for polytypic signals; c) An embedded hardware and real-time operating system with the industrial stability. A customized software architecture accompanied with the data acquisition device, named the DUT-SHM has been integrated by the state machine and event-driven architecture and featured with functions of modularization and multithreading for demands of SHM. This novel device has been applied to various civil engineering monitoring projects and rewarded the bronze medal of the 45$^{th}$ International Exhibition of Inventions of Geneva.

To reduce the uncertainty, imprecision and low reliability, the multi-sensor data fusion technique had better to be adopted. Dr. Li proposed an improved data fusion method based on the consensus algorithm for a multi-sensor system. In this method, the relation matrix is innovatively blurred to avoid the subjective error in determining the threshold value. And then, he developed an analytical approach for the seismic ground motions by applying the CWT, which focuses on the energy input to the structure. Considering that the wavelet packet transform (WPT) has the ability to clearly reflect the damage characteristics of structural response signals and the artificial neural network (ANN) is capable of learning in an unsupervised manner and of forming new classes when the structural exhibits change, Dr. Li proposed a multi-stage structural damage diagnosis method by using the WPT and ANN based on the "energy-damage" theory, in which, the wavelet packet component energy is first extracted to be damage sensitive feature and then adopted

as the input into an improved back propagation (BP) neural network model for damage diagnosis in a step by step mode.

Static displacement curvature of a structure could be used for the damage detection. However, it will also be influenced by varying environmental and operational conditions. Based on the unique characteristics of the curvature of a beam, Dr. Li proposed a new damage identification index, i.e., the combination of successive displacement curvature. The position coordinates of three successive nodes of a beam bearing concentrated loads, and consequently their corresponding curvatures, satisfy certain relationship. Once the relationship fails to meet the relationship, damage occurs and thus can be identified. Furthermore, influence of ambient temperature variation on the proposed damage index can be eliminated since successive displacement curvature bear similar trend under the same temperature condition, which is also the rationale of the so-called co-integration. Therefore, his method could eliminate the influence of changing environmental temperature without the structural data in a healthy condition, and has the ability to monitor and identify the damage location online.

Dr. Li and his team are renowned for their efforts in the use of SHM in civil engineering structures across China. He has integrated the understanding of unique design concepts with the practical need for effective monitoring structures and tremendously influenced and contributed to the implementation of SHM in practice.

The first design code in the field of SHM in China called “Design Standard for Structural Health Monitoring System (CECS 333: 2012)” was edited by Dr. Li (Editor-in-Chief) and his colleagues. The Standard has been widely circulated among practitioners and researchers in the world for consultation, and reviewed by a reviewing committee formed by China Association for Engineering Construction Standardization before putting it in force. It has induced a positive chain reaction for the revision of Bridge Design Standard in Australia as well as encouraging other countries, which do not have SHM included in their design specifications, to follow.

Dr. Li has established the “Joint Laboratory for Structural Health Monitoring and Control” with National Instruments Corporation, USA. They have jointly invented more than 10 patents related to smart sensing technology and novel sensors. More important, the developed technology innovation and methodologies have been applied in many real large-scale engineering projects in China, as most of the largest and most notable engineering structures built in recent years are in China and a demand for effective long term health monitoring becomes imminent.

Dr. Li has had a profound impact on SHM research and engineering education for near 30 years. Great accomplishments have been made by him in SHM field, and related technologies and methodologies have been applied into many actual large-scale engineering projects which promoted significantly the development of the discipline of SHM. It is a career filled with honors, patents, and publications. He is a world pioneer in development, research, innovation, and implementation of SHM technology, and has tremendously pushed the boundaries of SHM technologies.

# Electrochemical Applications for Clean Energy Generation/Storage and Corrosion Control

**by Jingli Luo, Member EUAS**

Short Biography

*Dr. Jingli Luo received her Ph.D from the McMaster University, Canada, in 1992 and is now a professor emeritus of chemical and materials engineering at University of Alberta, Canada and is Fellow of the Canadian Academy of Engineering. She served as Canadian Research Chair in Alternative Fuel Cells from 2004 to 2015 and was a member of (Discovery) Grant Selection Committee of Natural Sciences & Engineering Research Council of Canada (NSERC). Dr. Luo's outstanding achievements in research on alternative fuel cells and corrosion control are internationally known and widely acknowledged, and she is the member of Editorial Board, Electrochemical Energy Reviews (EER) (Springer-Nature publishing group). Dr. Luo pioneered several non-conventional fuel cells that co-generate electricity and value-added products; her latest invention, as a green technology, can eliminate $CO_2$, and her inventions represent significant advances in this field. Dr. Luo led three NSERC Strategic Projects and holds six US patents. She has published over three hundred papers in refereed journals and received, among other awards, the Morris Cohen Award in 2002 and the Canadian Metal Chemistry Award in 2014 from the Metallurgy and Materials Society in recognition of her outstanding contributions. Dr. Luo has supervised 125 graduate students and post-doctors, ten of them are now university professors.*

## Research Activities

Seeking new energy sources or converting industrial wastes to energy and value-added products has long been an engineering challenge. Fuel cells, as a clean energy source, require stable and active electrodes, and stable yet conductive electrolytes. Dr. Luo synthesized several novel materials for new generation of fuel cells with enormous economic benefits: the sulphur-tolerant and coking resistant catalysts enable the development of the SOFCs using non-conventional fuels such as $H_2S$-containing industrial syngas or natural gas. Traditionally, $H_2S$ must be removed from the fuels at high cost in industry prior to its use in the fuel cells. Elimination of this step in her novel fuel cell process makes fuel cells a more promising and

economic energy source. Another novel anode catalyst she developed can selectively oxidize $H_2$ without activating CO molecules; the SOFC with such an anode can use syngas as the feed and generate electricity while enriching CO with few deleterious contaminants. As a major technological breakthrough, the novel catalyst has resulted in the next generation of SOFC: a process for conversion of $CO_2$ + $CH_4$ to value added product, CO, and co-generation of electricity, surpassing the original concept of fuel cell and exemplifying the "green" technology via utilization of what is otherwise considered as waste or pollutant.

As a council member of International Corrosion Council (ICC) and Editorial Board member of Corrosion Science, Dr. Luo has extensive achievements in corrosion research: she developed a theoretical model for quantitative evaluation of the synergism of electrochemical and mechanical factors in erosion-corrosion based on non-equilibrium thermodynamics, electrochemistry and dislocation kinetics of carbon steels in slurry. She has also conducted extensive research work on corrosion of nuclear materials under extreme conditions and discovered various corrosion mechanisms for achieving better corrosion control.

**Selected Research Outputs**


(1) Zhou Chen, Tingting Fan, Ya-Qian Zhang, Jing Xiao, Minrui Gao, Nanqi Duan, Jiawei Zhang, Jianhui Li, Qingxia Liu, Xiaodong Yi* and Jing-Li Luo,* "Wavy $SnO_2$ catalyzed simultaneous reinforcement of carbon dioxide adsorption and activation towards electrochemical conversion of $CO_2$ to HCOOH,*" Applied Catalysis B: Environmental*., 261, 118243 (2020).

(2) Tengfei Li, Chao Yang, Jing-Li Luo,* Gengfeng Zheng,* "Electrolyte Driven Highly Selective CO2 Electroreduction at Low Overpotentials," *ACS Catalysis*, 9, pp. 10440−10447 (2019).

(3) Chong Sun, Subiao Liu, Jiankuan Li, Hongbo Zeng, Jing-Li Luo,* "Insights into the interfacial process in electroless Ni-P coating on supercritical $CO_2$ transport pipeline as relevant to carbon capture and storage," *ACS Appl. Mater. Interfaces*, 11, pp. 16243-16251 (2019).

(4) Xian-Zong Wang, Hong Luo, Jing-Li Luo,* "Effects of hydrogen and stress on the electrochemical and passivation behaviour of 304 stainless steel in simulated PEMFC environment," *Electrochimica Acta*, 293, pp. 60-77 (2019).

(5) Yuan-Yuan Hong, Xian-Zong Wang, Ken Cadien, Jing-Li Luo, "Transient Potential Induced Anodic Dissolution of 316L Stainless Steel in Sulfuric Acid Solution," *Journal of The Electrochemical Society*, 166, pp. C3355-C3363 (2019).

(6) Chong Sun, Hongbo Zeng, Jing-Li Luo,* "Unraveling the effects of $CO_2$ and $H_2S$ on the corrosion behavior of electroless Ni-P coating in $CO_2$/$H_2S$/Cl- environments at high temperature and high pressure," *Corrosion Science*, 148, pp 317-330 (2019).

(7) Bin Hua,* Meng Li, Wanying Pang, Weiqiang Tang, Shuangliang Zhao, Zhehui Jin, Yimin Zeng, Babak Shalchi Amirkhiz, and Jing-Li Luo,*

"Activating p-Blocking Centers in Perovskite for Efficient Water Splitting," *Chem*, 4, Issue 12, pp.2902-2916 (2018).

(8) Chong Sun, Jiankuan Li, Shuo Shuang, Hongbo Zeng, Jing-Li Luo,* "Effect of defect on corrosion behavior of electroless Ni-P coating in $CO_2$-saturated NaCl solution," *Corrosion Science*, 134, pp. 23–37 (2018).

(9) Subiao Liu, Xian-Zong Wang, Hongbiao Tao, Tengfei Li, Qi Liu, Zhenghe Xu, Xian-Zhu Fu, Jing-Li Luo,* "Ultrathin 5-Fold Twinned Sub-25 nm Silver Nanowires Enable Highly Selective Electroreduction of $CO_2$ to CO," *Nano Energy*, 45, pp. 456–462 (2018).

(10) Bin Hua, Meng Li*, Jing-Li Luo*, "A facile surface chemistry approach to bifunctional excellence for perovskite electrocatalysis", *Nano Energy*, 49, pp. 117-125 (2018).

(11) Ya-Qian Zhang, Meng Li, Bin Hua,* Yue Wang, Yi-Fei Sun, Jing-Li Luo,* "A strongly cooperative spinel nanohybrid as an efficient bifunctional oxygen electrocatalyst for oxygen reduction reaction and oxygen evolution reaction," *Applied Catalysis B: Environmental*, 236, pp. 413-419 (2018).

(12) Xian-Zong Wang, Triratna Muneshwar, Hongqiang Fan, Ken Cadien, Jing-Li Luo,* "Achieving ultrahigh corrosion resistance and conductive zirconium oxynitride coating on metal bipolar plates by plasma enhanced atomic layer deposition," *Journal of Power Sources*, 397, pp. 32-36 (2018).

(13) Subiao Liu, Hongbiao Tao, Li Zeng, Qi Liu, Zhenghe Xu, Qingxia Liu,* Jing-Li Luo,* "Shape-Dependent Electrocatalytic Reduction of $CO_2$ to CO on Triangular Silver Nanoplates," *J. Am. Chem. Soc.*, 139, pp. 2160–2163 (2017).

(14) Bin Hua, Meng Li, Ya-Qian Zhang, Yi-Fei Sun, Jing-Li Luo,* "All-in-one Perovskite Catalyst: Smart Controls of Architecture and Composition towards Enhanced Oxygen/Hydrogen Evolution Reactions," *Advanced Energy Materials*, DOI: 10.1002/aenm.201700666. (July 14, 2017).

(15) B. Hua,* N. Yan, M. Li, Y.F. Sun, Y. Q. Zhang, J. Li, T. Etsell, P. Sarkar, J.L. Luo,* "Anode-Engineered Protonic Ceramic Fuel Cell with Excellent Performance and Fuel Compatibility," *Adv. Mater.*, 28(40), pp. 8922-8926 (2016) (Oct. 26, 2016)

(16) Bin Hua, Ning Yan, Meng Li, Ya-Qian Zhang, Yi-Fei Sun, Jian Li, Thomas Etsell, Partha Sarkar, Karl Chuang and Jing-Li Luo,* "Novel layered solid oxide fuel cells with multiple-twinned $Ni_{0.8}Co_{0.2}$ nanoparticles: the key to thermally independent $CO_2$ utilization and power-chemical cogeneration," *Energy & Environmental Science*, 9, pp. 207-215 (2016).

(17) Bin Hua, Ya-Qian Zhang, Ning Yan,* Meng Li, Yi-Fei Sun, Jian Chen, Jian Li, and Jing-Li Luo,* "The excellence of both worlds: developing effective double perovskite oxide catalyst of oxygen reduction reaction for room and elevated temperature applications," *Adv. Funct. Mater.*, 26, pp. 4106-4112 (2016).

# Innovative Computing Methods in Cloud Computing, Big Data and Bioinformatics Applications

**by Yi Pan, Member EUAS**

Short Biography

*Dr. Yi Pan was born in Jiangsu, China. He entered Tsinghua University in March 1978 with the highest college entrance examination score among all the students who took the exams in Jiangsu Province in 1977.*

*Dr. Pan is currently a Regents' Professor and Chair of Computer Science at Georgia State University, USA. He has served as an Associate Dean and Chair of Biology Department during 2013-2017 and Chair of Computer Science during 2006-2013. Dr. Pan joined Georgia State University in 2000, was promoted to full professor in 2004, named a Distinguished University Professor in 2013 and designated a Regents' Professor (the highest recognition given to a faculty member by the University System of Georgia) in 2015.*

*Dr. Pan received his B.Eng. and M.Eng. degrees in computer engineering from Tsinghua University, China, in 1982 and 1984, respectively, and his Ph.D. degree in computer science from the University of Pittsburgh, USA, in 1991. His profile has been featured as a distinguished alumnus in both Tsinghua Alumni Newsletter and University of Pittsburgh CS Alumni Newsletter.*

*Dr. Pan has served as an editor-in-chief or editorial board member for 20 journals including 7 IEEE Transactions. He is the recipient of many awards including one IEEE Transactions Best Paper Award, four other international conference or journal Best Paper Awards, 4 IBM Faculty Awards, 2 JSPS Senior Invitation Fellowships, IEEE BIBE Outstanding Achievement Award, NSF Research Opportunity Award, and AFOSR Summer Faculty Research Fellowship. He has organized numerous international conferences and delivered keynote speeches at over 60 international conferences around the world.*

*Dr. Pan's current research interests include parallel and cloud computing, big data, deep learning, and bioinformatics. Dr. Pan has published more than 350 papers including over 200 SCI journal papers and over 90 IEEE/ACM Transactions papers. In addition, he has edited/authored 43 books. His research work has been cited more than 10,000 times in Google Scholar and his current h-index is 53.*

Below are some of his recent research work:

## 1. Novel Deep Learning Method for Predicting Epilepsy

Deep learning has been successfully used in many applications such as computer vision, automatic speech recognition, natural language processing, audio recognition, and medical imaging processing and disease diagnosis. Recently, our group has designed a method to detect a type of epilepsy - benign epilepsy with

centrotemporal spikes, which is the most popular epilepsy with children. In our method, we use three sources of data: hand-crafted features from MRI images based on doctors' knowledge, 3D MRI images and 4D functional MRI images. The final prediction decision is obtained by fusing the three prediction results through another neural network. Our idea is to take advantages of all three data sources which have different strengths and important features to achieve the best prediction results. We have done many experiments which show that the proposed method is truly better than any existing prediction method. Future improvement includes how to use more data sources.

## 2. Challenges and Improvements in Deep Learning Research

Neural networks, modeled after the human brain, contain a set of algorithms to recognize patterns via training a data set. Deep learning neural network architectures differ from traditional neural networks because they have more hidden layers and newer training algorithms. Deep learning networks can be trained in an UNSUPERVISED or SUPERVISED manner for both UNSUPERVISED and SUPERVISED learning tasks and hence can be applied in many applications. Deep learning is now producing many remarkable successes in computer vision, automatic speech recognition, natural language processing, audio recognition, bioinformatics and disease prediction and detection. Although various deep learning architectures and novel algorithms have been applied to many big data applications, better explainability, increasing prediction accuracy and speeding up the training process are still challenging tasks among others. In this research, our focuses are on proposing more effective architectures, intelligently freezing layers, effectively handling high dimensional data, designing encoding schemes, mathematical proofs, optimization of hyper-parameters, embedding logic and reasoning during training, result explanation and hardware support for deep learning. Some of our solutions and preliminary results in these areas will be presented and future research directions will also be identified.

## 3. Automatic Parallel Programming on Cloud Computing Platforms

Cloud computing has gradually evolved into an infrastructural tool for many scientific and business applications with intensive data or computing requirements. One of the challenges in cloud computing now is how to run software efficiently on cloud platforms since lots of classic sequential codes are not ready to be executed in parallel in cloud environments, resulting in long execution time and low efficiency. It is also costly and labor intensive to redesign and convert current sequential codes into cloud codes running on cloud programming models such as MapReduce or Spark. Thus, automatic translation from sequential codes to cloud codes is one of the directions that could resolve the problem of slow code migration from traditional computing platforms to cloud infrastructures. In this research, we propose and design several automatic translators (M2M, J2M and J2S) for cloud programming models MapReduce and Spark. Details of the design of our translators

and their performance results based on many experiments are presented. Performance comparisons with hand coded cloud programs are also studied. Our experimental results indicate that the translators not only can precisely translate the sequential codes such as MATLAB and Java codes into cloud codes, but also can achieve almost linear speedup in performance if the data sizes are big enough. In addition, their limitations and shortcomings will be identified and future directions in this area will also be provided.

## 4. Genome-Wide Disease Association through SNP Analysis

A genome-wide association study (GWAS) involves rapidly scanning markers across the complete sets of genomes of healthy and sick people to find genetic variations associated with a particular disease through analysis of SNPs. Once new genetic associations are identified, we can use the information to develop better strategies to detect, treat and prevent the disease. Although traditional single-locus statistical approaches have been standardized and led to many interesting findings, a substantial number of recent GWASs indicate that for most disorders, the individual SNPs explain only a small fraction of the genetic causes. Consequently, exploring multi-SNPs interactions in the hope of discovering more significant associations has attracted more attentions. In this research, we provide a critical review and comparison of several popular methods, i.e., BOOST, TEAM, epiForest, EDCF, SNPHarvester, epiMODE, MECPM, and MIC with multi-SNPs interactions considered. Several evaluation methodologies, including detecting powers, disease models for simulation, resources of real GWAS data, and the control of false discover rate, are also identified. We present several new results based on using clustering, cloud technologies, energy distribution difference, and new statistical models in this area. In particular, we show that cloud technology can not only speed up the computation, but also achieve better accuracy due to intelligent clustering of sequence data. We also describe a new, fast and powerful Bayesian method for detecting genome-wide multi-locus epistatic interactions on multiple diseases. All of our claims are validated through experimental results.

## 5. Protein Structure Prediction and Its Understanding Based on Machine Learning Methods

Understanding protein structures is vital to determining the function of a protein and its interaction with DNA, RNA and enzyme. The information about its conformation can provide essential information for drug design and protein engineering. While there are over a million known protein sequences, only a limited number of protein structures are experimentally determined. Hence, prediction of protein structures from protein sequences using computer programs is an important step to unveil proteins' three dimensional conformation and functions. As a result, prediction of protein structures has profound theoretical and practical influence over biological study. The explanation of how a decision is made during prediction is also important for improving protein structure prediction and guiding the "wet

experiments". In this research, we show how to use machine learning methods to improve the accuracy of protein structure prediction and to interpret prediction results. We report our research on using neural networks, Support Vector Machines combined with Decision Tree and Association Rule for protein structure prediction, rule extraction and prediction interpretation. Evaluation and comparisons of various prediction and rule extraction systems are presented and future research direction in this area are also identified.

**6. Biological Multiple Sequence Alignment: Scoring Functions, Algorithms, and Evaluations**

Aligning multiple biological sequences is a fundamental task in bioinformatics and sequence analysis. These alignments may contain invaluable information that scientists need to predict the sequences' structures, determine the evolutionary relationships between them, or discover drug-like compounds that can bind to the sequences. Unfortunately, multiple sequence alignment (MSA) is NP-Complete. In addition, the lack of a reliable scoring method makes it very hard to align the sequences reliably and to evaluate the alignment outcomes. In this research, we propose a new scoring method for use in biological multiple sequence alignment. Our scoring method encapsulates stereo-chemical properties of sequence residues and their substitution probabilities into a tree-structure scoring scheme. In addition to the new scoring scheme, we have designed an overlapping sequence clustering algorithm to use in our three new multiple sequence alignment algorithms. One of our alignment algorithms uses a dynamic weighted guidance tree to perform multiple sequence alignment in progressive fashion. The use of dynamic weighted tree allows errors in the early alignment stages to be corrected in the subsequence stages. Other two algorithms utilize sequence knowledge and sequence consistency to produce biological meaningful sequence alignments. The sequence knowledge-based algorithm utilizes the existing biological sequence knowledge databases such as Swiss-Prot to guide sequence alignment. When sequence knowledge databases are not available, the sequence consistency-based algorithm can utilize the consistency information from the input sequence to achieve a similar effect. Experimental results and theoretical analysis indicate that our new scoring function and alignment algorithms truly improve the current best multiple sequence alignment algorithms.

# Synthesis and Processing of Nanomaterials for Energy Storage and Structural Applications

## by Leon L. Shaw, Member EUAS

Short Biography

***Current Positions***

- *Rowe Family Endowed Chair Professor in Sustainable Energy, Department of Mechanical, Materials & Aerospace Engineering, Illinois Institute of Technology (IIT), Chicago, Illinois, USA*
- *Professor of Materials Science and Engineering, Department of Mechanical, Materials & Aerospace Engineering, Illinois Institute of Technology (IIT), Chicago, Illinois, USA*

***Education***

| | |
|---|---|
| *Ph. D.* | *Materials Science and Engineering, University of Florida, Gainesville, Florida, USA, 1992* |
| *Minor* | *Mechanics and Engineering Science, Univers. of Florida, Gainesville, Florida, USA, 1992* |
| *M. S.* | *Materials Science and Engineering, University of Florida, USA, 1992* |
| *M. Eng.* | *Mechanical Engineering, Fuzhou University, Fuzhou, Fujian, China, 1987* |
| *B. S.* | *Materials Engineering, Fuzhou University, Fuzhou, Fujian, China, 1980* |

***Professional Activities***

*Member Editorial Board for "Scientific Reports"*
*Member Editorial Board for "Batteries"*
*Member Editorial Board for "Journal of Sol-Gel Science and Technology"*
*Member International Advisory Committee of THERMEC' 2011, 2013, 2016, and 2018*
*Member ASM International*
*Member TMS*
*Member American Ceramic Society*
*Member Electrochemical Society*
*Guest Editor Metallurgical and Materials Transactions (1998), Materials Science and Engineering (1998,2001, 2007), Journal of Materials Engineering and Performance (2005), Journal of Materials Science (2011)*

***Awards and Honors***

*2019* *Member, EU Academy of Sciences (EUAS)*
*2019* *Keynote Presentation on "Coating as a Potent Method to Enhance the Specific Capacity, Charge Rate and Cycle Life of Cathodes for Next-Generation Li-ion Batteries" at the 2nd International Conference on Materials Science and Materials Chemistry, London, United Kingdom*
*2018* *Energy Award, International Association of Advanced Materials (IAAM)*
*2018* *Energy Award Lecture on "Hierarchical Design and Synthesis of Si Anodes for Next-Generation Li-ion Batteries" in Plenary Session at* ***European Advanced Materials Congress (EAMC 2018),*** *Stockholm, Sweden*
*2018* *Rave Award, Illinois Institute of Technology for outstanding student employment service*
*2018* *First Place in the poster competition at the 2018 Joint Advanced Photon Source/Center for Nanoscale Materials (APS/CNM) Users Meeting, Argonne National Laboratory, USA*
*2016* *Keynote Presentation on "Hierarchical Design and Synthesis of Nanomaterials to Enable High Capacity Rechargeable Battery Electrodes," at THERMEC'2016, Graz, Austria*
*2015* *Key Scientific Article contributing to the Excellence in Energy Research, Renewable Energy Global Innovations*
*2014* *Keynote Presentation on "High Voltage, High Capacity, Ambient Temperature Sodium-Based Flow Batteries" at Cleantech 2014, Washington DC, USA*
*2013* *Keynote Presentation on "Energy Storage Enabled by Nanomaterials and Advanced Processing" at ISPlasma 2013, Nagoya, Japan*
*2011* *NSF Highlights: "Next Generation Bone Implants: More Like the Real Thing"*
*2011* *Outstanding Poster Award, MS&T' 2011, Columbus, OH, USA*
*2010* *The John & Virginia Towers Distinguished Lecture, Michigan Technological University*
*2006* *Member, Connecticut Academy of Science and Engineering (CASE), Connecticut, USA*

*2006 "Highly Commended Paper for Excellence 2006", Emerald Group Publishing Limited*
*2006 Outstanding Faculty Member Award, the Materials Science and Engineering Program, University of Connecticut, Connecticut*
*2005 Fellow, World Academy of Materials and Manufacturing Engineering (AMME), Poland*
*2004 Fellow, ASM International*
*2003 Best Poster Award, the Solid Freeform Fabrication Annual Meeting, Austin, TX*
*2001 Outstanding Department Member Award, Department of Metallurgy and Materials Engineering, University of Connecticut, Connecticut*
*2000 Outstanding Junior Faculty Award, School of Engineering, University of Connecticut, Connecticut*
*1999 Outstanding Department Member Award, Department of Metallurgy and Materials Engineering, University of Connecticut, Connecticut*
*1999 Honorary Advisory Professorship, Harbin Institute of Technology, Harbin, China*
*1999 Honorary Guest Professorship, Fuzhou University, Fuzhou, China*
*1995 Olin Junior Faculty Development Award, Olin Corporation, Connecticut*
*1992 First Place of the ASM International Graduate Student Paper Contest, ASM International*
*1990 Lifetime Member of Alpha Sigma Mu (International Metallurgical Honorary Society)*

***Publications, Patents and Presentations***

- *Over 300 publications (including 3 edited books, 10 book chapters, 210+ archival refereed journal articles, 4 editorial materials, and 77 conference proceedings)*
- *9,400 non-self citations with a h-index of 52 and an i10-index of 168 (Google Scholar)*
- *3 US patents granted and 4 US patents pending*
- *290+ presentations including more than 100 invited talks, keynote presentations and plenary lectures at various national and international conferences as well as a wide range of universities in and outside the United States.*

Leon Shaw's research fields and scientific interests are in the areas of nanomaterials synthesis, processing and microstructure control for energy storage and structural applications as well as additive manufacturing. His group has developed integrated mechanical and thermal activation (IMTA) processes for synthesis of low cost, high purity nanomaterials. Examples of nanomaterials synthesized via the IMTA process include, but are not limited to, SiC, WC, $Si_3N_4$, TiN, CrN, WC-Co and their composites. The progress made in this area has been featured by many magazines including *Chemical Engineering*, *American Ceramic Society Bulletin*, *Sealing Technology*, *Cutting Tool Engineering*, and *Ceramic Industry*. His work in nano-coatings through thermal plasma spray has revealed that the phase content, grain size, hardness, density and wear resistance of nanostructured $Al_2O_3$-$TiO_2$ coatings exhibit a strong dependency on the spray temperature, which can be divided into three regimes, i.e. low, intermediate and high temperature regimes, according to the characteristics of the coating produced from the nanopowder. Furthermore, with the proper control of the ratio of the electrical power to the primary Ar gas flow rate, the coating sprayed using nanopowder feed displays a much better wear resistance than the counterpart sprayed using commercial coarse-grained powder feed. The fundamental understandings established by his group in collaboration with Professors Maurice Gell and Eric Jordon have paved the way for the eventual award of a coating's qualification for onboard ship applications under a United States' military standard (MIL STD 1687A). The technology for plasma spray of nano-coatings has been transferred to the US Navy, and currently there are multiple US Navy ships with these coatings in the field. Some key publications in these areas are as follows.


- R.-M. Ren, Z.-G. Yang and L. Shaw, "Synthesis of Nanostructured Silicon Carbide through Integrated Mechanical and Thermal Activation Process," *J. Am. Ceram. Soc.*, 85 [4] 819-827 (2002).
- L. Shaw, Z.-G. Yang and R.-M. Ren, "Synthesis of Nanostructured $Si_3N_4$/SiC Composite Powders through High Energy Reaction Milling," *Mater. Sci. Eng.*, A244 [1] 113-126 (1998).
- Z.-G. Yang and L. Shaw, "Synthesis of Nanocrystalline SiC at Ambient Temperature through High Energy Reaction Milling," *Nanostruct. Mater.*, 7 [8] 873-886 (1996).

- L. Shaw, D. Goberman, R.-M. Ren, M. Gell, S. Jiang, Y. Wang, T. D. Xiao and P. Strutt, "The Dependency of Microstructure and Properties of Nanostructured Coatings on Plasma Spray Conditions," *Surface and Coatings Technology*, 130, 1-8 (2000).
- M. Gell, E. H. Jordon, Y. H. Sohn, D. Goberman, L. Shaw, and T. D. Xiao, "Development and Implementation of Plasma Sprayed Nanostructured Ceramic Coatings," *Surface and Coatings Technology*, 146-147, 48-54 (2001).
- D. Goberman, Y. H. Sohn, L. Shaw, E. Jordan and M. Gell, "Microstructure Development of Plasma Sprayed Alumina – 13wt.% Titania Coatings Derived from Nanocrystalline Powders," *Acta Mater*., 50 [5] 1141-1152 (2002).

Leon Shaw has also made contributions in the area of surface nanocrystallization and hardening to enhance material's tensile strength and fatigue resistance. His research activities in this area focus on processing-microstructure-property relationships and modeling of surface nanocrystallization process. The studies by his group show that the enhancement in the fatigue resistance is derived from a combination of a nanocrystalline surface layer, a work-hardened surface region, and residual compressive stresses at the surface. The investigation of the surface nanocrystallization mechanisms reveals that the grain refinement of face-centered-cubic (FCC) crystals with low stacking fault energy proceeds with ubiquitous deformation twinning, which is complemented by dislocation activity. These discoveries have led to many journal publications along with book chapters for *Encyclopedia of Tribology, Bulk Nanostructured Materials, CRC Materials Processing Handbook,* and *Nanostructured Metals and Alloys: Processing, Microstructure, Mechanical Properties and Applications*. Some key publications in these areas include:

- K. Dai, J. Villegas, Z. Stone and L. Shaw, "Finite Element Modeling of the Surface Roughness of 5052 Al Alloy Subjected to a Surface Severe Plastic Deformation Process," *Acta Mater*., 52 [20] 5771-5782 (2004).
- J. C. Villegas, L. Shaw, K. Dai, W. Yuan, J. W. Tian, P. Liaw, and D. L. Klarstrom, "Enhanced Fatigue Resistance of a Nickel-Based Hastelloy Induced by a Surface Nanocrystallization and Hardening Process," *Phil. Mag. Lett*., 85 [8] 427-438 (2005).
- J. C. Villegas and L. Shaw, "Nanocrystallization Process and Mechanism in a Nickel Alloy Subjected to Surface SPD," *Acta Mater*., 57, 5782-5795 (2009).
- L. Shaw, "Surface Nanocrystallization and Hardening," an Invited Chapter for *Encyclopedia of Tribology*, Q. Jane Wang & Yip Wah Chung (eds.), Springer Science, Inc., USA, 2012, DOI: 10.1007/978-0-387-92897-5.
- K. Lu and L. Shaw, "Bulk Materials with a Nanostructured Surface and Coarse-Grained Interior," an Invited Chapter for the book of *Bulk Nanostructured Materials*, M.J. Zehetbauer and Y.T. Zhu, Eds., Wiley-VCH Publishers, 2009, pp. 649-671.
- L. Shaw and Yuntian T. Zhu, "Multiscale Processes in Surface Deformation," an Invited Chapter for *CRC Materials Processing Handbook*, J. Groza, J. Shackelford, E. Lavernia and M. Powers, Eds., CRC Press, Boca Raton, FL, 2007, pp. 31-1 – 31-16.

Lately, Leon Shaw has focused on nanomaterials synthesis and processing for energy storage, particularly in the areas of hydrogen storage materials, Li-ion batteries, Na-ion batteries, and redox flow batteries. In the area of hydrogen storage materials, the focus is on synthesis and processing of nanostructured $LiNH_2$, $Li_2NH$, LiH, $LiBH_4$ and $MgH_2$ materials to achieve hydrogen release and uptake near room temperature with high gravimetric densities. Recent work on a new composite mixture of nano-$LiBH_4$ + nano-$MgH_2$ has resulted in reversible release and update of 5.0 wt.% $H_2$ at 265 $^oC$. This reversible storage capacity is the highest one ever reported for the $LiBH_4$ + $MgH_2$ system at temperature $\leq$ 265 $^oC$. In the area of rechargeable batteries, research has been focused on synthesis and processing of nanostructured Si anodes, novel coatings on $Li(Ni_xMn_yCo_z)O_2$ cathodes, Li-S batteries, structural defect control of $NaCrO_2$ cathodes, and hybrid Na-based flow

batteries. The most prominent advancement made in the area of rechargeable batteries is the design and synthesis of Si micro-reactor powder that exhibits unusual properties with ultrafast charging/discharging capability (10 to 15 min), high specific capacity (800 mAh/g), and long-lasting cycle life (1,000 cycles) simultaneously. Silicon micro-reactor powder is synthesized via a simple and industrially scalable method, which can pave the way for practical applications of Si micro-reactors in the future. The advancements made in the areas of rechargeable batteries and hydrogen storage materials have led to multiple keynote presentations, plenary lectures, and "Energy Award" in 2018 presented by International Association of Advanced Materials (IAAM) as well as news release by *DOE* Environmental Molecular Sciences Laboratory **(***EMSL), The Hydrogen Journal, Pacific Northwest National Laboratory (PNNL), the Battelle Newsletter,* and *Renewable Energy Global Innovations.* Some key publications in these areas are as follows.


- Z. Ding, Y. Lu, L. Li, and L. Shaw, "High Reversible Capacity Hydrogen Storage through Nano-$LiBH_4$ + Nano-$MgH_2$ System," *Energy Storage Mater.*, 20, 24-35 (2019).
- W. Osborn, T. Markmaitree, and L. Shaw, "Long-Term Hydriding and Dehydriding Stability of the Nanoscale $LiNH_2$ + LiH Hydrogen Storage System," *Nanotechnology*, 20, 204028 (2009).
- J. Z. Hu, J. H. Kwak, Z. Yang, X. Wan, and L. Shaw, "Direct Observation of Ion Exchange in Mechanically Activated LiH+$MgB_2$ System Using Ultra-High Field Nuclear Magnetic Resonance Spectroscopy," *Appl. Phys. Lett.*, 94, 141905 (2009).
- X. Wan, T. Markmaitree, W. Osborn, and L. Shaw, "Nanoengineering-Enabled Solid-State Hydrogen Uptake and Release in the $LiBH_4$ plus $MgH_2$ System," *J. Phys. Chem. C*, 112, 18232-18243 (2008).
- C. Chen, W. Yao, Q. He, M. Ashuri, J. Kaduk, Y. Liu, and L. Shaw, "Tunable $LiAlO_2$/$Al_2O_3$ Coating through a Wet-Chemical Method to Improve Cycle Stability of Nano-$LiCoO_2$," *ACS Appl. Energy Mater.*, 2, 3098-3113 (2019).
- M. Ashuri, Q. He, Y. Liu, S. Emani, and L. Shaw, "Synthesis and performance of nanostructured silicon/graphite composites with a thin carbon shell and engineered voids," *Electrochim. Acta*, 258, 274-283 (2017).
- M. Sawicki, A. Ortiz, M. Luo and L. Shaw, "Structural-defect-controlled electrochemical performance of sodium ion batteries with $NaCrO_2$ cathodes," *ChemElectroChem*, 4, 3222-3230 (2017).
- L. Chen, N. L. Dietz Rago, I. D. Bloom, and L. Shaw, "New Insight into the Electrode Mechanism of Lithium Sulfur Batteries via Air-Free Post-Test Analysis," *Chem. Commun.*, 52, 9913-9916 (2016).
- M. Ashuri, Q. He, Y. Liu, K. Zhang, S. Emani, M. S. Sawicki, J. S. Shamie and L. Shaw, "Hollow silicon nanospheres encapsulated with a thin carbon shell: an electrochemical study," *Electrochim. Acta*, 215, 126-141 (2016).
- J. S. Shamie, C. Liu, L. Shaw, and V. L. Sprenkle, "Room temperature, hybrid sodium-based flow batteries with multi-electron transfer redox reactions," *Scientific Reports*, 5, 11215 (2015).


Novel nanomaterial synthesis and processing are expected to continuously lead to advanced materials with new functionalities and superior properties. In particular, microstructure control and crystal defect manipulation made available by novel nanomaterial synthesis and processing have the potential to result in new materials with unprecedented properties for energy storage and structural applications in the future.

# Unusual Photophysical Phenomenon the Aggregation-Induced Emission (AIE) & the Exploration of High-Tech Applications of AIE Luminogens (AIEgens)

**by Ben Zhong Tang, Member EUAS**

Short Biography

*Tang received his BSc degree from South China University of Technology (China) in 1982 and his PhD degree from Kyoto University (Japan) in 1988. He performed postdoctoral work at the University of Toronto (Canada) before joining the Department of Chemistry at the HKUST as Assistant Professor in 1994 and became Chair Professor in 2008. He was elected to the Stephen Kam Chuen Cheong Professor of Science and the Fellow of the Royal Society of Chemistry in 2013 and the Chinese Academy of Sciences in Nov 2009. He has published more than 1,400 peer-reviewed research papers and delivered upward of 420 invited talks at international conferences. His papers have been cited over 79,000 times, with an h-index of 131. He was listed by Thomson Reuters and Clarivate Analytics as a Highly Cited Researcher in two categories, Chemistry and Materials Science, in 2014-2018.*

*Tang's scientific discoveries have often been highlighted by prestigious news media, such as C&EN (ACS), Chemistry World (RSC), Materials Views (Wiley-VCH), Chemical Technology (RSC), Asia Materials (Nature Publishing Group), Advanced Materials (Wiley-VCH), High-Tech Materials Alerts (Wiley), Polymer News (G&B), and Noteworthy Chemistry (ACS). His research papers have been illustrated as front cover images of Acc. Chem. Res. (ACS), Adv. Funct. Mater. (Wiley), Chem. Commun. (RSC), Macromolecules (ACS), Polymer (Elsevier), J. Polym. Sci. Part A (Wiley), J. Mater. Chem. (RSC), etc.*

*Tang is Editor-in-Chief of Materials Chemistry Frontiers (RSC) and RSC Polymer Chemistry Series (RSC), and Editor of Advances in Polymer Science (Springer) and Science China: Chemistry (Science China Press). He is sitting in the editorial board of a dozen of international scientific journals. He has received a number of awards over the years, notably the Distinguished Young Scholars Award in 2002 (National Science Foundation of China), the Croucher Senior Research Fellowship in 2007 (Croucher Foundation), the second-class State Natural Science Award in 2007 (Chinese Government), the Wang Baoren Award also in 2007 (Chinese Chemical Society), the Khwarizmi International Award in 2014 (IROST), the title of "Honorary Citizen of Guangzhou" in 2015, the HLHL Foundation's Prize for Scientific and Technological Progress in 2017, and the first-class State Natural Science Award also in 2017 (Chinese Government).*

Tang's most important contribution to science to date must be his pioneering work on the discovery of an unusual photophysical phenomenon known as aggregation-induced emission (AIE) and the exploration of high-tech applications of AIE luminogens (AIEgens).

Light is indispensable to all life forms and civilization. To acknowledge the significant role of light in scientific discoveries and technological innovations, the United Nations has proclaimed 2015 the International Year of Light and Light-Based Technologies. Light is emitted from luminophores. The development of new luminescent materials has allowed us to gain unprecedented knowledge, opening a new avenue to scientific achievement and societal development. Many luminescent materials such as quantum dots, hybrid nanoparticles and fluorescent proteins have been developed and applied in biological sensing and imaging applications. However, they exhibit several disadvantages such as toxicity to living cells, complicated operating procedures and interference with the conformations and dynamics of macromolecular biological targets. The properties of organic dyes, on the other hand, can be tuned through simple modulation of their structures. However, they tend to form aggregates in aqueous media or in living cells, which quenches their bright emissions. This phenomenon of aggregation-caused quenching (ACQ) has greatly limited the degree to which bioanalytes could be labeled with dye molecules and forced researchers to instead use dilute solutions with low sensitivity and photostability for sensing applications (left panel of Figure 1). Various approaches have been adopted to eliminate the luminophore aggregation but with only limited success because aggregate formation is an intrinsic process when luminogenic molecules are in close vicinity in the condensed phase.

**Figure 1**. Fluorescent photographs illustrating the photophysical phenomena of (left) aggregation-caused quenching (ACQ) and (right) aggregation-induced emission (AIE).

In 2001, Tang discovered a novel system, in which luminogen aggregation played a constructive, instead of destructive, role in the light-emitting process. For example, hexaphenylsilole is non-luminescent when dissolved in tetrahydrofuran (THF) but becomes highly emissive when aggregated in aqueous mixtures with high water contents (right panel in Figure 1). He coined the term of AIE for this uncommon phenomenon because the non-luminescent silole molecules were induced to emit by aggregate formation (*Chem. Commun.* **2001**, 1740). AIE is thus the exact opposite of the ACQ effect discussed above. Through systematic investigations, Tang proposed that restriction of intramolecular motions in the aggregate state was the main cause of the AIE effect (*Chem. Mater.* **2003**, *15*, 1535). Tang's mechanistic model has now been well accepted and widely used by other research groups in the world to explain their experimental observations.

Tang's discovery changed people's way of thinking of the light emitting process in the aggregate state and attracted much interest among scientists. Since Tang's pioneer work in 2001, hundreds of laboratories around the world are now performing AIE research, as evidenced by the exponentially increasing numbers of publications and citations on this theme over the year (Figure 2). The "fabrication, properties and cell imaging applications of aggregation-induced emission compounds" is ranked second in the fields of Chemistry and Materials Science in the list of Top 100 Research Fronts compiled by Thomson Reuters. Several international conferences on AIE have been held in recent years and

attracted scientists from different countries. A New Feature article published by Nature said that "The nanolight revolution is coming" and listed AIEgens as one of the unique luminescent materials that can revolutionize high technology applications (*Nature* **2016**, *531*, 26). Following the approval from the State Ministry of Science and Technology, Tang and his colleagues established the Hong Kong branch of the Chinese National Engineering Research Centre for transforming the academic results into commercial products (https://drive.google.com/open?id=1Gk4rnvBpHs-3o0dAKKVKXBFzDpEEQ95b).

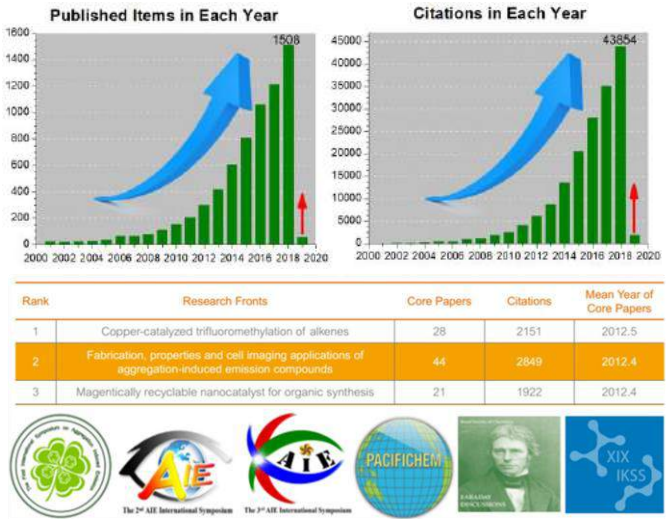


**Figure 2.** (Upper) Histograms showing annual numbers of papers and citations on AIE (data retrieved from Web of Science on January 20, 2019). (Middle) "Fabrication, properties and cell imaging applications of aggregation-induced emission compounds" is ranked 2nd in the areas of Chemistry and Materials Science in the list of Top 100 Research Fronts compiled by Thomson Reuters in 2015. (Lower) International conferences on AIE.

Tang has also devoted his effort to the exploration of high-tech applications of AIEgens, which has been summarized in his recent review articles (e.g.: *ACS Omega* **2018**, *3*, 3267–3277; *Biomaterials* **2017**, *146*, 115–135; *Chem. Rev.* **2015**, *115*, 11718–11940; *Adv. Mater.* **2014**, *26*, 5429–5479; *Chem. Soc. Rev.* **2014**, *43*, 4494; *Acc. Chem. Res.* **2013**, *46*, 2441; *Chem. Soc. Rev.* **2011**, *40*, 5361). In principle, the AIE effect can be utilized in all applications involving aggregation. For example, Tang has fabricated organic light-emitting diodes using AIEgens with aggregation-induced delayed fluorescence as emitting layers, which show excellent electroluminescence (EL) efficiencies of 59.1 cd $A^{-1}$, 65.7 lm $W^{-1}$ and 18.4%, and a negligible current efficiency roll-off of 1.2% at 1000 cd $m^{-2}$. Those with amplified chirality can even emit circularly polarized EL with high external quantum efficiency of up to 9.3% and EL dissymmetry factor of up to ±0.02. Various chemosensors based on AIE luminogens for the assays of pH, explosives, carbon dioxide, amines, ions, latent fingerprints, hazardous species, chirality, etc. have been developed by Tang. AIEgens have been successfully used as fluorescence "turn-on" or "light-up" biosensors, DNA visualizers, and probes for biological processes such as protein fibrillation. The AIE effect enables specific imaging of organelles, cells, microorganisms and tissues at molecular, cellular and tissue levels. The aggregates of AIEgens can stay inside cells and remain visible for a prolonged period of up to 21 passages, permitting monitoring of the growth of a specific type of cell line. Multifunctional systems constructed from AIEgens have been developed for biomedical diagnosis and therapy. Since some AIEgens can distinguish cancer cells from normal cells, AIE can provide an array of possibilities with great potential for fluorescence imaging-involved theranostic systems, ranging from reactive oxygen species promoted photodynamic therapy, to photoacoustic imaging associated with

photothermal therapy. The AIE dots enjoy the advantages of high emission efficiency, large Stokes shift, good biocompatibility and superb photostability. Their performances are superior to their counterparts of inorganic semiconductor quantum dots in long-term, non-invasive, in vitro cell tracing, opening a new avenue in the development of fluorescent probes for imaging cellular structures and monitoring biological processes. The best AIE dots can be 40 times brighter than quantum dots. Now, researchers are reporting other materials like clusters of gold atoms, not just small organic molecules, can undergo AIE as well. Tang has proven that many AIE luminogens are intelligent or smart materials, whose luminescence properties change in response to external stimuli or environmental variations, such as electric field, photonic irradiation, mechanical force, solvent polarity, temperature, vapor, and pH. This makes them promising for applications in areas like pressure sensors, information storages and security inks.

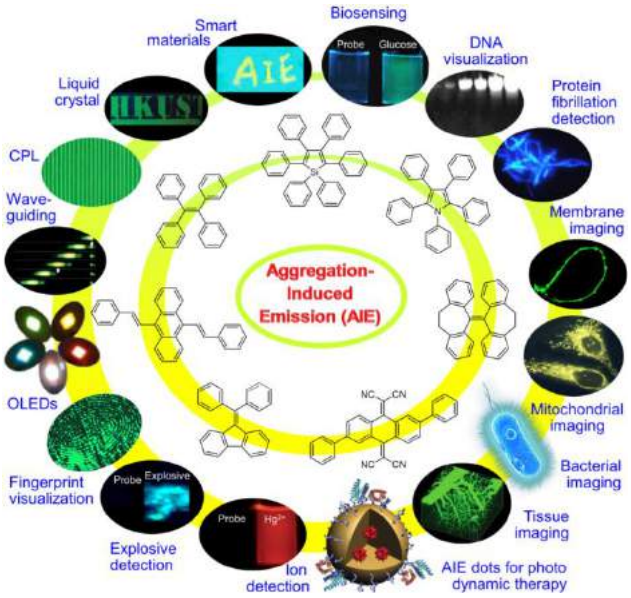


**Figure 3.** Examples of technological applications of AIEgens.

In conclusion, Tang's discovery on AIE is of great scientific value and has far-reaching technological implications. It overturns the general belief that the luminophore aggregation quenches light emission. Thanks to the enthusiastic efforts of Tang and other researchers in the world, AIE has now developed into an emerging area of research. The breakthrough is expanding the frontier of knowledge and may lead to the rewriting of photophysics textbook.

# Stochastic Optimal Control Problems with Fixed Terminal Time & First Exit Time

## by Kok Lay Teo, Member EUAS

Short Biography

***EDUCATION AND QUALIFICATIONS:***

- *PhD in Electrical Engineering, the University of Ottawa, Canada, 1974.*
- *MASc in Electrical Engineering, the University of Ottawa, Canada, 1971*
- *BSc in Telecommunications Engineering, Ngee Ann Technical College, 1968.*

***Employment History:***

- *John Curtin Distinguished Professor, Department of Mathematics and Statistics, Curtin University, Perth, Australia (From January 2011).*
- *Professor and Head, Department of Mathematics and Statistics, Curtin University of Technology, Perth, Australia (January 2005-December 2010).*
- *Chair Professor and Head, Department of Applied Mathematics, The Hong Kong Polytechnic University, Hong Kong (December 1998 – December 2004).*
- *Professor of Applied Mathematics, School of Mathematics and Statistics, Curtin University of Technology, Australia, December 1996 - November 1998.*
- *Associate Professor, Department of Mathematics, The University of Western Australia, Australia, November 1988 - November 1996.*
- *Associate Professor, Department of Industrial and Systems Engineering, National University of Singapore, Singapore, December 1984 - October 1987.*
- *Lecturer and Senior Lecturer, School of Mathematics, University of New South Wales, Australia, July 1974 - December 1984.*

***RESEARCH GRANTS***

***From Australian Research Council (won each year from 1994 to 1998):***

***Discovery Grants***

***1994-1998:*** *A$832,778 (won each year from 1994 to 1998**)***

***1998:*** *A$210,000 (equipment grant)*

***1999-2005:*** *I was with Hong Kong Polytechnic University*

***2006-2008****: A$300,000;* ***2008-2010****: A$240,000;* ***2011-2014:*** *A$315,000;* ***2014-2017:*** *$285,000;* ***2019-2021****: $450,000*

***Linkage Grants***

***2013-2016:*** *A$500,000;* ***2014-2017:*** *A$428,000.*

***From Research Grants Council of Hong Kong Competitive Earmarked Grants:***

***2000-2003****: HK$635,817;* ***2001-2004****: HK$782,762;* ***2002-2005:*** *HK$890404;* ***2003-2006****: HK$565723.*

***2001-2004****: HK$2,000000 from the Centre for Multimedia Signal Processing of the Department of Electronic and Information Engineering.*

***PLENARY/KEYNOTE LECTURES:*** *Presented over 30 keynote/plenary lectures*

***AWARDS and HONOURS INCLUDE:***

- *John Curtin Distinguished Professor, Department of Mathematics and Statistics, Curtin University, Perth, Australia (From January 2011) – John Curtin Distinguished Professor is the highest rank professor at Curtin University.*
- *Distinguished Vising Chair Professor, School of Management Science and Engineering, Tianjin University of Finance and Economics, Tianjin 300222, P.R. China, 2019-2021.*
- *Fellow of the Australian Mathematical Society*
- *My paper, entitled "The control parameterization method for nonlinear optimal control: A survey", by Lin, Loxton and Teo, Journal of Industrial and Management Optimization, 2014, was a winning paper in the prestigious Emerald Citations of Excellence for 2017.*

- *Winner of the 2013 John de Laeter Research Leadership Award, Curtin University. This is the highest award given by Curtin University.*
- *Listed in the Essential Science Indicators (ESI) in the field of Engineering.*
- *Two international conferences and 3 special journal issues were dedicated to professor Teo.*

***EDITORIAL POSITIONS:***

***Editor-in-Chief:*** *(i) Industrial and Management Optimization (from 2005); (ii) Numerical Algebra, Control and Optimization (from 2011); (iii) Cogent Mathematics (from 2014).*

***Member of editorial Board:*** *(i) Automatica; (ii) Journal Optimization Theory and Applications; (iii) Journal of Global Optimization; (iv) Discrete and Continuous Dynamic Systems, Series A; (v) Applied Mathematical Modelling; (vi) Optimization and Engineering; (vii) Pacific Journal of Optimization; (viii) Optimization Letters.*

***POSTDOCTORIAL FELLOWS AND POST-GRADUATE STUDENTS:*** *45 post-doctoral fellows/visiting research fellows. 40 PhD students.*

***PUBLICATION****: Over 500 papers published in reputable scholarly journals.*

## Highlight of Some Research Contributions

- Stochastic Optimal Control Problems with Fixed Terminal Time and First Exit Time: Necessary conditions for optimality; and existence of optimal controls
- Optimal Control of Various Distributed Parameter Systems - particularly systems governed by parabolic partial differential equations with various boundary and initial value conditions: Necessary conditions for optimality; and existence of optimal controls
- Optimal control of systems governed by ordinary differential equations with or without time delay: Necessary conditions for optimality; and existence of optimal controls; and numerical computational methods for solving optimal control problems subject to terminal equality or terminal inequality constraints as well as continuous inequality constraints.
  - For numerical computation methods, control parameterization technique was proposed, where the control function is approximated by piecewise constant function or piecewise linear function with the heights of these approximate functions treated as decision variables. For the continuous inequality constraints, the constraint transcription method is introduced to approximate it by a series of inequality constraints in integral form (called canonical inequality constraint). Gradient formulas of the cost functional, terminal equality or inequality as well as canonical inequality constraints are derived in a unified manner. The optimization techniques can then be used to solve these approximate optimal control problems. These methods are supported by the analysis of convergence property.
  - The switching points of the piecewise functions can be optimized to improve efficiency. The time scaling transformation technique is introduced. Then, each of the optimal parameter selection problems with switching times also taken as decision variables is transformed equivalently to standard optimal parameter selection problem involving an additional piecewise constant function with its heights as decision variables.
  - This time scaling transform has become a powerful tool to deal with optimal control problems governed by switched systems. It has been extended to hybrid time scaling transform to deal with optimal control problems with time delay.

- Exact penalty function method is developed to solve optimal control problems subject to continuous inequality constraints for which the penalty parameter is not required to tend to infinity.
  - The constraint transcription method and exact penalty function function methods have been applied to solve many semi-infinite optimization problems arise in signal processing.
- New risk measure under min-max rule; and chance constraints. Distributionally robust optimization theory is introduced when the probability distribution is uncertain.

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IEEE Transactions on Signal Processing, Vol. 66, Issue 22, pp. 6016 – 6030, 2018.

# Acid Catalysis & Asymmetric Catalysis for C-C Bond Formation by Chiral Lewis and Brønsted Acids

## by Hisashi Yamamoto, Member EUAS

Short Biography

***Education***

| | |
|---|---|
| *B. S.* | *Kyoto University, 1967 (Prof. H. Nozaki, Thesis Director)* |
| *Ph. D.* | *Harvard University, 1971 (Prof. E. J. Corey, Thesis Director)* |

***Professional:***

| | |
|---|---|
| *1971-1972* | *Researcher, Toray Industries, Inc. (Prof. J. Tsuji, Adviser)* |
| *1972-1976* | *Instructor, Kyoto University (Prof. H. Nozaki, Adviser)* |
| *1976-1977* | *Lecturer, Kyoto University* |
| *1977-1980* | *Associate Professor, University of Hawaii* |
| *1980-1983* | *Associate Professor, Nagoya University* |
| *1983-2002* | *Professor, Nagoya University* |
| *2003-* | *Professor Emeritus, Nagoya University* |
| *2002-2012* | *Professor, The University of Chicago* |
| *2012-* | *Professor Emeritus, The University of Chicago* |
| *2012-* | *Professor and Director of Molecular Catalyst Research Center, Chubu University* |
| *2012-* | *Research Supervisor, JST Crest Project of Molecular Technology* |
| *2014-* | *Research Supervisor, JST-ANR Joint Project of Molecular Technology* |
| *2016-2018* | *President of Chemical Society of Japan* |

*Hisashi Yamamoto is an internationally recognized scholar whose contributions to organic chemistry span a wide range: from articulating and demonstrating new concepts of designer acid catalysis, to elucidating the stereochemical foundations of organic reactions, and to the creative invention of powerful new synthetic methods and their applications including for his new catalytic peptide synthesis. His distinctive contributions to all of these endeavors are characterized by originality and creativity. The breadth of his research accomplishments reflects an intellectual virtuosity in the application of chemical principles to important synthetic and mechanistic problems. His most important contributions are summarized below, highlighting both the scope and depth of his accomplishments over the past 45 years. Most noteworthy of these numerous achievements are the novel aspects of Lewis and Brønsted acid catalysts he has brought to light in selective organic synthesis since the 1970s. During his career, he has discovered a wide variety of powerful new synthetic reactions, reagents, and catalysts based on acid catalysis. Through his dedicated efforts, Lewis and Brønsted acids are now recognized as major tools in the synthesis of both simple and complex organic molecules. Among Yamamoto's many superb contributions, the following are especially worthy of mention.*

*Yamamoto has published over 550 papers and over 145 reviews, which have been cited more than 30,000 times (50,000 including books), with an h-index of 96 (113 by Google).*

*His contributions have been recognized by his being a recipient of, among others, the Prelog Medal (1993), the Chemical Society of Japan Award (1995), Le Grand Prix de la Fondation Maison de la Chimie (2002), the National Prize of Purple Medal (Japan) (2002), the Tetrahedron Prize for Creativity in Organic Chemistry (2006), the Japan Academy Award (2007), the Grand Prize of the Synthetic Organic Chemistry of Japan (2009), the ACS Award for Creative Work in Synthetic Organic Chemistry (2009), Fellow of Amer. Academy Arts and Science (2011), the Noyori Prize (2011), the Fujiwara Prize (2012), and the Roger Adams Award (2017) which is the highest award for organic chemistry in the US, Orders of the Sacred Treasure, 2018, The Person of Cultural Merit, 2018, Barluenga Lectur. medal, 2018, Member of EU Academy of Sciences, 2019.*

**Designer Acid Catalysis**

Yamamoto was intrigued by the chemistry of carbonyl group-Lewis acid complexes and introduced the unusually bulky organoaluminum reagents methylaluminum bis(2,6-di-tert-butyl-4-methylphenoxide) (MAD) and aluminum tris(2,6-diphenylphenoxide) (ATPH). These reagents were successfully utilized for the selective alkylation of cyclic ketones and aldehydes to generate equatorial alcohol and an *anti*-Cram-type product, respectively, for *trans*- and *cis*-selective Claisen rearrangement, for regioselective and exo-selective Diels-Alder reaction, and for epoxide-aldehyde rearrangement. The ATPH-aromatic carbonyl complex selectively reacts with nucleophiles at the *para*-position of the aromatic ring to generate cyclohexadiene derivatives. Besides these unexpected contributions to Lewis acid chemistry, his research in the area of organoaluminum chemistry has had a great impact on synthetic organic chemistry. The strong Lewis acidity of organoaluminum compounds appears to account for their strong tendency to form a stable 1:1 complex. Thus, the coordination of designer Lewis acid to molecules invariably causes a change in reactivity and, though coordinated by Lewis acid, the group may be activated or deactivated depending upon the type of reaction. Furthermore, with the coordination of organic molecules, an auxiliary bond can become coupled to the reagent and promote the designed reaction. In short, the reagents make a combined Lewis acid-Lewis base attack on a substrate with less activation energy, a field opened by Yamamoto's highly original early studies, which began in 1973. His aluminum amide reagents for epoxide rearrangement, biogenetic-type terpene synthesis, and the Beckmann rearrangement-alkylation reaction sequence are notable examples. Various Lewis acid-coordinated heterocyclic compounds are reported recently to activate specific positions of a molecule for CH activation, which originated in Yamamoto's Lewis acid chemistry. Based on these careful investigations of selective Lewis acid/Lewis base complexation, he proposed several basic principles for acetal chemistry, which are now used in selective ring opening and alkylation processes for various asymmetric syntheses. More recently, his ATPH catalyst is now used for the 1000-ton scale synthesis of perfumes in Japan.

Finally, using this crucial understanding of Lewis and Brønsted acid catalysis, he achieved super silyl (tris(trimethylsilyl)silyl) chemistry, which can realize double or triple aldol reactions in a single pot to generate a number of stereogenic centers in the molecule. Otherwise unattainably high diastereoselectivity in this cascade reaction makes this process a so-called "second generation of Mukaiyama aldol reaction", which can produce up to an eleven-hydroxyl polyketide structure only in three steps in a stereospecific manner. These findings open the new chapter for a polyketide synthesis in modern organic chemistry.

**Asymmetric Catalysis for C-C Bond Formation by Chiral Lewis and Brønsted Acids**

In what is likely to become his most significant chemical legacy, Yamamoto has formulated a new paradigm for the chiral catalysis of reactions of main group elements by demonstrating chiral Lewis and Brønsted acid-catalyzed asymmetric processes. In the early 1980s, he first introduced chiral binaphthol as a key ligand for chiral Lewis acid catalysts. This work was the forerunner of a vast quantity of present-day research on $C_2$ symmetry-based chiral Lewis acid catalysts, now known as privileged ligands. Based on his knowledge of organoaluminum chemistry, he designed an organoaluminum chiral catalyst using 3,3'-disubstituted binaphthol for the first asymmetric hetero-Diels-Alder reaction in 1988. It was his Brønsted acid/Lewis acid combined system that offered him a unique opportunity, as this produced the most efficient asymmetric carbon-carbon formations based on a Lewis acid catalyst. Thus, his discovery of tartaric acid-based catalysts (CAB catalyst) and amino acid-based catalysts (oxaborolidine-type catalyst) led to the first and the most general enantioselective Diels-Alder reaction of a broad range of dienes and dienophiles. The same catalyst was shown to be the first efficient one for asymmetric aldol, ene, and allylation reactions. His recently uncovered silver-catalyzed aldol and allylation process has provided a new entry into the creation of quaternary carbon stereogenic centers for asymmetric synthesis. A similar concept was employed for his

catalytic asymmetric protonation, which is capable of creating a long-sought enantio-face-selective protonation that induces asymmetric and biomimetic polyene cyclization. The use of 8-hydroxyquinole-based chiral Lewis acid catalysis was a recent contribution of his to acid catalysis. The catalyst is designed as a rigid metal complex of *cis*-β configuration, which provides the metal center with $C_1$ chirality. The ligand turned out to be a brand new "privileged ligand" for asymmetric synthesis; catalytic asymmetric pinacol coupling, NH reaction, Mukaiyama-Michael addition, Pudovik reaction, Strecker reaction, hydrocyanation, Nagata-Michael addition, and nitroso Diels-Alder reaction are now able to proceed with complete enantioselectivity (>99%ee). In fact, most of the asymmetric carbon-carbon bond-formation processes recognized today are based on Yamamoto's early discoveries.

Recently, he designed several chiral Brønsted acid catalysts with high reactivity for various asymmetric transformations. The original Akiyama-Terada catalyst is effective for nitrogen containing molecules. However, his phosphoramide catalyst could activate oxygen containing molecule and greatly expand the utility of the catalyst with >99%ee. This field of chemistry is now rapidly growing are as organocatalysis and Yamamoto is the pioneer of this important area of chiral super Brønsted acid catalysis.

**From "Reagent Controlled Reaction" to "Substrate Controlled Reaction"**

Yamamoto has also contributed significantly in the area of catalytic asymmetric oxidation reactions. One example is the nitroso-aldol reaction originating from his invention of O-nitroso aldol reaction over 10 years ago. Asymmetric epoxidation of homo- and bis-homoallylic alcohols was achieved first in his laboratory. His tungsten chemistry was a real groundbreaking discovery for oxidation using this non-toxic metal catalyst. Sequential epoxidation/ring opening will be used as a new strategy to generate >99.9%ee amino alcohol synthesis. The following is a list of catalytic asymmetric processes developed by Yamamoto: O-nitroso aldol and N-nitroso aldol synthesis; nitroso-Diels-Alder reaction; epoxidations of homo- and bis-homoallylic alcohol; N-oxidation and S-oxidation of hydroxyl amine and hydroxyl sulfide. Most of these reactions are classified as substrate-controlled (functional group directable) chemical reactions: Nonbonding interactions contributed by substrate substituents provide the dominant stereochemical control element for chemical transformations.

Yamamoto published a very important paper in 2015 as a modern substrate controlled chemical reaction, reporting a catalyst system employing two independent metals in the catalyst. The two metals are independent to each other: one metal holds the substrate and the other metal is responsible for the desired reaction at the appropriate. This enzyme-like catalyst using two independent metal centers is responsible for effective asymmetric epoxidation, sulfoxidation, and amine-oxide formation. Direct condensation of carboxylic acids with alcohols or amines is the most important transformation of organic synthesis. His zirconium- or hafnium-catalyzed esterification and boron-catalyzed amidation were groundbreaking studies. More recently, Yamamoto discovered Lewis acid catalyzed amide synthesis based on his concept of "substrate controlled chemical reaction". With this knowledge in hand, he finally succeeded to open a new door for "catalytic peptide synthesis" using his Ta/Nb Lewis acid catalyst as a substrate controlled chemical reaction as a key concept, solving a century-old unsolved and most difficult problem in organic synthesis. His new method is not only providing a truly catalytic peptide synthesis but also solving the problem of racemization of peptides, which was the nightmare for classical peptide synthesis many years.

# Double Wall & Jet Array Cooling - Turbine Blade Heat Transfer & Flow Dynamics

## by Phil Ligrani, Member EUAS

Short Biography

*Eminent Scholar in Propulsion, Professor of Mechanical and Aerospace Engineering, Department of Mechanical and Aerospace Engineering, Propulsion Research Center, 5000 Technology Drive, University of Alabama at Huntsville*

***PROFESSIONAL PREPARATION***

| | | |
|---|---|---|
| *University of Texas at Austin* | *Mechanical Engineering* | *Bachelor of Science, 1974* |
| *Stanford University* | *Mechanical Engineering* | *Master of Science, 1975* |
| *Stanford University* | *Mechanical Engineering* | *Doctor of Philosophy, 1980* |

***APPOINTMENTS***

| | |
|---|---|
| *2014 – present* | *Eminent Scholar in Propulsion, Professor of Mechanical and Aerospace Engineering, Department of Mechanical and Aerospace Engineering, University of Alabama* |
| *2010 – 2014* | *Professor of Aerospace & Mechanical Eng, Saint Louis University* |
| *2010 – 2013* | *Director of Graduate Programs, Parks College, Saint Louis University* |
| *2006 – 2009* | *Statutory Professor, Department of Engineering Science, University of Oxford* |
| *2006 – 2009* | *Director, Rolls-Royce UTC (University Technology Centre)* |
| *1997 – 2006* | *Professor, Department of Mechanical Engineering, University of Utah* |
| *2002 – 2006* | *Adjunct Professor, Department of Bioengineering, University of Utah* |
| *1992 – 1997* | *Associate Professor, Department of Mechanical Engineering, University of Utah* |

***ARCHIVAL JOURNAL PUBLICATIONS AND RELATED ITEMS.***

*As of December 2019, Dr. Ligrani is author or co-author of more than 190 publications in archival journals, including the International Journal of Heat and Mass Transfer, the ASME Transactions-Journal of Turbomachinery, the ASME Transactions-Journal of Engineering for Gas Turbines and Power, the ASME Transactions-Journal of Heat Transfer, the ASME Transactions-Journal of Fluids Engineering, the Journal of Fluid Mechanics, the AIAA Journal, Experiments in Fluids, Physics of Fluids, the AIAA Journal of Heat Transfer and Thermophysics, the International Journal of Rotating Machinery, Separation Science and Technology, Sensors and Actuators A: Physical, and the Journal of Microcolumn Separations. He is also author of 9 book chapters, and about 144 conference presentations and publications. A number of these are invited conference presentations at international meetings, at locations which include Korea, France, the Ukraine, Croatia, Germany, England-United Kingdom, and Belgium. From 1994 to 2019, he has also presented approximately 182 lectures at different institutions and establishments, including many invited lectures. From 2010 to 2020, he presented or is scheduled to present 7 Invited Keynote Papers, 7 Invited Papers, and 8 Invited Plenary Keynote Papers at different international conferences. Current SCOPUS Reference Citation H-INDEX is 42. Current GOOGLE SCHOLAR Reference Citation H-INDEX is 45.*

***EDITOR ACTIVITIES.***

*From 1998 to 2000, Dr. Ligrani served as Guest Editor for a Special Topical Issue for Measurement Science and Technology. He has also served as Associate Editor for the ASME Transactions-Journal of Heat Transfer from 2003 to 2006, and from 2010 to 2014, and as Associate Editor for the ASME Transactions-Journal of Fluids Engineering from 2005 to 2008. Present editor duties include: (i) Member of the Distinguished Editorial Review Board for the Advances in Transport Phenomena, Book Series with Springer Publishing Corporation (since 2006), (ii) Editorial Board Member, Power and Thermal Engineering Processes and Equipment Journal, Published by the National Technical University "Kharkov Polytechnic Institute", Russia and Ukraine (since 2015), (iii) Editorial Board Member, International Journal of Innovative Works in Engineering and Technology (IJIWET) (since 2015), (iv) Associate Editor, Journal of Propulsion Technology (JPT) Journal, Published by CNPIEC, P. R. China (since 2015), (v) International Editorial Board Member, Industrial Thermal Engineering Journal, Published by Thermogasdynamics Department, National Academy of Sciences of Ukraine, Kiev, Ukraine (since 2018), (vi) Editorial Board Member, Advances in Aerodynamics (AIA) Journal. Published by the Chinese Society of Aerodynamics (CSA), and the China Aerodynamics Research and Development Center (CARDC), P. R. China (since 2018), (vii) Associate Editor, Energies Journal (since 2018), (viii) Associate Editor, ASME Transactions-Journal of Journal of Engineering for Gas Turbines and Power (2018-2021).*

***SELECTED RECENT HONORS, AWARDS, ACADEMIC RECOGNITIONS***

*● ASME IGTI Outstanding Service Award 2019. ● 2019 University Distinguished Research Award for Excellence. University of Alabama in Huntsville, Huntsville, Alabama, USA. ● Outstanding Senior Faculty Member Award for 2019. College of Engineering, University of Alabama in Huntsville, Huntsville, Alabama, USA. ● Guest Professor. School of Mechanical Engineering, Shanghai Jiao Tong University, Shanghai, P. R. China. 2019 to Present. ● Outstanding Mechanical Engineer of the Year Award 2016, ASME – American Society of Mechanical Engineers, NAS - North Alabama Section, USA. ● Distinguished Advisory Professor, Inje University, South Korea, 2010 to 2020. ● Distinguished Lecture Award, 2011, CEAS Distinguished Lecture Series, College of Engineering, University of Wisconsin, Milwaukee, Wisconsin, USA. ● Distinguished Editorial Review Board membership for Springer Publishing Corporation. ● Carl E. and Jessie W. Menneken Faculty Award for Excellence in Scientific Research. ● NASA Space Act Tech Brief Award for "Development of Subminiature Multi-Sensor Hot-Wire Probes." ● Silver Winner for the Annual 26th Educational Advertising Awards for the Higher Education Marketing Report.*

Dr. Ligrani has a strong past and present record of working with many different collaborators and co-workers, from many locations throughout the world. Additional information on selected, currently active research projects is provided within sections which follow. **(i) Traditional Heat Transfer and Fluid Mechanics Investigations** involving electronics cooling, heat transfer augmentation, drag reduction, turbulent boundary layers, flows in channels with dimpled surfaces, flows in curved channels, elastic turbulence, slot impingement cooling, and macro-scale pumps and pump flows. Also included are **aerodynamics investigations with *high-speed, compressible flows at transonic and supersonic Mach numbers***, including SWBLI – Shock Wave Boundary Layer Interactions. Related projects involve **transonic and supersonic experimental testing**. Research interests also include experimental diagnostics in high speed flows, and air breathing propulsion. **(ii) Air Breathing Engines - Gas Turbine Heat Transfer, Cooling, and Aerodynamics Losses**, including internal cooling, film cooling, impingement cooling, cooling of extremities, aerodynamic performance including aerodynamic losses, and transonic turbine flows and heat transfer. This subject area includes the effects of uses of bio-fuels, synthetic fuels, and renewable energy sources in relation to gas turbines and gas turbine heat transfer and cooling technologies. Note that an important area of turbomachinery research interest involves heat transfer and aerodynamics investigations with *high-speed, compressible flows at transonic and supersonic Mach numbers*, including linear cascade studies. **(iii) Micro-Fluidics and Millimeter-Scale-Fluidics**, including micro-pump flows, and the effects of slip phenomena on gas and liquid flows in micro-scale passage flows with and without surface roughness, including the effects of hydrophobic surfaces and elastic turbulence. **(iv) Experimental Techniques**, including development of millimeter-scale multiple-hole pressure probes, subminiature hot-wire anemometry, and infrared thermography

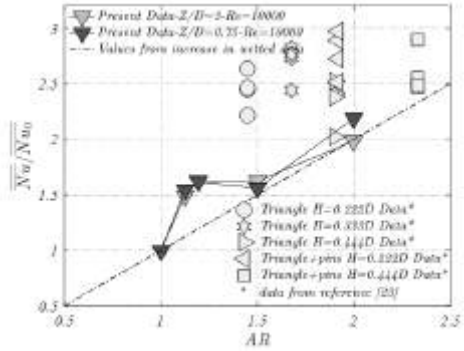
**DOUBLE WALL COOLING RESEARCH INVESTIGATIONS**

Provided are new effusion cooling data for both surfaces of full coverage effusion cooling plate. For the effusion cooled surface, measured are spatially-resolved distributions of surface adiabatic film cooling effectiveness, and surface heat transfer coefficients (measured using transient techniques and infrared thermography). For the impingement cooled surface, measured are spatially-resolved distributions of surface Nusselt numbers (measured using steady-state liquid crystal thermography). To produce this cool side augmentation, impingement jet arrays at different jet Reynolds numbers, and cross flow cooling at different cross flow Reynolds numbers, are employed. Experimental data are given for a sparse effusion hole array, with spanwise and streamwise impingement hole spacing such that coolant jet hole centerlines are located midway between individual effusion hole entrances. Considered are comparisons of hot-side effusion plate

results for a mainstream flow passage with contraction ratio CR of 1 and for a mainstream flow passage with contraction ratio CR of 4. These results are given for main flow Reynolds numbers $Re_{ms}$ of 89,900 to 95,800. For this main flow Reynolds number range, four different combination values of crossflow Reynolds number and impingement Reynolds number are tested for each CR value, which are associated with four different values of initial blowing ratio BR. The resulting variations of surface adiabatic film cooling effectiveness and surface heat transfer coefficients are due to three competing phenomena, whose relative influences change with streamwise location. These include increased turbulent mixing and transport result from effusion coolant jets, decreased magnitudes of local blowing ratio with streamwise location, and significant streamwise acceleration, which induces local boundary layer re-laminarization.

**IMPINGEMENT JET ARRAY COOLING RESEARCH USING TARGET SURFACES WITH SPECIAL TEXTURES AND SURFACE ROUGHNESS DISTRIBUTIONS.**

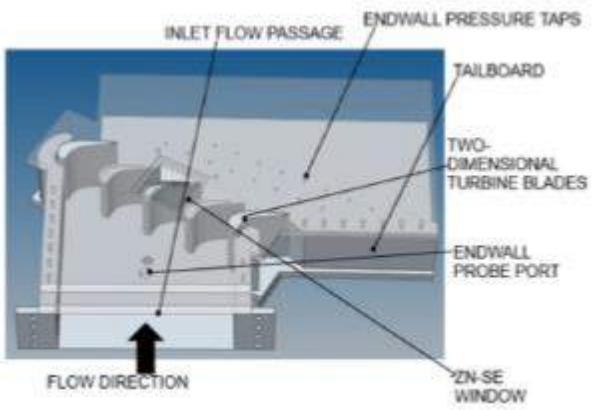
Experimental results are obtained along target surfaces with a variety of different surface roughness and surface micro pin-fins arrangements. The use of arrays of micro pin fins for installation in different application environments is made possible by recent developments in additive manufacturing. Considered are effects of impingement jet Reynolds number, jet-to-target plate distance, micro pin-fin shape, and micro rectangle pin-fin height. Area-averaged Nusselt number variations for the different data sets are a result of the effects of increased wetted surface area, turbulent transport and turbulent mixing, thermal conduction resistance from pin-fin material, and local flow separations and recirculation regions. When compared at a particular streamwise location, impingement jet Reynolds number, and jet-to-target plate distance, area-averaged Nusselt number ratios generally increase with height for the rectangle micro pin-fins. The attached figure shows area-averaged Nusselt number ratio variation with wetted area ratio for impingement jet Reynolds numbers of 10000 to 11100.




**TURBINE BLADE HEAT TRANSFER RESEARCH WITH INNOVATIVE FILM COOLING CONFIGURATIONS.**

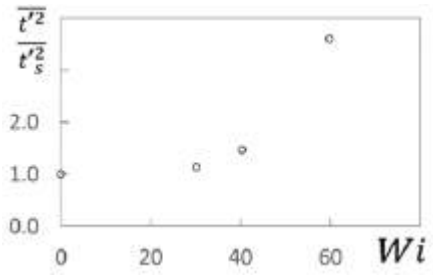
Currently, there is a deficit of experimental data for surface heat transfer characteristics and thermal transport processes associated with tip gap flows, and a lack of understanding of performance and behavior of film cooling as applied to blade tip surfaces. Of interest is development of a two-dimensional linear cascade with appropriate cascade airfoil flow periodicity. Included are boundary layer flow bleed devices, downstream tailboards, and augmented cascade inlet turbulence intensity. The present linear cascade approach allows experimental configuration parameters to be readily varied. Tip gap magnitudes are scaled so that ratios of tip gap to inlet boundary layer thickness, ratios of tip gap to blade axial chord length, and ratios of tip gap magnitudes to blade true chord length match engine hardware configurations. Ratios of inlet boundary layer thickness to tip gap range from 3 to 5. Innovative film cooling configurations are utilized for one blade tip configuration, and scaled engine components are modelled and tested with complete external cooling arrangements. Results are obtained with engine representative transonic

Mach numbers, Reynolds numbers, and film cooling parameters, including density ratios, which are achieved using foreign gas injection with carbon dioxide. Presented within the attached figure is a three-dimensional view of the turbine blade cascade which is employed for the investigation.



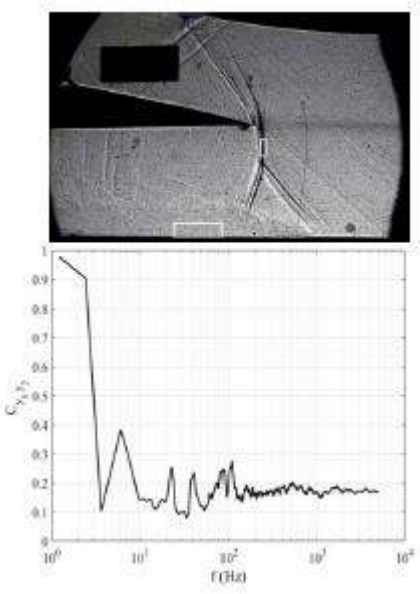

**THERMAL TRANSPORT AND CONVECTIVE HEAT TRANSFER ENHANCEMENTS FROM ELASTIC INSTABILITIES.**

The influences of elastic instabilities on convective heat transfer, within a rotating Couette flow arrangement are experimentally determined. Different concentrations of polyacrylamide in 65 percent sucrose solutions are used, along with solutions with 65 percent sucrose only, as different magnitudes of shear stress and strain rate are imposed upon the flow field. Transition and development of elastic instabilities are characterized, along with convective heat transfer enhancements. The resulting increased levels of mixing, transport, and effective diffusion from elastic instabilities give Nusselt numbers which are as high as 3.0, within a spsecific rotating Couette flow location, for the highest polymer concentration and highest shear shear rate considered, whereas zero shear rate values (obtained with zero rotation) are in the vicinity of 1.0. Nusselt number enhancement ratios are then as high as 2.4, relative to conditions associated with pure sucrose solution flows (with no polymers present), when compared at the same shear rate. Variations of spectra of static temperature fluctuations, and mean-square magnitudes of fluctuating static temperature provide evidence of increased flow irregularities and unsteadiness (relative to pure sucrose solution flows), which are believed to result from instability induced polymer twisting, unsteadiness, and convolutions. Shown within the attached figure are variations of normalized and time-averaged magnitudes of the mean-square of flow static temperature fluctuations (measured within the rotating Couette flow environment) for a 4.19 rad/s disk rotational speed and a shear rate of 21.28 1/s. Here, ratios are provided relative to pure sucrose solution values. These data are consistent with Nusselt number variations with shear rate and disk rotational speed for different polymer concentrations, since both types of data increase substantially as Weissenberg number becomes greater than 30.



**INVESTIGATIONS OF SHOCK WAVE UNSTEADINESS.**

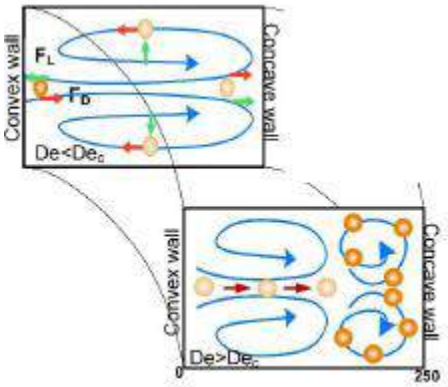
Despite over fifty years of research on shock-wave-boundary-layer-interaction unsteadiness, the source, origin, and propagation direction of the unsteadiness remains controversial and a debated topic. The present research effort considers normal shock wave unsteadiness characteristics, using a newly-developed, supersonic wind tunnel, which is located at the University of Alabama in Huntsville, USA. The wind tunnel test section includes a two flow passage arrangement, where each passage is separated by a shock wave holding plate. The top wall for the top passage is contoured relative to the streamwise flow direction, and a choking flap is located at the downstream portion of the bottom flow passage. With this arrangement, the Mach number at the test section inlet is 1.54, and total air mass flow rate is approximately 12.5 kg/s. Of particular interest are spatially- and temporally-varying shock wave characteristics, which are quantified using shadowgraph flow visualization images, magnitude squared coherence variations with frequency, and time lag magnitude variations with frequency, where these last two quantities are determined for different flow locations relative to shock wave locations. The attached figure shows a shadowgraph flow visualization image, which illustrates the presence of a normal shock wave, lambda foot, and separated turbulent boundary layer within the lower flow passage, and an oblique shock wave system within the upper flow passage. Note that flow direction is from right to left. White boxes within this figure indicate the regions used to correlate the shock wave and the downstream boundary layer. The magnitude squared coherence, shown in the attached figure, depicts pronounced coherence at Strouhal numbers of 0.00263, 0.00526, and 0.01315, where the associated length scale is the magnitude of inlet boundary layer thickness. Associated time lags variations with frequency indicate that the perturbations that occur at Strouhal numbers of 0.00263 and 0.01315 occur in the downstream boundary layer prior to occurring in the shock wave. The perturbation at a Strouhal number of 0.00526 occur in the shock wave first.



**DEAN FLOW DYNAMICS AND CELL SORTING WITHIN CURVILINEAR SPIRAL MICROCHANNELS.**

A wide range of microfluidic cell-sorting devices has emerged in recent years, based on both passive and active methods of separation. Curvilinear channel geometries are often used in these systems, due to presence of secondary flows, which can provide high throughput and sorting efficiency. Most of these devices have been designed on the assumption that there are counter-rotating Dean vortices, present in the curved rectangular channels, which exist in the state of steady rotation and amplitude. The presence of multiple vortices for Dean numbers greater than a critical

value thus has important effects upon the focusing of particles and cells in spiral microchannels. The overall effect of the vortices is to shift radial positions of the particles from the convex wall towards the concave wall of the channel, as shown within the adjacent figure, which illustrates the behavior of red blood cells. Overall, such results illustrate the importance of secondary flows, Dean instabilities, and the magnitude of Dean number in regard to fluid mixing, particle separation, and cell focusing for sorting techniques where microchannels are employed.



# New Investigations in Flat Panel Technolgies

## by Vladimir Chigrinov, Member EUAS

Short Biography

*Professor Vladimir G. Chigrinov is Professor of Hong Kong University of Science and Technology since 1999. He is an Expert in Flat Panel Technology in Russia, recognized by the World Technology Evaluation Centre, 1994, and SID Fellow since 2008. He is an author of 6 books, 25 reviews and book chapters, about 300 journal papers, more than 656 Conference presentations, and 112 patents and patent applications including 32 US patents in the field of liquid crystals since 1974. He got Excellent Research Award of HKUST School of Engineering in 2012. He obtained Gold Medal and The Best Award in the Invention & Innovation Awards 2014 held at the Malaysia Technology Expo (MTE) 2014, which was hosted in Kuala Lumpur, Malaysia, on 20-22 Feb 2014. He is a Member of EU Academy of Sciences (EUAS) since July 2017. He got A Slottow Owaki Prize of SID in 2018 http://www.ee.ust.hk/ece.php/enews/detail/660. He is 2019 Distinguished Fellow of IETI (International Engineering and Technology Institute). http://www.ieti.net/news/detail.aspx?id=184 http://www.ieti.net/memberships/Fellows.aspx*

*The last five years research on azodye photoalignment and its application.*
*We have made the following research in the last years since 2016.*

1. *Application of photoalignment in photonics devices: switches, lenses, optical vortex, q-plates, fibers, nanorods, Airy beams, Angular momentum beams and switchable gratings*
2. *Investigation of photoaligned surfaces and liquid crystal (LC) physical properties for displays and photonics applications*
3. *Synthesis and characterization of new azodye materials and mixtures for photoalignment*
4. *Azodye investigation for displays and optical films (polarizers, nanorods, fibers, lenses, gratings): optimal processing, gray levels, dependence on physical parameters of the flexible surface and LC*

1. DA CHEN, HUIJIE ZHAO, KEXIN YAN, DONG XU, QI GUO, LINGHAO SUN, FAN WU, VLADIMIR G. CHIGRINOV,AND HOI-SING KWOK, Interference-free and single exposure to generate continuous cycloidal alignment for large-area liquid crystal devices, **Optics Express,** Vol. 27, No. 20/30, pp. 29332-29339 (2019).

Interference-free and single exposure to generate continuous cycloidal alignment for large-area liquid crystal devices

**Abstract**

An approach for generating cycloidal pattern of liquid crystal (LC) molecules based on interference-free and single exposure is illustrated. The spatial manipulation of polarization state is achieved using birefringent prism and wave plates. And then, the spatially variant polarization of exposure beam is transferred to LC molecules by azo-dye photo-sensitive layer. Consequently, the LC samples fabricated shows periodically cycloidal texture and diffraction efficiency more than 99%. The measured period A and diffraction angle are in good consistency with theoretical results. Thus, this exposure method provides an effective and robust way for fabricating large-area LC elements, therefore paving the way for widespread applications of high-performance diffractive LC devices.

2. Qi Guo , Kexin Yan, Vladimir Chigrinov, Huijie Zhao, and Michael Tribelsky, Ferroelectric Liquid Crystals: Physics and Applications, **Crystals,** 2019, 9, 470, pp1-21.

Ferroelectric Liquid Crystals: Physics and Applications

**Abstract**

Electrooptic modes with fast response and high contrast ratio are highly desirable in modern photonics and displays. Ferroelectric liquid crystals (FLCs) are especially promising for fulfilling these demands by employing photoalignment technology in FLC cells. Three electrooptic modes including surface stabilized FLC (SSFLC), deformed helix ferroelectric (DHF) mode, and electrically suppressed helix (ESH) mode are reviewed with the corresponding electrooptic effects like bi- and multi-stable switching, continuous modulation of grayscale or phase, and high contrast switching. The general operation principles FLC electrooptic modes are described, and then the characteristics of each modes for potential applications are summarized. With the advantages of controllable anchoring energy, the photoalignment provides FLC samples with uniform alignment and high contrast ratio. The fast FLCs with a high resolution and high contrast can be used in the next generation display including field sequential color FLC microdisplays, as well as switchable 2D/3D televisions.

3. Rybakov, V. V. Belyaev, S. Kumar, V. G. Chigrinov and V. A. Zhachkin, Molecular relaxation of components of LC mixture 2f- 3333 (ROLIC) for dual-frequency electrooptic shutters, **Liquid Crystals**, Vol. 46, No. 12, pp. 1861–1867 (2019).

Molecular relaxation of components of LC mixture 2f-3333 (ROLIC) for dual-frequency electrooptic shutters

**Abstract**

Dual-frequency liquid crystal materials are used in fast response electrooptic modulators in different devices for digital information displaying and processing. In an NLC mixture 2f-3333 (ROLIC, Switzerland) there are components with lateral dipole moment. Their molecular relaxation is investigated by a method of dielectric spectroscopy. Values of relaxation time and its activation energy, molecular friction coefficient, rotational diffusion are obtained. They are compared with data obtained by other methods like LC viscosimetry.

4. Jiatong Sun, Deng, K. L., Sang, J. X., Gong, X. H., Liu, Y., Shang, J. H., Liu, H., Zhang, Y. H., Guo, Q., and Vladimir.G. Chigrinov, The effect of chiral dopant on the rewriting speed of optically driving liquid crystal display , **Liquid Crystals**, DOI: 10.1080/02678292.2019.1662106

The effect of chiral dopant on the rewriting speed of optically driving liquid crystal display

**Abstract**

Mixing liquid crystal with chiral dopant for increasing the response speed of optical driving liquid crystal display was investigated in this paper. It is demonstrated that by adding chiral dopant, rewriting time could be decreased from 30 s to 20 s with good repeatability. Without adding other steps in the process of making cells, this improvement is due to the stronger elastic energymaking LC molecules twist more easily.

5. J. T. Sun, L. H. Ren, K. L. Denga, T. Wang, Q. Guo, J. X. Sanga, Y. Liu, H. Liua, J. H. Shanga, and V.G. Chigrinov, Greyscale generation for optically driving liquid crystal display, **Liquid Crystals**, Vol. 46, No. 9, pp. 1340–1344 (2019).

Greyscale generation for optically driving liquid crystal display

**Abstract**

It is very difficult to display greyscale for an optically driving liquid crystal display (ODLCD) because the driving unit and display unit are separate, and there are no electronics in the display part of ODLCD. In this paper, two greyscale generation methods are proposed to achieve this goal. Six and nine grey levels are separately achieved through the two methods.

6. Ma, Y, Tam, Alwin M. W , Gan, X. T,Shi, L. Y, Srivastava, A. K., Chigrinov, V. G. **,** Kwok, H. S., Zhao, J. L., Fast switching ferroelectric liquid crystal Pancharatnam-Berry lens, **Optics Express,** Vol. 27, No. 7, pp. 10079-10086 (2019).

**Abstract**

A ferroelectric liquid crystal (FLC) cell with continuously alignment structure is realized by a polarization hologram method for fabricating a Pancharatnam-Berry (PB) lens. which is employed as a concave/convex lens. The PB phase can be maintained by the optical axis in-plane switching: meanwhile, its diffraction efficiency can be tuned in a certain range by electrically controlling azimuthal angle and optical biaxiality of the smectic helical structure realized by deformed helix ferroelectric liquid crystals. The measured diffraction efficiency of the fabricated device is up to 87% and the response time can be 300 mu s with a low electric voltage. The FLC PB lens can have potential applications in existing optical devices and the realization of FLC with continuous alignment structure can be further used for other LC-based optical devices.

7. Qi Guo, Lin Xu, Jiatong Sun, Xiaoqian Yang, Hongwei Liu, Kexin Yan, Huijie Zhao, V. G. Chigrinov and H. S. Kwok, Fast switching beam steering based on ferroelectric liquid crystal phase shutter and polarisation grating, **Liquid Crystals**, Vol. 46, No. 9, pp. 1383–1388 (2019).

Fast switching beam steering based on ferroelectric liquid crystal phase shutter and polarisation grating

**Abstract**

We report on fast-switching and high-efficient optical beam steering based on a polymerisable liquid crystal polarisation grating (PG) in combination with ferroelectric liquid crystal (FLC) phase shutter. The PG was fabricated in a convenient single-step holographic exposure process using photo-sensitive azo-dye material as alignment layer for liquid crystal (LC) director. A binary electro-optical FLC was employed for circular polarisation selection, which enables the electro-tunable steering of the combined system. The efficiency of 95.7% with 82 mu s switching time is obtained for 1064nm laser. This work provides a versatile candidate for non-mechanical beam steering devices.

# Investigations in Atmospheric Propagation & Microwave Biophysics

## by André Vander Vorst, Member EUAS

Short Biography

*André Vander Vorst was born in Brussels in 1935. At high school, he studied classical humanities, including Latin and Greek. He graduated in 1958 as an electrical and mechanical engineer at the UC Louvain (UCL), Belgium, from which he received his Doctoral degree in 1965. During his thesis he spent six weeks working at Philips Natuurkundig Laboratorium, Eindhoven, The Netherlands. As a research associate, he was at M.I.T 1964-1965 where he received a M.Sc. degree in microwaves, and at Stanford University 1965-1966, both in radioastronomy. In 1966, he founded the Microwave Laboratory at UCL, which he headed for 35 years. His research interests were successfully loaded waveguides and cavities, atmospheric propagation up to 300 GHz, opto-microwaves, humanitarian demining, and bio-microwaves. He has been teaching in four Belgian Universities on electromagnetics, transmission lines, and microwaves. He also taught analogue and hybrid computation, antennas, and microwave and satellite communications. He supervised 27 doctoral theses and about 200 engineer's theses.*

*Prof. Vander Vorst has authored and co-authored seven books, a number of book chapters, and more than 300 papers in peer-reviewed journals and conference proceedings. His last book, RF/Microwave Interaction with Biological Tissues, with A. Rosen and Y. Kotsuka as co-authors was published by Wiley U.S.A. in 2006.*

*Through his academic career at UCL, Prof. Vander Vorst has been Head of EE Department 1970-1972, Dean of Engineering 1972-1975, Vice-President of the Academic Council 1973-1975, and President of the Open School in Economic and Social Politics 1973-1987.*

*Over the last 50 years, Prof. Vander Vorst has been actively involved in developing the International microwave community. In 1967-2001 he was chairing Student Activities Committee and Educational Activities Committee and setting up Chapter Coordination Committee in I.E.E.E. Region 8. He was a corresponding member of the Organizing Committee of the first European Microwave Conference (EuMC) in London 1969, Chair EuMC Technical Program Committee in Brussels 1973, and Chair EuMC in Liège 1984. Ha has been a reviewer for every EuMC since 1969. He is a founder member of the European Microwave Association (EuMA) and has been EuMA Secretary General for 18 years. In the latter function he has set up and developed EuMA Headquarters. He is now appointed Secretary Emeritus and Data Protection Officer.*

*His service to the microwave community Prof. Vander Vorst has done also under the umbrella of I.E.E.E. MTT Society, in which he has been active in 1985-2006. He is a Life fellow of the I.E.E.E. and obtained a number of awards including the Microwave Career Award 2004 from I.E.E.E MTT-S and the Propagation Award 2019 of the European Association for Antennas and Propagation (EurAAP).*

*He is an associate member of Belgian Academia of Letters and Science, a member of Academia Europaea, the Electromagnetics Academy, and EU Academy of Sciences. He is an Honorary Member of Belgian National Committee or URSI. He has been a member of National Health Council in both Belgium and The Netherlands. He has been cited in a number of Who'sWho.*

*He loves music and has conducted choirs for more than 40 years.*

*He has five children and twelve grandchildren.*

From 1960 to 1964, André Vander Vorst investigated fast switching of magnetic cores for his doctoral thesis. As a research associate with a post-doctoral fellowship, he spent two years in the USA: 1964-1965 at M.I.T. and 1965-1966 at Stanford University to specialize in microwaves, in the Laboratory of Radio-astronomy in both institutions. In 1966, back in Belgium he founded the Microwave Laboratory at the Université catholique de Louvain (UCL) and started research on propagation in loaded waveguides and cavities, which has the been the subject of several doctoral theses. Some typical publications are mentioned for each research topic mentioned.

The first doctoral thesis in the Laboratory was by F. Gardiol, 1966-1969, who analytically investigated the impact of a one-dimensional inhomogeneity on waveguide propagation, that is the effect of a ferrimagnetic slab in a rectangular waveguide [1].

Simultaneously, A. Vander Vorst started developing numerical analysis for propagation in diverse inhomogeneously loaded microwave transmission lines by means of variational principles [2]. He produced a numerical version of the variation-iteration method presented by Morse and Feshbach, *Methods of Theoretical Physics*, Part 1 and 2, McGraw-Hill, 1953.
In 1969, he obtained the first numerical solution of a second-order partial derivative eigenvalue equation, describing the propagation in a rectangular waveguide loaded by inserts. The method he developed was used extensively by himself and by several doctoral students.

A number of doctoral students then investigated the impact of inhomogeneity on miscellaneous propagating structures, like microstrips, fin lines, and p-i-n transmission lines, as well as opto–induced effects on transmission lines [3]-[8].
The research started in 1966 with propagation in lossless closed structures at X-band and ended up with propagation on lossy distributed structures at frequencies up to 100 GHz. In 2002, he co-authored with I. Huynen a research book on variational principles and distributed circuits [9].

Atmospheric propagation has been a research interest of A. Vander Vorst from 1968 until about year 2000 [10]. In 1970, he set up two horizontal links at 11.6 and 35 GHz, respectively, for measuring atmospheric propagation parameters, operating for a five-year period [11]. This has been the subject of the first of his five consecutive COST projects on atmospheric propagation, which covered both horizontal links and slant paths.

He was the Belgian participant to the Orbital Test Satellite (OTS) of the European Space Agency (ESA), 1978-1983. He obtained for this significant funding from the Belgian State (equivalent to 5 million EUR at today's value) to obtain one transmitting-receiving fixed television station at 14 GHz (up, 2 kW) and 11 GHz (down), as well as two receiving stations at 11 GHz, one fixed and one mobile [12]-[14].

Then, he was together with D. Vanhoenacker-Janvier the Belgian participant to the Olympus experiment of ESA, 1988-1993. They again obtained significant funding from the Belgian State and PTT Department, respectively, to set up two receiving stations at 12.5 and 30 GHz and 12.5 and 20 GHz in both polarisations at both frequencies, respectively. Measurements made at Louvain-la-Neuve included attenuation, depolarisation and scintillation at 12.5 and 30 GHz and radiometry in two polarisations at 12 and 35 GHz [15]. Fast measurements were available, every 34 ms, especially in view of investigating the time scale of the scintillation effects.

These experimental tools have stimulated original atmospheric propagation investigations in theory, experiment, and simulation as well. The OTS stations have been the occasion for the Laboratory to be one of the three research centres to experimentally point out the microwave scintillation phenomena, which have been then extensively investigated by D. Vanhoenacker-Janvier in her doctoral thesis and later.

Site-shielding, in particular by a knife-edge obstacle, has been investigated with measurements from 8 to 94 GHz [16]. The research then evaluated the bit-error rate prediction of atmospheric communications links [17]. It continued until the year 2000 with the evaluation of some special effects related to the structure of linearly tapered slot antennas including the Vivaldi antenna, up to some tens of GHz [18].

A. Vander Vorst conducted research on atmospheric propagation of EM waves at frequencies up to 300 GHz [19]. He has been involved in EM wave propagation since 1994, start of his stay in the US, until the end of his active professional career.

Microwave biophysics has been another subject of interest of A. Vander Vorst. The project started at the end of the seventies by designing and implementing a system for sterilizing air, eliminating bacteria by microwave heating, in the form of a flux to proceed to open air surgeries. This system was patented and commercialized.

Experimental work has been going on with rabbits from 1987 through 1994, for the doctoral thesis by J. Teng. The first step was devoted to developing a method for microwave acupuncture by inserting a miniature cable into acupuncture points and exciting these by injecting microwaves in the cable with the advantage of having a quantitative method for measuring analgesia. The purpose was to excite the nervous system for detecting an analgesic effect by exciting some specific points. Results were positive [20].

The second step consisted of the development of a method to measure in the cervical centre of

pain the effect of analgesia [Fig. 1]. This showed that with this procedure the composition of the cervical liquid in the pain centre is modified similarly to what is obtained when ingesting analgesic products [21].

In the third experimental step, a method was developed for measuring in the cervical centre of pain the effect of an electric impulse applied to a rabbit's foot in the absence or the presence of analgesia produced by microwave acupuncture. Simultaneously, the deformation of the impulse was measured as a function of microwave acupuncture on the nervous system and in particular the spinal cord, by inserting a microwave micro-antenna inside of the backbone [22]. The purpose was to investigate whether a non-thermal microwave effect could be experienced. The result was negative [23].

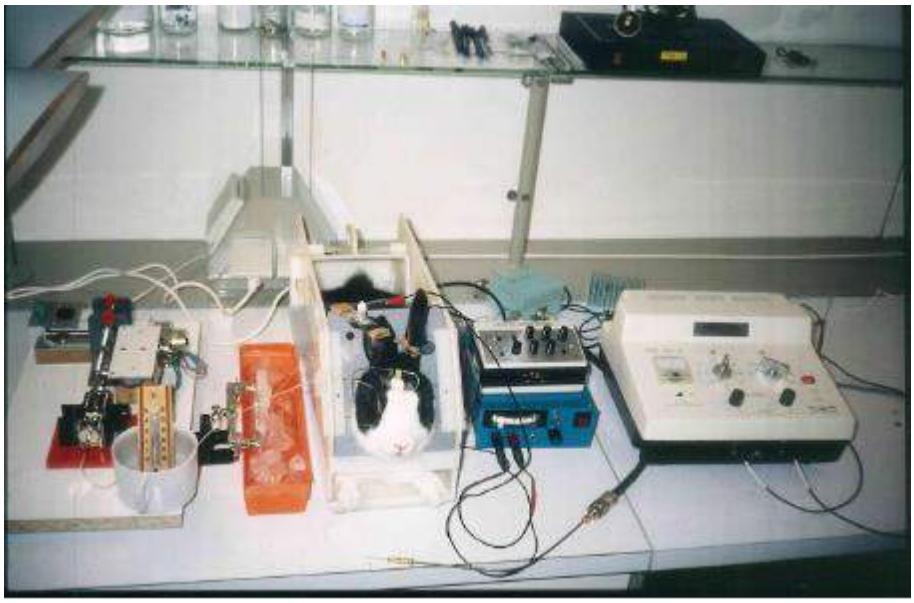


Figure 1. Measuring pain threshold on a rabbit as a function of antalgic microwave acupuncture

A cooperation went on with colleagues of the School of Medicine in the years 1993-1997 to evaluate the effect of magnetic induction produced by a coil to implant on a mouse for obtaining a muscular reinforcement. The result was positive [24].

Dielectric parameters and blood absorption have been measured from 2 to 110 GHz [25] and a review of microwave effects on nervous system and nervous fibre has been performed [26].
Research has then been more oriented toward biological effects and medical applications [27] and more specifically to biological effects on living systems and especially human beings [28]. Face heating at the occasion of a telephone conversation has been measured in direct view of a base station, in stairs and in the basement of a building, respectively, with the measurement of an increase of 0.7°C after 10 minutes in the basement [29].

Specific very low frequency magnetic field measurements have been made on spontaneous bioelectric activity of neurons [30] while dielectric absorption microwave power has been evaluated at the scale of nucleic acids [31].

Microwave exposure of rats has been prepared, performed and evaluated from 1998 through 2009, for the doctoral thesis of D. Adang. They were submitted to a microwave level corresponding to the calculation by WHO of the limit for the human being, taking into account however a factor 10 for difference of length between the human being and the rat. The exposure duration has been long: 2 hours per calendar day of 70% of the rat lifetime which was 30 months. There were four groups of 31 rats, including three groups exposed to three different microwave schemes, respectively, and one sham-exposed group, with in particular exposure to 970 MHz CW. Fifteen

blood parameters were analysed 6 times on the 124 rats, yielding more than 10.000 biological data, together with behavioural effects and mortality. A combination of positive and negative results has been obtained on monocytes, behavioural effects, and mortality, respectively [32][33].

Planar antennas have been designed and evaluated in view of medical applications, from 2005 through 2013, being mainly the subject of the doctoral thesis of H. Halheit. This necessitated the evaluation of a radiating structure, the operating frequencies, the influence of the substrate on the resonance frequencies of the antenna and their bandpass, the power necessary for medical applications, and mutual coupling between the elements. It also necessitated the evaluation of the electric characteristics of biological tissue and of the electric influence of heterogeneity [34].

A number of presentations have been made in medical symposia [35].

At the request of the Editor of the Wiley Series in Microwave and Optical Engineering, a research book was written on the subject of RF/Microwave interaction with biological tissues and published by Wiley U.S. in 2006, with PhD students as a prime target [36].

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# Progress on the Next Generation of Subsea Production System

## by Menglan Duan, Member EUAS

Short Biography

*Professor of Mechanical Engineering and Ocean Engineering.*
*Dean of College of Safety and Ocean Engineering at China University of Petroleum, Beijing, China.*
*Over 200 publications in high quality scientific journals.*
*Project Manager for over 150 Projects in Ocean Engineering, Mechanical Engineering and Petroleum Engineering.*
*Chairman of Subsea Technology Committee of the International Ships and Offshore Structures Congress (ISSC).*
*Chairman of China Branch of the Society for Underwater Technology (SUT).*
*Chairman of Industry-University Joint Committee of the Chinese Society of Theoretical and Applied Mechanics (CSTAM).*
*Visiting Professor at Federal University of Rio de Janeiro.*
*Founding Editor-in-Chief of Frontiers in Fossil Fuel Engineering, Editor-in-Chief of Development and Application of Ocean Engineering, and Editorial Board Members of 16 international journals.*
*Member of the EU Academy of Sciences.*
*Founding and Executive Chairman of the Annual SUT Technical Conference.*
*Founding and Executive Chairman of the China-Brazil Deepwater Forum.*

The amount of oil and gas production in the world has increased sharply in the past decade, and about 90% is from the deep waters. Subsea production systems (SPS) which cover all the equipment and installations are very important to the development of deepwater oil and gas fields. The Offshore Engineering Structures and Equipments Group of the China University of Petroleum has devoted its group for ten years to innovative development of the SPS and the research has been applied to South Sea of China, publishing about 100 patents and over 200 technical papers. A new concept of next generation of SPS has been proposed by Prof. Duan to further reduce the risks and cost of the subsea production of oil and gas. The main points of the concept are presented as follows:

1) A new type of subsea floating manifold which meets the requirement that the gravity center should be under the buoyant center has been designed. The key point of the design is the position of the buoy. Considering the buoy maybe block the sight of the operator when it is mounted at the bottom, we employ the distributed buoys at the corner of the manifold, as is shown in Fig. 1. Each buoy's mass and buoyancy are calculated. Once one buoy is flooded, other buoys can also provide enough buoyancy to make the manifold suspended under water. The inner design of the buoy is shown in Fig. 2.

**Fig. 1** Design of the suspended manifold

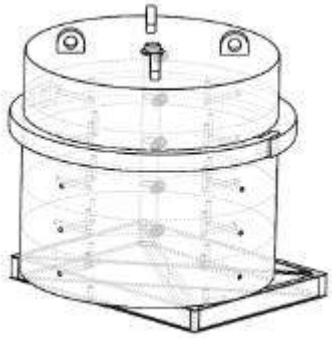


**Fig. 2** Design of the buoy

2) A new model of deepwater functional chamber which can realize the functions of production and installation has been proposed, meeting the structural strength, basic stability, cabin installation and demolition, maintenance and repair requirements. The functional chamber features a multi-cabin design with a distributed layout, as is shown in Fig. 3. For the external pressure resistant structure of the chamber, titanium alloy is used. The buckling calculation of the single-layer cylinder structure and the T-beam structure are carried out by nonlinear theory and variational method. In the research of foundation bearing load, a new design of wellhead with suction anchor is formed. The basic stability problem of the wellhead is analyzed by calculating the ultimate bearing capacity of the pile foundation. The maintenance plan for the functional chamber under different working conditions is also proposed, which is divided into three phases: the minor repair phase, the intermediate repair phase and the overhaul phase.

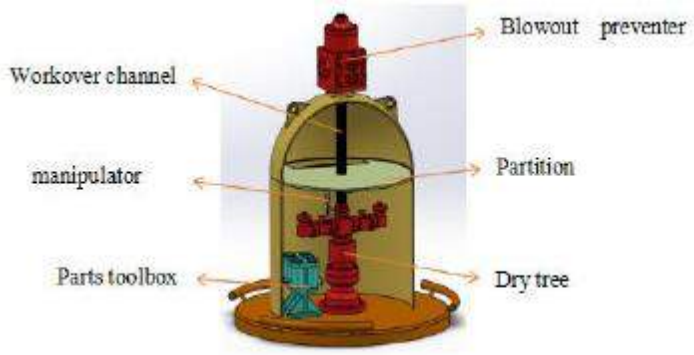



**Fig. 3** Sketch of the internal equipment layout of the functional chamber

3) An intelligent self-warning coating based on phosphotungstic acid fluorescence composite is developed to realize the partial self-healing and self-reporting function of the flexible pipes, as shown inf Fig. 4. In addition, nanoparticle-graphene oxide is prepared to improve the mechanical property of the pipeline. Pulse position modulation is adopted to realize the ultrasonic energy conversion and wireless communication technology.

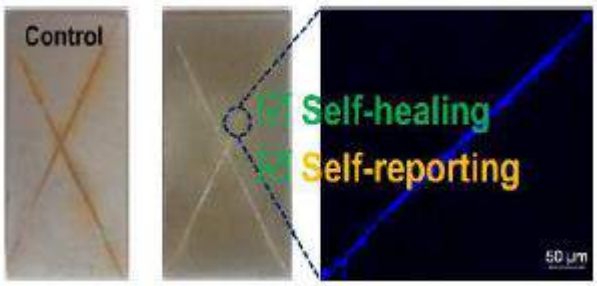



**Fig. 4** Self-warning coating for the flexible pipes

4) The traditional methods to prevent the appearance of hydrate and wax mainly include electrical heating, chemical injection, etc. A new concept that phase change material can be used to realize flow assurance was proposed. A super-oleophobic nano membrane is developed to avoid the formation of hydrate and wax. The in-lab experiment was conducted, showing that the super-oleophobic coating works for the common metal materials used in the pipelines, as shown in Fig. 5.

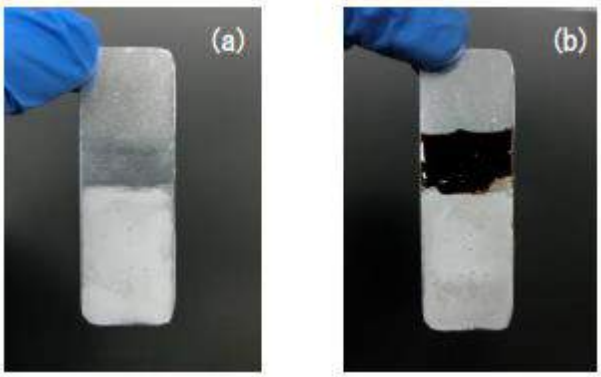



**Fig. 5** Metal with (a) or without (b) the super-oleophobic coating after immersing the oil

5) In the production of oil and gas, severe slug flow can lead to sharp changes of the pressure of the equipment, which may cause serious damage to production process. Methods usually used to eliminate slug flow mainly include throttling, gas lifting, PID (proportional-integral-derivative) control, etc. However, these methods all have an apparent shortcoming that the production flow rate will decrease during the exploitation. A new method based on multiphase flow transient simulation using OLGA is used to predict the slug flow pattern in the subsea pipeline, as is shown in Fig. 6. The proposed method can not only eliminate the serious slug flow by using the instant responses, but also realize the automatic control of the system.

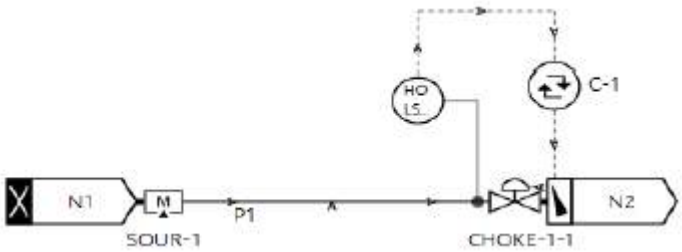



**Fig. 6** Pipeline model for OLGA simulation of slug flow conditions

# Recent Trends in Biomedical Materials & Clinical Biochemistry

## by Pankaj Vadgama, Member EUAS

Short Biography

***CURRENT APPOINTMENTS***

*2000- Director IRC in Biomedical Materials, Queen Mary University of London*
*2000 - Professor of Clinical Biochemistry, Queen Mary University of London*
*2000 - 15 Honorary consultant Chemical Pathologist Barts Health NHS Trust*
*2003 - 15 Head of NHS Clinical Service (Appointed NHS Consultant 1983)*
*2015- Visiting Professor Southern Medical University Guangzhou, China*
*2017 - Visiting Professor University of Grenoble Alps*

***ACADEMIC QUALIFICATIONS***

*1971 MB, BS Newcastle University*
*1976 BSc Chemistry (1st Class Hon) Newcastle University*
*1977 Member (later Fellow) Royal College of Pathologists*
*1984 PhD Newcastle University*
*1994 Fellow Royal Society of Chemistry*
*2001 Fellow Institute of Materials Minerals and Mining*
*2002 Fellow Institute of Physics*
*2006 Fellow Royal Society of Medicine*
*2008 Chartered Scientist (Institute of Materials, Minerals and Mining)*
*2010 Fellow Royal Society of Biology*

***ACADEMIC APPOINTMENTS***

*1977-1980 MRC Training Fellow Newcastle University*
*1983-1988 Director Biosensor Research Group Newcastle University*
*1988-2000 Professor of Clinical Biochemistry, Manchester University*
*1998-2000 Professor of Biomedical Materials, Manchester University*
*1991-1997 Head of Department of Medicine, Manchester University (Salford)*
*1993-1996 Postgraduate Dean, Faculty of Medicine, Manchester University*
*1996-1998 Research Dean, Faculty of Medicine, Manchester University*
*1998-2000 Head of Division of Biomedical Engineering, Manchester University*

***Editorial Board Positions***

*Editorial Board: Physiological Measurement, Medical Engineering and Physics, Bioanalytical Reviews, Functional Biomaterials, Medical Devices and Sensors, 3D Printed Systems and Materials, Journal of Biochemistry and Molecular Biology Research, Chinese Chemical Letters. Guest Editor for Analytical and Bioanalytical Chemistry: (i) Thin film characterisation (ii) Membrane based sensors. Sub-Editor Biomaterials Series (RSC). Editor for (i) Bioelectrochemistry for the Encyclopedia of Interfacial Chemistry, Surface Science and Electrochemistry (ii) Bioinstrumentation and Bioinformatics for the Encyclopedia of Biomedical Engineering (Elsevier).*

***National/International Committees***

*Member EPSRC (Engineering and Physical Science Research Council): Materials Strategic Advisory Team (SAT) (2004/5/7/8); Healthcare (2005). Member, Institute of Materials Minerals and Mining Smart Materials Committee, Nanotechnology Committee, Biomedical Applications Division and External Advisory Committee. National Measurement Systems (NMS) Grants Committees for Materials and Modelling (2002 – 15) and Innovation R&D (2012-15); NPL(National Physical Laboratory)/LGC (Laboratory of the Government Chermist) projects. Past EPSRC grants panel memberships (includes as chair of some panels) from 1986: Materials, Structural Materials, Chemistry, Multidisciplinary (Engineering), Health Care, Analytical Science, Mechanical and Medical Engineering, Follow-on Funding, DTCs (Doctoral Training Centres), Master's Training*

*Packages, Sensors' Policy Group, SMART Technologies, Basic Sciences, Life Science Interface, Engineering Fellowships (Senior/Advanced). Nanotechnology Strategy Working Group (co-author, section on nanomedicine) (2005). ROPA (Realising our Potential) Panels EPSRC, MRC (Medical Research Council) (1995-96). MRC Joint Research Equipment Initiative Panel (JREI, 1996-7). Royal Society of Chemistry, Industrially-Sponsored Award in Electroanalytical Chemistry (1997, 2000). Member of Organisation and Delivery of Healthcare Task Force (Foresight Healthcare, 1999-2000). Member Academy of Medical Sciences/Foresight Working Group on the Detection and Identification of Infectious Disease (2004). Member Institution of Electrical Engineers Professional Group S9 (Biomedical Engineering, 1990-93). Chair (i) R&D (ii) Point of Care Testing committees, Division of Pathology Barts Health NHS Trust (2002-2011). Member BBSRC Strategic Research Studentships Panel 2004, LINK Program Medical Technologies and Molecular Sensors (1994-2001), Foresight LINK awards (2001). European Space Agency Advisory Panel on bioassay under microgravity (2000). Various EU FP IV & V Panels: Biotechnology, Biomedical and Health Research, Cell Factory, Growth, Standards, Measurements and Testing (1993-2000). Chair DTI Building up Biomaterials (BuB) Materials Healthcare Advisory Group (2001-2003). Member UK delegations (x3) to Japan (Biomaterials) and Singapore (x1) (Materials). Roadmap Champion for Diagnostics for human health, RSC (2010). Member Manchester Commonwealth Games 2002 Scientific Congress Committee.*

*RAE (Research Assessment Exercise, UK) Panel member Materials (2008). External Assessor Faculty of Engineering, University of Coimbra, Portugal (2013), Founder member biennial international conference series: Biomaterials Interfaces (2007-). Chair RSC Chemistry in Medicine Panel (2010). Chair, Steering Committee EPSRC IRColl Interdisciplinary Research Collaboration) in Bionanotechnology, University of Oxford (2003-5), Member 4th Generation Light Source (4GLS) Advisory Group, Daresbury. Member, international task force on environmental carcinogens (Halifax Project, 2014). Advisor, UK Biobank Project (2004). Member Special Inquiry into Regenerative Medicine Research at UCL.*

*RAE Advisor University of Manchester, REF Advisor University of Central Lancashire. Academic promotions advisor (Rutgers, Cranfield, Ulster, Manchester, Leeds, Flanders). Advisor, Engineering – Materials Faculty research quality, Limerick (2011). Cranfield University Senate committee panel member on Biomedicine MScs (2013). External advisor on the reorganization of the Chemistry Department, University of Surrey (2001). Scrutineer for Fellowship/Membership applications to the Institute of Materials Minerals and Mining. External assessor for staff appointments, PhD applications for Nazarbayev University (2014). Advisor to University of Ege (Turkey) on summer school biotechnology rolling Programme. International advisory member (vice-chair) of Uganda based research training foundation; advice on training needs and external funding, eg secured for geological sciences MScs. Co-Chair UK – China Biomaterials Partnership (2006-9). Global Initiative of Academic Networks (GIAN, India)) lecture course at University of Tezpur (2016). Host to Commonwealth Fellows India (Tezpur, 2015; Aligarh Muslim University, 2003), PhD Fellow (Government of Pakistan, 2017). NMS research project advisor, LGC (2005-07).*

*Chair UK Foresight Panel on Biomaterials and member of Materials, Smart Materials panel (2004) (co-author, strategy documents). Member, DTI Innovation and Growth Team (2006), Member UK Standards Group on ISO TC 229; nanotechnology nomenclature (2006 -). Chair of ISO Working Group on Nanomedicine and member Working Group on Nanobiotechnology (2006 – 2010). Member BSI Committees on Nanotechnology, Botechnology and Cell Therapies.*

*Member DFG Review Panel for German Excellence Initiative: Materials 2005,2007). Member Finland Research Council panel on Bioscience and Engineering (2008). Grants reviewing national funding councils: Australia, Quatar, Hong Kong, Portugal, Austria, Netherlands, Italy, Ukraine, Kazakhstan, Netherlands, Romania.*

***RECENT COLLABORATIONS***

*-EPSRC Program grant on elite athlete monitoring (ESPRIT) with Loughborough University Imperial College and UK Sport (£600k) (2011-15)*

*-DoH Dual function nano-silver incorporated polymers for medical device antimicrobial coatings*

*– 2 projects (total £263 k) (2010 – 2014) Rainbow Medical Ltd*
*-EU Marie Curie exchange with five China Universities: Microsystems and Bioanalysis Platforms for Health Care (£78k) (2010 – 14)*
*-Industrial CASE Studentship on polymer bioadhesives with UEA, TWI (2012 -16)*
*-EU Marie Curie exchange with three China Universities Advanced biomaterials for generative medicine (£39k) (2010 – 15)*
*-UKIERI collaboration with Central Electronics Engineering Research Institute, India on Micro/nanofluidics for diagnostics (£65k) (2014 -16).*
*-TSB/BBSRC grant on Blood brain barrier model for drug permeability and toxicity testing with Kirkstall Ltd and Leeds University. (£52k) (2014-15)*
*- DoH Anti-bacterial 'Fill & Flush' Urinary Catheter Development with University of Southampton (£61k) (2017 -19)*
*- Newton Institutional Links Grant (Egypt) Renewable Energy Driven Hybrid Desalination System for Remote Areas (£115, 647) (2016 – 18)*

**Research**

**Anastasova S, Sphehar-Delese A, Bickham D, Uebel P, Schmidt M, Russell P and Vadgama P (2012) 'Stabilised biosensing using needle based recess electrodes' Electroanalysis 24, 529-538.**

Abstract

A recess disk electrode for amperometric monitoring of oxygen and glucose is reported. The basic design of sensor is a needle structure for easy implantation, embodying a gold filled silica capillary with a 80 mu m inner diameter working electrode. Recess and inlaid disc electrodes, placed inside stainless steel tubes which served as a counter/reference electrode, were compared. The working electrode surface was modified with different treatments and barrier membranes to achieve selectivity for the analytes of interest. The basic needle format is ideal for in vivo use, and the format is easily extendable to other analyte targets. The sensors show linear working range for oxygen up to 160 mmHg partial pressure of oxygen, and for glucose from 1 to 10 mM. Bio-fouling, as assessed by exposure to bovine serum albumin, was significantly reduced. Response times for the recess construct was increased but remained within the acceptable range for physiological monitoring. The operational stability of the sensors is demonstrated as well as the interference-free detection of peroxide in the presence of physiologically relevant levels of ascorbic acid, uric acid, acetaminophen, and catechol. Preliminary in vivo tests showed excellent response towards glucose.

**Chang, H, Khan, R, Rong, Z, Sapelkin A, Vadgama P (2010) "Study of albumin and fibrinogen membranes formed by interfacial crosslinking using microfluic flow" Biofabrication DOI: 10.1088/1758-5082/2/3/035002.**

Abstract

Microfluidics enables scale reduction in sample volume with obvious benefits for reagent conservation. In contrast to conventional macro-scale flow, microfluidics also offers unprecedented control over flow dynamics. In particular, laminar flow is readily achieved, allowing for new analytical and synthetic strategies. Here, two parallel flows of buffer and xylene were used to create a stable liquid-liquid interface within linear micro-channels. These, respectively, carried protein (albumin or fibrinogen) and an acyl chloride to effect protein crosslinking. This created robust, micro-membranes at the interface that

bisected the fluid channel. Membrane formation was self-limiting, with fibrinogen membranes showing greater solute permeability than albumin, based on dye transport (Ponceau S, Meldola Blue). The crosslinker isophthaloyl dichloride led to thinner, less permeable membranes than terephthaloyl chloride. Larger surface area membranes formed at a static liquid-liquid interface served as a more physically accessible model and allowed precise electrochemical determination of acetaminophen, catechol and peroxide diffusion coefficients, which confirmed the greater fibrinogen permeability. Scanning electron microscopy (SEM) of the membranes also indicated a higher population of discrete nanopores at the fibrinogen surface. A crosslinking pH had a strong effect on overall permeability. Adhesion of B50 neuronal cells was demonstrated, and it is proposed that the membranes could facilitate cell growth through bidirectional nutrient supply in a micrbioreactor format.

**Hakimi O, Gheysens T, Vollrath F, Grahn MF, Knight, DP, Vadgama P (2009) "Modulation of cell growth on exposure to silkworm and spider silk fibers", Journal of Biomedical Materials Research 92A, 1366-1372.**

Abstract

Recent years have seen an increased interest in the use of natural and modified silks for tissue engineering. Despite longstanding concerns regarding the biocompatibility of silk sutures, only a few studies have been carried out to investigate the biocompatibility of natural silk fibers. Here, we report an in vitro assessment of the effect of nonmodified, degummed silks on cells. We describe the effects of degummed silk fibers as well as extracted sericin on cell metabolism and proliferation. Endothelial cells directly exposed to native degummed Bombyx mori and Antheraea pernyi silks showed lower rates of proliferation and metabolism than nonexposed cells. A similar but milder effect was observed for cells in direct contact with Nephila edulis egg sack fibers. Sericin and silk-conditioned medium had no negative effect on cell proliferation except in medium supplemented with 5% bovine serum prior to conditioning with A. pernyi silk. The toxicity of A. pernyi was negligible after thorough enzymatic treatment of the fibers with trypsin. It is, therefore, proposed that A. pernyi silk contain one or more cytotoxic components, which need to be removed prior to medical use.

**Nair G, Gargiuli J, Shiju NR, Rong Z, Shapiro E, Drikakis D, Vadgama P (2006) 'in situ fabrication of crosslinked protein membranes using microfluidics', ChemBioChem, 7, 1683-1689.**

Abstract

We report a novel technique for preparing cross-linked protein membranes within microchannels by using; an interfacial cross-linking reaction. Glass microchannels with a Y input were assembled by using a simple adhesive bonding technique to achieve dual, parallel laminar flows. Membrane formation utilised an interfacial reaction at the liquid-liquid interface, which involved bovine serum albumin (aqueous solution with a flow rate of 300 mu L min(-1)) and terephthaloyl chloride (xylene solution with a flow rate of 700 mu L min(-1)), to form thin (similar to 25 mu m) cross-linked films along the length of the channel under the continuous pressure-driven laminar flow. Such microfabricated membranes could extend the separation potential of any microfluidic structure provide a stable barrier layer: Furthermore, degradation of the membane was possible by using an alkali sodium dodecyl sulfate solutio whichled to the complete disappearance of the

membrane. These membranes could facilitate additional modification to allow for different permeability properties by controlled degradation. The one-step in situ membrane-fabrication methodology reported here generated precisely localised membranes and avoided the complexities of`subcomponent assembly, which require complicated alignment of small; preformed membranes. This methodology could 'become the basis for sophisticated microseparation systems, biosensors and several "lab-on-a-chip" devices.

**Rong Z, Leitao E, Popplewell J, Alp Burcak, Vadgama P (2008) "Needle enzyme electrode for lactate measurement *in vivo*", IEEE Sensors Journal, 8, 113-120.**

Abstract

Electrochemical lactate needle enzyme electrodes were fabricated based on lactate oxidase with a conventional hydrogen peroxide detection regimen with a linear range up to 7 mM, response time similar to 3 min, and sensitivity similar to 1 nA/mM. A negatively charged inner (sulphonated polyether ether sulphone-polyether sulphone) membrane was applied for ensuring selectivity by limiting oxidazible anion diffusion to the Pt working electrode; polyurethane outer membrane layers were dip coated over the enzyme layer to limit substrate diffusion to the enzyme layer to achieve: 1) stir independence and 2) a low oxygen requirement. Lactate was monitored subcutaneously in rats during controlled haemorrhage and hypovolaemic shock. Tissue lactate showed agreement with blood lactate before haemorrhage and for limited haemorrhage (up to 2 ml blood withdrawal from 16 ml total blood volume) but with blood loss above 3 ml the tissue lactate rise was less pronounced than in blood. Loss of intercompartmental equilibrium due to diffusion limitation is suggested as a factor in causing this difference. An experimental in vitro model was developed which employed the needle lactate electrode within a cylindrical collagen gel to monitor inward diffusion of lactate as a basis for determining lactate diffusion coefficient. The high precision measurement gave a diffusion coefficient consistent with report values $3.54^{-6}$ x $10cm^2/s$. The simplified experimental approach could allow lactate transport studies across tissue analogues.

**Ateh DD, Vadgama P, Navasaria HA (2006) "Culture of human keratinocytes on polypyrrole-based conducting polymers", Tissue Engineering 12, 645-655.**

Abstract

Variously loaded polypyrrole films, including those containing proteins and polysaccharides, were prepared on gold-coated polycarbonate coverslips. The characteristics of human keratinocytes were studied on these films by microscopy, biochemical assays, and immunocytochemistry. We found keratinocyte viability to be load dependent. For chloride, polyvinyl sulphate, dermatan sulphate, and collagen-loaded polypyrrole films, keratinocyte viability as assessed by the AlamarBlue assay was respectively 47.22, 60.43, 87.71, and 22.65% of tissue culture polystyrene controls after 5 days. This was found to require a previously unreported polymer washing step prior to cell seeding due to the observed toxicity of untreated films. In the case of bare polycarbonate and gold substrates, viability was respectively 75.44 and 61.04% of tissue culture polystyrene controls after 5 days. Keratinocytes stained positive for PCNA (proliferation), K10 (suprabasal differentiation), and K16 (hyperproliferation) markers although cell morphology was poor for organotypical cultures on dermatan-loaded polypyrrole compared with de-epidermalized dermis. From our studies, we concluded that optimized polypyrrole films adequately support keratinocyte growth in submerged cultures with some

improvements needed for organotypical cultures. Polypyrrole composites are attractive candidates for tissue-engineering applications since they may incorporate biomolecules and are electrically addressable with the potential to both direct and report on cell activity.

**Rigby GP, Crump PW, Vadgama P (1996) "Stabilized needle electrode system for in vivo glucose monitoring based on open flow microperfusion" Analyst 121, 871-875.**

Abstract

Preliminary in vitro studies and in vivo performance of amperometric glucose needle enzyme electrodes incorporating an open microflow technique, in which the sensor surface is subjected to a flow of fluid, are reported, Initially using a slow flow (60 mu l h(-1)) of isotonic phosphate buffer over the enzyme electrode tip, an interface was created which reduced cellular/protein fouling for electrode measurements in whole blood, Here a minor reduction in electrode response (apparent only at high glucose concentration) occurred which was not cumulative and therefore not associated with fouling, The protection afforded by the moving aqueous film was independent of fluid composition; the use of isotonic/hypertonic buffer, addition of anticoagulant (1% m/v heparin) or enhanced fluid viscosity (addition of 1% v/v glycerol) did not affect the system, Implantation of the electrode and its microflow cannula into subcutaneous tissue in rats was associated with a decreased buffer flow (30 mu l h(-1)) and had the effect of (i) reducing electrode stabilization (30 min), (ii) accelerating 'pick up' of tissue glucose changes after intravenous glucose (1-2 min lag) or insulin (3-7 min lag) and (iii) achieving a correlation between tissue and blood glucose values under dynamic conditions ($r(2) = 0.98$, $y = 0.99x + 0.23$), Reassessment of the electrode response in vitro, following a 4 h monitoring period, provided a sensor response within 3% of the original electrode sensitivity, indicating little or no surface fouling and avoiding the requirement for repeated in vivo calibrations at least over the initial implantation period.

**Desai MA, Vadgama PM (1992) "Bicarbonate and other buffer systems can enhance the rate of $H^+$ diffusion through mucus *in vitro*" Biochimica et Biophysica Acta 1116, 43-49.**

Abstract

The effect of various diffusible buffers on mucus H+ permeability, and in particular the potency of the HCO3-/CO2 buffer system relative to other selected buffers is reported here. The diffusional resistance of mucus and water was demonstrated to be dependent on buffer concentration, and the contrast between the two types of layer was most pronounced for low D(H+) values near neutrality. This concentration dependence was most marked with mucus layers in the buffer systems investigated. Furthermore, the nature and pK(a) values of the diffusible buffer systems used in this study had a profound effect on measured D(H+) The effect was particularly striking in the case of HCO3- buffer with mucus. Possible implications of these in vitro findings in mucosal protection from acid are discussed.

# New Contributions in Aletrnative Energy

## by Arthur Ragauskas, Member EUAS

Short Biography

*Arthur Ragauskas held the first Fulbright Chair in Alternative Energy and is a Fellow of American Association for the Advancement of Science, the International Academy of Wood Science and TAPPI. In 2014, he assumed a Governor's Chair for Biorefining based in University of Tennessee's Department of Chemical and Biomolecular Engineering, with a complementary appointment in the UT Institute of Agriculture's Department of Forestry, Wildlife, and Fisheries and serves in the US Energy and Environmental Sciences Directorate, Biosciences Division, at ORNL. His research program is directed at understanding and exploiting innovative sustainable bioresources. This multifaceted program is targeted to develop new and improved applications for nature's premiere renewable biopolymers for biofuels, biopower, and bio-based materials and chemicals. His research program has been sponsored by NSF, USDA, DOE, GA Traditional Industry Program, a consortium of industry partners, and several fellowship programs which is summarized in 488 publications. His Fulbright sponsored activities at Chalmers University of Technology, Sweden were focused on the forest biorefinery and new biofuel conversion technologies for lignocellulosics. Currently, Dr. Ragauskas manages a research group of graduate students, postdoctoral research fellows, a research scientist, and visiting scientists. He is the recipient of the 2014 TAPPI Gunnar Nicholson Gold Medal Award, the ACS Affordable Green Chemistry award, 2017 AIChE Green Processing Award, 2017 Academia Distinguished Service Award, and his students and postdocs have won several awards, including the ACS graduate research award, ORNL UT-Battelle Award, and Supplementary Performance Award (ORNL).*

*Ragauskas is an Associate Editor for Biofuels, Bioproducts and Biorefining, Biofuels, BioEnergy Research, Industrial Biotechnology, Taiwan Journal of Forest Service, TAPPI J., Holzforschung, Journal of Biobased Materials and Bioenergy, Journal of Petroleum Technology and Alternative Fuels, The Open Biotechnology Journal, Current Biotechnology, and J. Wood Chemistry and Technology. He is an editorial board member of Sustainability and Journal of Chemical Technology and Biotechnology. Ragauskas has served on several advisory boards and review panels including: Austrian Science Fund, European Commission Research Directorate, National Science Academy, J. Paul Getty Trust, NSF, USDA, DOE, ARAP-E, NSERC, TAPPI Research Management Committee, Netherlands Organization for Scientific Research (NWO), Swedish Foundation for Strategic Research, Swedish VINN Excellence Center, Swedish Knowledge Foundation, VTT Technical Research Centre of Finland, ERA Chemistry, Swiss National Science Foundation, Finnish Academy of Science Norway Research Council, The Technology Foundation STW, Agence Nationale de la Recherche and Singapore Agency for Science, Technology and Research. Dr. Ragauskas has been an invited visiting professor at Universidade da Beira Interior, Portugal; Chalmers University of Technology, Sweden; Royal Institute of Technology/ STFi, Stockholm, Sweden; and Southeast University, China, and South China University of Technology, China.*

### Ragauskas Governor Chair Mission Statement

As an academician, Ragauskas' core belief is that a professor can only be as successful as the students he educates, mentors, and graduates. As such, Ragauskas' academic mission has been, and remains, the cornerstone of his career objectives. These career objectives include:

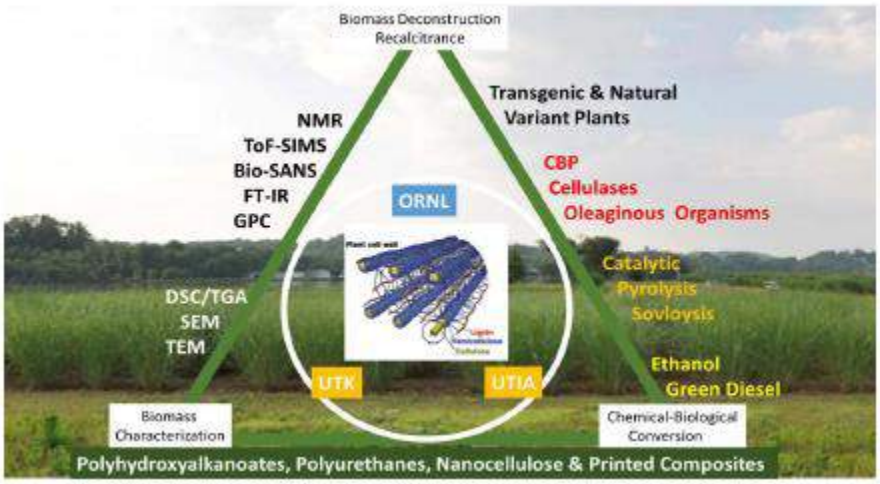
- Develop a challenging and enriching educational and research experience that facilitates the intellectual development of UTK/UTIA students and postdoctoral fellows and supports the mission of the Department of Chemical and Biomolecular Engineering, and Center for Renewable Carbon.

- Recruit, educate, and develop the next generation of scientists that will be nationally/internationally recognized leaders in green chemical engineering of biofuels, bio-derived materials, and chemicals.
- Develop a nationally/internationally recognized research center for sustainable green chemical engineering of biorefining, leveraging the exceptional researchers and research infrastructure located at ORNL, UTK, and UTIA.

## Research Accomplishments and Activities

Ragauskas assumed the ORNL-UTK-UTIA Governor's Chair in Biorefining position in June 2014. This UTK faculty position, jointly funded by UTK/UTIA and ORNL, is focused on developing a fundamental research and academic program in sustainable biomass biorefining. As highlighted in Ragauskas' 2018 invited seminar at the Birmingham Science Museum (England), his research program is focused on three central overlapping focus areas (see **Figure 1**) including:

- Fundamental lignocellulosic properties of plant cell walls and their relationship to biological biorefining of biomass to biofuels.
- Valorization of biomass components for bio-derived materials
- Development of new tools and methodologies for biomass characterization.




F**ig. 1**. Summary of Ragauskas' ORNL, UTK, UTIA Governor Chair Research in Biorefining.

During this period, his research group has published over 175 manuscripts, of which greater than 90% were joint ORNL-UTK-UTIA publications. Ragauskas' publications are acknowledged internationally with a **Google H-index of 84**, **i10 index of 338** and **greater than 30,000 citations**. These overall accomplishments were acknowledged last year by Publons (Clarivate Analytics), who named Ragauskas as one of the world's most highly cited researchers in his field for 2018. The impact of these studies was recognized in a series of awards, including (i) Nominated to Sigma Xi (2019); (ii) Fellow Royal Society of Chemistry (2018); (iii) Green Process Engineering American Institute of Chemical Engineers Award (2017); (iv) The University of California, Bourns College of Engineering – Center for Environmental Research and Technology, Distinguished Service Award (2017).

### *ORNL Focused Activities*

Five representative publications that have been published since Ragauskas assumed the Governor's Chair position include:

1. Downregulation of pectin biosynthesis gene GAUT4 leads to reduced ferulate and lignin-carbohydrate cross-linking in switchgrass. Li M.; Yoo C.G.; Pu Y.; Biswal A.K.; Tolbert A. K; Mohnen D.; Ragauskas A.J.; *Communications Biology* (2019) 2, 22.
2. Sugar release and growth of biofuel crops are improved by downregulation of pectin biosynthesis. Biswal, A.K.; Atmodjo, M.A.; Li, M.; Baxter, H.L.; Yoo, C.G.; Pu, Y.; Lee, Y.C.; Mazarei, M.; Black, I.M.; Ji-Yi, Z.; Ramanna, H.; Bray, A.L.; King, Z.R.; LaFayette, P.R.; Pattathil, S.; Donohoe, B.S.; Mohanty, S.S.; Ryno, D.;Yee, K.; Thompson, O.A.; Rodriguez Jr., M.; Dumitrache, A.; Natzke, J.; Winkeler, K.; Collins, C.; Yang, X.; Tan, L.; Sykes, R.W.; Gjersing, E.L.; Ziebell, A.; Turner, G.B.; Decker, S.R.; Hahn, M.G.; Davison, B.H.; Udvardi, M.K.; Mielenz, J.R.; Mark, D.F.; Nelson, R.A.; Parrott, W.A.; Ragauskas, A.J.; Stewart Jr., N.C.; Mohnen, D. *Nature Biotechnology* (2018) 36(3), 249-257.
3. Insights of biomass recalcitrance in *Populus* trichocarpa natural variants for biomass conversion. Yoo, C.G.; Yang, Y.; Pu, Y.; Meng, X.; Muchero, W.; Yee, K.; Thompson, O.; Rodriguez, M.; Bali, G.; Engle, N.L.; Lindquist, E.; Singan, V.; Schmutz, J.; DiFazio, S.; Tschaplinski, T.J.; Tuskas, G.; Chen, J.G.; Davison. B.H.; Ragauskas, A. *Green Chemistry* (2017) 19(22), 5467-5478.
4. A study of poplar organosolv lignin after melt rheology treatment as carbon fiber precursors. Sun, Q.; Khunsupat, R.; Akato, K.; Tao, J.; Labbe, N.; Gallego, N.C.; Bozell, J.J.; Rials, T.G.; Tuskan, G.A.; Tschaplinski, Timothy J.; Naskar, A.K.; Pu, Y.; Ragauskas, A.J. *Green Chemistry* (2016) 18(18), 5015-5024.
5. Cross-linked poly(methyl vinyl ether-co-maleic acid)/poly(ethylene glycol)/nanocellulosics foams via directional freezing. Liang, L.; Huang, C.; Hao, N.; Ragauskas, A.J. *Carbohydrate Polymers* (2019) 213, 346-351.

The first two publications, in the Nature family of publications, are representative of Ragauskas' collaborative efforts within BESC and CBI. In both of these publications, advanced analytical methodologies were employed to determine the structure and molecular properties of cellulose, hemicellulose, and lignin in the native and transgenic switchgrass samples grown by researchers at UTK and University of Georgia. These fundamental studies highlighted the unique role that lignin-carbohydrate complexes (LCC) contribute to reduced recalcitrance in the knockdown expression of GalactUronosylTransferase 4 (GAUT4) in switchgrass when compared to wild type (WT) switchgrass. The reduction in LCC linkages was hypothesized to facilitate lignin migration allowing for improved cellulase deconstruction after a hot water pretreatment.

In light of the continuing controversies of LCC and methods of detecting these structures, Ragauskas was invited to submit a critical analytical review on this topic, along with research colleagues from the Royal Institute of Technology (Sweden), to Green Chemistry journal and this work was just recently published: A Critical Review on the Analysis of Lignin Carbohydrate Bonds in Plants. Giummarella, N.; Pu, Y.; Ragauskas, A.; Lawoko, M. *Green Chemistry* (2019) 20, 1573 - 1595.

The third publication is representative of Ragauskas' *Populus* research within BESC and CBI. Working with a team of ORNL researchers, he has examined the sugar release performance of natural *Populus* variants and correlated their biomass recalcitrance properties to the fundamental structure of cellulose, hemicellulose, and lignin. Among the physicochemical properties of poplar, the lignin content, lignin molecular weight, lignin S/G ratio, and cellulose accessibility were found to strongly correlate with sugar release. The results demonstrated that the lignin content was negatively correlated with sugar release, whereas the lignin molecular weight, lignin S/G ratio, and cellulose accessibility were positively associated with poplar sugar release. These changes in biopolymer structures were then related by differential gene expression (DEG) to identify potential target gene groups that are correlated with recalcitrance factors. These results provide valuable information for future biomass studies to understand the novel genes and their regulatory mechanism in forest genetics and apply this to tree breeding for enhancing biomass utilization.

In all of these recalcitrance studies, lignin is a by-product that was historically viewed as either

a waste product or, at best, a product for combustion. Starting with Ragauskas' publication in Science titled "Lignin Valorization: Improving Lignin Processing in the Biorefinery" (Ragauskas, A.J.; Beckham, G.T.; Biddy, M.J.; Chandra, R.; Chen, F.; Davis, M.F.; Davison, B.H.; Dixon, R.A.; Gilna, P.; Keller, M.; Langan, P.; Naskar, A.K.; Saddler, J.N.; Tschaplinski, T.J.; Tuskan, G.A.; Wyman, C.E. *Science*, (2014) 344(6185), 1246843-1-1246843-10) he has focused on utilizing lignin as a feedstock for novel material applications. A key focus of these studies is to demonstrate that lignin structure is a critical factor in controlling its physiochemical properties. This hypothesis was clearly illustrated in paper 4, whereby Ragauskas demonstrated viscosity properties of lignin at elevated temperatures could be altered by lignin's degree of polymerization and structural features. Comparable findings have also been reported in related studies, including: (i) Linking lignin source with structural and electrochemical properties of lignin-derived carbon materials. Li, W.; Zhang, Y.; Das, L.; Wang, Y.; Li, M.; Wanninayake, N.; Pu, Y.; Kim, D.Y.; Cheng, Y.T.; Ragauskas, A.J.; Shi, J., *RSC Advances* (2018) 8(68), 38721-38732. (ii) Understanding lignin fractionation and characterization from engineered switchgrass treated by an aqueous ionic liquid. Liu, E.; Li, M.; Das, L.; Pu, Y.; Frazier, T.; Zhao, B.; Crocker, M.; Ragauskas, A.J.; Shi, J. *ACS Sustainable Chemistry & Engineering* (2018) 6(5), 6612-6623. (iii) Mechanism-Guided Design of Highly Efficient Protein Secretion and Lipid Conversion for Biomanufacturing and Biorefining. Xie, S.; Sun, S.; Lin, F.; Li, M.; Pu, Y.; Cheng, Y.; Xu, B.; Liu, Z.; Sousa, L.C.; Dale, B.E.; Ragauskas, A.J.; Dai, S.Y.; Yuan, J.S. *Advanced Science*, doi.org/10.1002/advs.201801980.

In addition to genetic factors controlling the structure of lignin in bioresources, the extraction of lignin from biomass and its impact on lignin structure has been clearly defined in a series of publications, including CBI studies working with researchers at University of California, Riverside. Examining the structure before and after CELF pretreatment, lignin structure was shown to exhibit a significant decrease in DP and an accompanying decrease in β-aryl ethers (Note: depending on CELF reaction conditions) as reported in: Hybrid Catalytic Biorefining of Hardwood Biomass to Methylated Furans and Depolymerized Technical Lignin. Seemala, B.; Meng, X.; Parikh, A.; Nagane, N.; Kumar, R.; Wyman, C.E.; Ragauskas, A.J.; Christopher, P.; Cai, C.M. *ACS Sustainable Chemistry & Engineering* (2018) 6(8), 10587-10594. In contrast, the use of Consolidated Biomass Processing (CBP) yields residual lignin with minimally changes in structure, as reported in: Elucidating the structural changes to Populus lignin during consolidated bioprocessing with *Clostridium thermocellum*. Akinosho, H. O.; Yoo, C. G.; Dumitrache, A.; Natzke, J.; Muchero, W.; Brown, S.D.; Ragauskas, A.J., *ACS Sustainable Chemistry & Engineering* (2017) 5:9, 7486–7491.

The later finding is an important discovery since it allows future lignin valorization studies to be directly tied to the structural nature of lignin in plants. Currently, most pretreatments alter the structure of lignin, hence pretreatment lignin valorization studies need to consider both the structure of lignin in the starting biomass and the impact of pretreatment.

These key discoveries were made possible by the collaboration between researchers in the Biosciences Division at ORNL and Ragauskas' team members. These findings provide a valuable tool for researchers to tune the structure of lignin for a variety of chemical, biological, and material applications. Ragauskas has highlighted these opportunities in several publications, including: (i) Defining Lignin Nanoparticle Properties through Tailored Lignin Reactivity by Sequential Organosolv Fragmentation Approach (SOFA). Liu, Z.H.; Hao, N.; Shinde, S.D.; Pu, Y.; Kang, X.; Ragauskas, A.; Yuan, J.S. *Green Chemistry* (2019) 21(2), 245-260; (ii) High Shear Homogenization of Lignin to Nanolignin and Thermal Stability of Nanolignin-Polyvinyl Alcohol Blends. Nair, S.S.; Sharma, S.; Pu, Y.; Sun, Q.; Pan, S.; Zhu, J. Y.; Deng, Y.; Ragauskas, A.J. *ChemSusChem* (2015) 7(12), 3513-3520; (iii) Fast Fractionation of Technical Lignins by Organic Co-solvents. Wang, Y.Y.; Li, M.; Cai, C.; Wyman, C.; Ragauskas, A.J. *ACS Sustainable Chemistry and Engineering* (2018) 6(5), 6064-6072.

Key to Ragauskas' research program is the development of new analytical tools to characterize the structure of biomass. Over the past five years, this has been accomplished in several fields, including: (i) Novel whole-cell NMR methodology, for example, Elucidating Structural

Characteristics of Biomass using Solution-State 2D NMR with a Mixture of Deuterated Dimethylsulfoxide and Hexamethylphosphoramide. Yoo, C.G.; Pu, Y.; Li, M.; Ragauskas, A.J., *ChemSusChem* (2016) 9(10), 1090-1095; (ii) Phosphitylation/$^{31}$NMR to characterize lignin from biomass pretreatment, for example, Determination of Hydroxyl Groups in Biorefinery Resources via Quantitative 31P Nuclear Magnetic Resonance Spectroscopy. Meng, X.; Crestini, C.; Ben, H.; Hao, N.; Pu, Y.; Ragauskas, A.J.; Argyropoulos, D.S., *Nature Protocols* (2019) accepted; (iii) ToF-Sims to investigate surface topochemistry of biomass and recalcitrance, for example, see: Determining the Syringyl/Guaiacyl Lignin Ratio in the Vessel and Fiber Cell Walls of Transgenic Populus Plants. Tolbert, A.K.; Ma, T.; Kalluri, U.C.; Ragauskas, A.J. *Energy & Fuels* (2016) 30(7), 5716-5720; (iv) SANS investigation into biomass pretreatment and recalcitrance, for example, Understanding Multiscale Structural Changes During Dilute Acid Pretreatment of Switchgrass and Poplar. Pingali, S.V.; Urban, V.S.; Heller, W.T.; McGaughey, J.; O'Neill, H.; Foston, M.B.; Li, H.; Wyman, C. E.; Myles, D.A.; Langan, P.; Ragauskas, A.; Davison, B.; Evans, B.R., *ACS Sustainable Chemistry & Engineering* (2017) 5(1), 426-435; (v) Hemicellulose-cellulose composites reveal differences in cellulose organization after dilute acid pretreatment. Shah, R.; Huang, S.; Pingali, Sai V.; Sawada, D.; Pu, Y.; Rodriguez, M.; Ragauskas, A.J.; Kim, S.H.; Evans, B.R.; Davison, B. H.; Hugh, O.N., *Biomacromolecules* (2018) 20(2), 893-903.

In addition to these energy-focused studies, Ragauskas is actively involved in the utilization of bioresources for bio-derived materials with a special emphasis on the utilization of lignin and nanocellulose. His nanocellulose studies are directed at engineering the relative orientation of crystalline nanocellulose (CNC) and cellulose nanofibrils (CNF) for advanced composites for material and human health applications. These studies employ novel methodologies including chemical crosslinking, directional freezing and layer-by-layer synthesis, as reported in: (i) Preparation and characterization of nanocellulose-polyvinyl alcohol multilayer film by layer-by-layer method. Hou, Q.; Wang, X.; Ragauskas, A.J. *Cellulose* (2019) 26(8), 4787-4798; (ii) Cross-linked poly(methyl vinyl ether-co-maleic acid)/poly(ethylene glycol)/nanocellulosics foams via directional freezing. Liang, L.; Huang, C.; Hao, N.; Ragauskas, A.J. *Carbohydrate Polymers* (2019) 213, 346-351; (iii) Porous artificial bone scaffold synthesized from a facile in situ hydroxyapatite coating and crosslinking reaction of crystalline nanocellulose. Huang, C.; Hao, N.; Bhagia, S.; Li, M.; Meng, X.; Pu, Y.; Yong, Q.; Ragauskas, A.J. *Materialia* 4 (2018) 237-246.

An innovative aspect of these studies is defining the fundamental molecular orientation and chemical properties of nanocellulosics to physicochemical properties. A key finding in the bone scaffold studies was that the sulfonate groups in CNC acts as a binding site for hydroxyapatite. In addition, Ragauskas has shown that crosslinking CNC stabilizes the artificial bone scaffold in water. As Ragauskas' fundamental program in bio-derived materials develops, there are obvious applications in the field of advanced wound healing, organ scaffolds, active membrane separation, and advanced functional composites. A basic premise of all these investigations is that the material properties of bio-derived composites are directly related to the structure of the starting biomass polymers, and hence, these properties are controlled by plant genetics. To provide a clear foundation for the relationship between plant genetics, plant polymers, and bio-derived composites we have initiated a new projects directed at Cell Printing of Bio-Derived Composites.

In summary, Dr. Ragauskas' vision has been to leverage academic-research accomplishments in lignocellulosic chemistry to develop a nationally and internationally recognized program for fundamental sustainable green chemistry engineering of biorenewables for biofuels, bio-derived materials, and chemicals at ORNL, UTK, and UTIA

# Resilience of Structures and Infrastructure under Extreme Transient Loads

## by Adnan Ibrahimbegovic, Member EUAS

Short Biography

*M. Adnan Ibrahimbegovic (PhD UC Berkeley, USA, Hab. Univ. Paris 6, France) is Professor Classe Exceptionnelle, Senior Fellow of IUF-Institute Universitaire de France and holder of a Chair in Computational Mechanics at UTC. He was attributed a number of research awards, including Alexander von Humboldt Research Award in 2005, IACM Fellow Award in 2006 and Slovenian Research Award in 2007, 'Classe Exceptionnelle' highest-rank of French University Professors in 2009, and Senior Member of IUF in 2015. He has also received many international awards: Chair 'Claude Levy-Strauss' for French Professor at University Sao Paulo, Brazil in 2012, 2016, 2020 ; Chair 'Åsgard' for French Professor at NTNU Trondheim, Norway in 2013 ; Mercator-Professor TU Braunschweig, Germany in 2014 ; Invited Professor KAIST-Korea Advanced Institute of Science and Technology, South Korea, 2014, 2016 ; Invited Professor TUBITAK, ITU-Istanbul Technical University, Turkey, 2014 ; WCP-World Class Professor program for Indonesia – with Technical University of Indonesia, Depok, Jakarta, Indonesia in 2017 ; 2018. His former collaborators (total: 53, including 40 doctoral theses, 10 post-docs and 3 habilitations), are presently at elite engineering schools in Paris (Ecole Centrale Paris, Ecole des Ponts Paris, ESTP), institutes of technology (PEER/UC-Berkeley, ZHAW -Zurich University of Applied Sciences, TU Braunschweig, UTC-Compiègne, INSA-Toulouse), French universities (University Paris X, University Lille 1, University de Nantes) and large industry groups, (AREVA, EDF, Lafarge, Renault) ; as well as professors in 11 different countries: France, Mexico, Czech Republic, Slovenia, Vietnam, Algeria, Bosnia, Croatia, Hungary, Turkey, Netherlands. He has over 600 publications, including close to 200 scientific papers in referred journals, resulting with h-index = 48.*

### Abstract

In this work we address the challenge pertinent to validating resilience of large engineering structures, both in terms of integrity to failure and ability to recover under extreme transient loads. Of particular interest are the effects of combined transient loads in industrial domains, such as civil and mechanical engineering. The effect of combined extreme transient loadings on a structure is not well understood— whether the source is man-made, such as an explosion and fire, or natural, as an earthquake or extreme wind loading. A critical assessment of current knowledge is timely (with Fukushima-like disasters or terrorist threats).

The central issue in all these problems is structural integrity, along with their transient nature, their unexpectedness, and often the uncertainty behind their cause. No single traditional scientific discipline provides full answer, but a number of tools need to be brought together: nonlinear dynamics, probability theory, some understanding of the physical nature of the problem, as well as modeling and computational techniques for representing inelastic behavior mechanisms. The paper also covers model building for different engineering structures and provides detailed presentations of extreme loading conditions. A number of illustrations are given: quantifying a plane crash or explosion induced impact loading, quantifying the effects of strong earthquake motion, quantifying the impact and long-duration effects of strong stormy winds — along with a relevant framework for using modern computational tools. The proposed approach considers the levels of reserve in existing structures, and ways of reducing the negative impact of high-risk situations by employing more sound design procedures.

## 1. Introduction and Motivation

This paper deals with important challenge on validating the durability and lifetime integrity of massive composite structures under extreme transient loads. The illustrative examples concern: earthquake, airplane impact, fires or tsunamis (see Figure 1). Special attention is given to costly massive structures or infrastructure with 'irreplaceable' components, which are characterized by a number of different failure modes that require the most detailed description and interaction across the scales. We would like to significantly improve the currently dominant approach of mode superposition, which is applicable when there is a linear relationship between external forces and corresponding structure-infrastructure response.

The key issue we address pertains to use of the material damage as the source of damping. Here, one needs to define nonlinear inelastic models, which pertains to any particular material. It can accommodate any among the most frequently used materials in engineering applications, such as steel, concrete and masonry. We conclude with clear recommendations on how to define the damping forces. Usual damping capacity is defined as the damping ratio of the energy dissipated in one cycle of oscillation to the maximum amount of energy accumulated in the structure, with viscous nature of damping forces. An alternative advocated here is to use the material damage and interface damping, much dependent upon the type of material, as well as on manufacturing method. By taking into account that the material characteristics vary due to material heterogeneities, which can be described by replacing the material parameters with random variables of random fields. Such a coupled nonlinear mechanics-probability computations provide the reliable estimation of influence that the material damage can have on structural damping, leading to the same asymptotic response as viscous damping, but described with much more reliable path to constructing predictive models. This is illustrated for some of the most frequently used structure materials.

**Fig. 1** Three examples of extreme natural and man-made hazards studied by PI: a) failure of Tacoma bridge; (nested parallel) fluid-structure computations of flutter-instability produced by forced long-term oscillations induced by wind (Ibrahimbegovic 2014); b) Impact by tsunami of Samoa island; model quantifying impact on a structure by water column (Ibrahimbegovic 2014); c) Terrorist threat for NPP structure under impact of large airplane; model quantifying damage to structure due to airplane crash (Ibrahimbegovic 2009a).

## 2. Main Objectives

The main objective in better damage and failure modes interpretation is development of novel Mesh-in-Element (MIEL) Multiscale Method capable of representing strain field heterogeneities induced by evolution (and interaction) of localized failure mechanisms in massive structure, pertaining to micro scale (FPZ-fracture process zone), macro scale including softening (macro cracks) and non-local macro scale (bond-slip for long fiber reinforcement). The objective of MIEL Multiscale Method is also to provide capabilities for quantifying the risk of premature localized failure through probability description of initial defects (microstructure heterogeneity) and uncertainty propagation through scales. The novel scientific concept to be explored pertains to multiscale formulation and solution

of coupled nonlinear mechanics-probability problem replacing the standard homogenization approach that can only provide average (deterministic) properties of heterogeneous composites. This concept is of interdisciplinary nature with Mechanics (defining probability distribution) and Applied Mathematics (providing uncertainty propagation) combined in order to capture the influence of heterogeneities and fine scale defects on premature failure.

The most important challenge concerns the ability to provide the sound, probability-based explanation of damping exponential asymptotic decay at the structural level, without resorting to classical viscous model but with different failure modes observed for different size specimens and real structure heterogeneities typical of composite materials (see Figure 2).

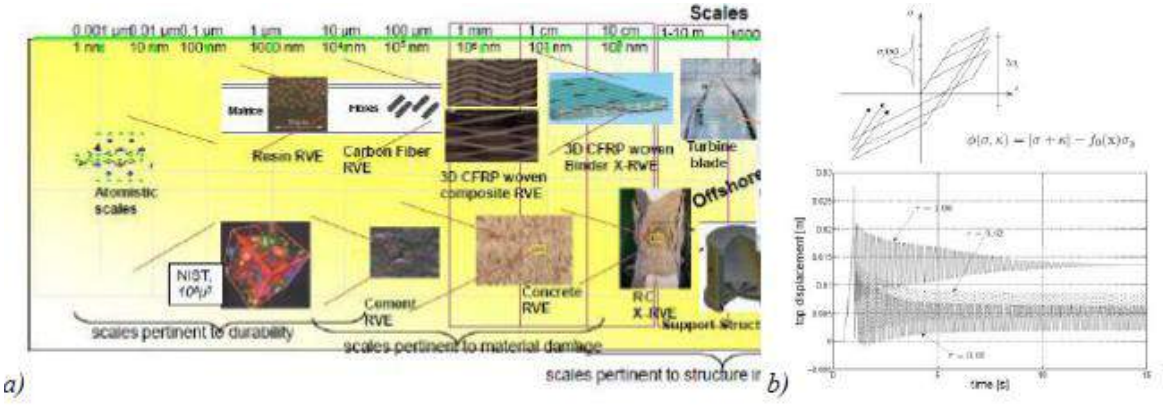



**Fig. 2** Mesh-In-Element (MIEL) multiscale method – a) failure modes for 3D carbon-epoxy woven composite and for reinforced concrete; b) hysteresis loops for heterogeneous materials with material parameters probability distribution described by random fields, producing the structural response characteristic of exponential asymptotic decay.

## 3. Concluding Remarks on Current and Future Research

The biggest potential gain concerns changing the resilience validation procedures for massive structures that are beyond the size suitable for testing at present. The scientific gains concern providing the Mesh-in-Element (MIEL) Multiscale Method that connects computations with design studies (optimization), testing (identification) and safety verification (monitoring) of massive composite structures. The scientific gains also concern further placing the proposed method within multiphysics framework, along with the original use of goal oriented error estimates to provide sufficiently reliable interpretation of extreme conditions (e.g. fluid or heat flow) and the code-coupling software implementation to quickly integrate existing simulation codes within such a framework.

The main technological gain is in development of the open source computational tools that can speed-up testing, innovation and decision-making in complex composite systems. Of special interest is the strategy that allows integrating the existing legacy software products that are used to verify and validate safety of particular components assembled within such complex systems. There are multiple challenges in solving any such problem pertaining to: theoretical formulation, discrete approximation, algorithmic stability and robustness, and finally informatics developments capable of integrating existing legacy

codes.

Further details on point of departure in the current research and developments to follow are given in our recent works (Ibrahimbegovic et al. 2003a, 2003b, 2003c, 2003d, 2004, 2005, 2007, 2008, 2009a, 2009b, 2009c, 2010a, 2010b, 2011, 2012, 2014, 2015, 2016, 2017, 2018, 2019).

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# Distributed Resilient Secondary Control of DC Microgrids against Unbounded Attacks

**by Frank Lewis, Member EUAS**

Short Biography

***Frank Lewis*** *(S'70–M'81–SM'86–F'94) received the bachelor's degree in physics and electrical engineering and the M.S.E.E. degree from Rice University, Houston, TX, USA, in 1971, the M.S. degree in aeronautical engineering from the University of West Florida, Pensacola, FL, USA, in 1977, and the Ph.D. degree in electrical engineering from the Georgia Institute of Technology, Atlanta, GA, USA, in 1981.*

*He is currently a Distinguished Scholar Professor and Distinguished Teaching Professor with the University of Texas at Arlington, Fort Worth, TX, USA and the Moncrief-O'Donnell Chair of the University of Texas at Arlington Research Institute, Fort Worth, TX, USA. He has authored six U.S. patents, numerous journal special issues, journal papers, and 20 books, including Optimal Control (Wiley), Aircraft Control (Wiley), Optimal Estimation (Wiley), and Robot Manipulator Control (CRC Press), which are used as university textbooks worldwide. His research interests include feedback control, intelligent systems, cooperative control systems, and nonlinear systems.*

*Prof. Lewis is a member of the National Academy of Inventors. Fellow IEEE, Fellow IFAC, Fellow AAAS, Fellow U.K. Institute of Measurement & Control, PE Texas, U.K. Chartered Engineer. UTA Distinguished Scholar Professor, UTA Distinguished Teaching Professor, and Moncrief-O'Donnell Chair at the University of Texas at Arlington Research Institute. He works in feedback control, intelligent systems, cooperative control systems, and nonlinear systems. He is author of 7 U.S. patents, numerous journal special issues, 420 journal papers, 20 books, including the textbooks Optimal Control, Aircraft Control, Optimal Estimation, and Robot Manipulator Control. He received the Fulbright Research Award, NSF Research Initiation Grant, ASEE Terman Award, Int. Neural Network Soc. Gabor Award, U.K. Inst Measurement & Control Honeywell Field Engineering Medal, IEEE Computational Intelligence Society Neural Networks Pioneer Award, AIAA Intelligent Systems Award, AACC Ragazzini Award.*

**Abstracts 2019**

## Distributed Resilient Secondary Control of DC Microgrids against Unbounded Attacks

Shan Zuo, Frank L. Lewis, Fellow, IEEE, Ali Davoudi, Senior Member, IEEE

### Abstract

This paper develops a fully distributed attackresilient secondary control framework for DC microgrids, in the presence of unknown unbounded attacks on both voltage and current communication networks. The secondary control of each converter consists of an average consensus-based voltage regulator and a consensus-based current regulator, by using relative information from neighboring converters. This distributed control manner relies on a communication network and, therefore, could be prone to malicious attacks that deteriorate consensus protocols and even destabilize the overall microgrid. In contrast to the existing remedies for bounded disturbances/faults, this paper considers the unbounded attacks that are intentionally designed to maximize the damage to the microgrids. An adaptive attack-resilient secondary control framework is established, and validated in a hardware-in-the-loop environment.

### Conclusion

We have formulated a distributed attack-resilient secondary control problem for DC microgrids, in the presence of unknown unbounded attacks. We have considered the unbounded attacks injected to both the voltage and current communication networks. A fully distributed adaptive control framework has been developed to achieve bounded global voltage regulation and proportional load sharing simultaneously. Experimental results and comparisons between the proposed attack-resilient and the standard secondary controllers under unbounded attacks demonstrate the effectiveness of the proposed approach.

## Time-Varying Output Formation-Containment of General Linear Homogeneous and Heterogeneous Multi-Agent Systems

Shan Zuo, Yongduan Song, Senior Member, IEEE, Frank L. Lewis, Fellow, IEEE, Ali Davoudi, Senior Member, IEEE

**IEEE TRANSACTIONS ON CONTROL OF NETWORK SYSTEMS**

**Abstract**

This paper investigates the time-varying output formation-containment control of general linear homogeneous and heterogeneous multi-agent systems (MAS). This control aims at making each follower's output reach an agreement on the time-varying formation reference, namely, the centroid of the multiple leaders' outputs, and keep a prede_ned time-varying offset with respect to it. Distributed static output-feedback (OPFB) and dynamic OPFB control protocols are first constructed for homogeneous and heterogeneous MAS, respectively, using only neighboring relative output information and a timevarying formation compensation signal. It is proved that the time-varying output formation-containment problem is solved by making certain output formation-containment errors go to zero asymptotically. Then, local sufficient conditions and explicit local design procedures are provided for both homogeneous and heterogeneous MAS. It is shown that the state/output consensus problems, the state/output containment problems, the state/output formation control problems, the time-varying state/output formation-tracking problems with a single leader, and target enclosing problems of homogeneous/heterogeneous MAS can all be treated as special cases of this paper. Finally, numerical simulations validate the effectiveness of the proposed control protocols.

**Conclusion**

We have defined the control problem of time-varying output formation-containment of general linear homogeneous and heterogeneous MAS. The control objective is to make each follower's output reach an agreement on the time-varying formation reference, i.e., the centroid of the leaders' outputs, and keep a time-varying offset with respect to it. We have proposed control protocols using static output-feedback and dynamic output-feedback designs for homogeneous and heterogeneous MAS, respectively. Both control protocols use only a linear combination of relative output measurement. We have provided local sufficient conditions and explicit local procedures for these controllers. The effectiveness of the proposed control protocols has been verified by simulated case studies.

# New Contributions in Inorganic Materials Chemistry

## by Glen Deacon, Member EUAS

Short Biography

*Glen Deacon graduated BSc(Hons) (HI) and PhD from the University of Adelaide (CSIRO and AAEC Scholarships, an ICIANZ Fellowship, and the Senior Tutorship at Lincoln College). Postdoctoral research work was carried out with Professor Sir Ronald Nyholm FRS at University College London (CSIRO Overseas Scholarship, ICI Fellowship) with additional collaboration with Professor Alwyn Davies FRS (UCL) and Dr John Green (NPL Teddington).*

*He was appointed to a lectureship at Monash in 1966, and received accelerated promotion to Senior Lecturer (1971) and Reader (1975). For his research work on Main Group Element Chemistry he was awarded the DSc degree of the University of Adelaide in 1972. He became a Fellow of the Royal Australian Chemical Institute in 1975. In 1994 he was appointed to a Personal Chair in Chemistry and was Professor of Chemistry from 2002-2012 when he was appointed Professor Emeritus. In 2005-6, he was also a Senior Adviser in the Monash Research Office.*

*Glen Deacon has achieved international recognition in several areas of Inorganic and Inorganic Materials Chemistry, particularly the Chemistry of Main Group Elements, Rare Earths, Precious Metals (including platinum anti-cancer compounds), Small Cyano Anions, New Materials (semi-conductor dopants and precursors) and Corrosion Inhibitors. He has received extensive research funding both alone and in research teams, e.g. from ARC (more than 50 grants including support from the Centre for Green Chemistry), ACCV, and GIRD, and is involved in extensive National and International (e.g. Germany, UK, France, Japan) research collaboration. He has supervised or jointly supervised 24 postdoctoral workers, 16 research assistants, and 50 PhD, 4 MSc, 6 MEnvSci and over 70 BSc(Hons) graduates. Over 500 papers have been published in refereed journals and several book chapters have been published. Considerable consulting/contract research has been carried out for industry and government agencies, and a patent is in commercial use.*

*Glen Deacon held a Visiting Lectureship at the University of Western Australia (1991), Guest positions at Universität Dortmund, Technische and Frei Universität Berlin, Universität Hannover, Universität Leipzig, Universität Tübingen, Universität Stuttgart, Universität Duisburg, KIT and Universität zu Köln, and was a Senior Academic Visitor, Queen Mary College, University of London and James Cook University, and has been Visiting Professor and Foundation Lecturer in Inorganic Chemistry, University of Sydney. Since 1987, he has given over 200 invited lectures/seminars at National and International (UK, USA, Germany, Netherlands, Eire) Conferences, Universities, Research Organisations etc. In 2006, he was awarded the Terrae Rarae Prize for Rare Earth Chemistry and in 2007 received the Burrows Award of the Royal Australian Chemical Institute for Inorganic Chemistry. From 2002-2004, he served on the Committee of Experts of the Australian Research Council. In 2012, the $SO_3$ elimination synthesis of organometallic compounds discovered by the Deacon group in the 1970s, was named the Deacon reaction (Organometallics, 2012, 31, 1801).*

**Replacing mercury: Syntheses of lanthanoid pyrazolates from free lanthanoid metals, pentafluorophenylsilver, and pyrazoles, aided by a facile synthesis of polyfluoroarylsilver compounds**

Zhifang Guo, Jenny Luu, Victoria Blair, Glen B. Deacon, Peter C. Junk

Eur. J Inorg Chem . 2019, 1018-1029

**Abstract**

The polyfluorophenylsilver complexes $[Ag_2(C_6F_4Br\text{-}4)_2(py)_3]$ (py = pyridine) (**1**) and $[\{Ag_2R_2(py)_2\}_n]$ [R = $C_6F_5$ (**2**); $C_6F_4Br$-3 (**3**); $C_6F_4H$-4 (**4**)] were prepared in reasonable yields by reactions of silver(I) oxide with the appropriate polyfluorobenzenes in pyridine. This simple and convenient synthesis is selective and does not lead to debromination of $C_6HF_4Br$-(3 or 4). Complex **1** is dinuclear with $AgR_2$ and $Ag(py)_3$ units linked by a bridging polyfluoroaryl group and Ag···Ag interactions, whereas **2-4** are polymeric with alternating $AgR_2$ and $Ag(py)_2$ units similarly linked. The trivalent lanthanoid pyrazolates, $[Ln(Ph_2pz)_3(py)_2]\cdot 2thf$ ($Ph_2pz$ = 3, 5-diphenylpyrazolate; Ln = Yb, **5**, Er**, 6**, Dy, **7**, Lu, **8**; thf = tetrahydrofuran), $[Ho(Ph_2pz)_3(py)(thf)]$ (**9**), $[Ln(Ph_2pz)_3(py)(dme)]\cdot solv$ (Ln = Tb, solv = 1.75PhMe, **10**, Gd, solv = 1.5dme, **11**; dme = 1, 2-dimethoxyethane; PhMe = toluene), $[Ln(Ph_2pz)_3(thf)_3]$ (Ln = La, **12**, Ce, **13**, Nd**, 14**), $[Ln(t\text{Bu}_2pz)_3(py)_2]$ ($^t\text{Bu}_2pz$ = 3, 5-di-tert-butylpyrazolate; Ln = Yb, **15**, Tm**, 16**, Ho, **17**, Dy, **18**), $[Yb(Phtpz)_3(py)_2]\cdot PhMe$ (**19**) (Phtpz = 3-Phenyl-5-(2'-thienyl)pyrazolate) and $[Nd(ttfpz)_3(dme)_2]$ (**20)** (ttfpz = 3-(2'-thienyl)-5-(trifluoromethyl)pyrazolate) have been prepared by redox transmetallation/protolysis (RTP) reactions employing lanthanoid metals, pentafluorophenylsilver and the corresponding pyrazoles (pzH) in donor solvents. This is a new synthetic route in which $AgC_6F_5$ replaces the more commonly used $Hg(C_6F_5)_2$ or $HgPh_2$. Yields are good to excellent if long crystallization times are used but the heavier Ln metals require activation with iodine to induce reaction. The monomeric structures exhibit $\eta^2$-bound pyrazolate ligands with eight-coordinate metal atoms for complexes **5-9** and **15-19**, nine-coordinate metal atoms for complexes **10-14**, and ten-coordinate metal atoms for complex **20**.

**Trapping $CS_2^{2-}$ and $S_3^{2-}$ Between Two Ytterbium Formamidinates.**

Daniel Werner, Glen B. Deacon, and Peter C. Junk

Inorg. Chem. 2019, 58, 1912-1918

**Abstract**

Treatment of $[Yb^{II}(DippForm)_2(thf)_n]$ (n = 2 (**1Yb**·2thf), n = 1 (**1Yb**·1thf); DippForm = *N*,*N*′-bis(2,6-diisopropylphenyl)formamidinate), with either excess $CS_2$ or $S_8$ gives $[Yb^{III}{}_2(DippForm)_4(CS_2)]$ (**3**) and $[Yb^{III}{}_2(DippForm)_4(S_2)_{0.5}/(S_3)_{0.5}]$ (**4**) respectively. **3** is a new addition to an exclusive class of compounds containing the $CS_2$ dianion, and **4** is the first crystallographically characterized example of a rare-earth tri-sulfide complex.

**Trinuclear and Mononuclear Lanthanoid Complexes Containing 2-Methyl-8-quinolinolate: Synthesis, Structures and Magnetic Properties**

Nurul F. Ghazali, Wasinee Phonsri, Keith S. Murray, Peter C. Junk, Glen B. Deacon, and David R. Turner

Eur. J. Inorg Chem. 2019, 2549-2557

**Abstract**

Two series of new complexes containing the 2-methyl-8-quinolinolate ($MQ^-$) ligand have been prepared at elevated temperatures. Lighter elements yield trinuclear complexes $[Ln_3(MQ)_9(HMQ)]\cdot 5H_2O\cdot 3MeOH$ (1Ln, where Ln = Pr, Eu, Gd, Tb, Dy and Ho) by solvothermal reaction and heavier lanthanoids yield the mononuclear complexes $[Ln(MQ)_3(HMQ)]\cdot HMQ\cdot MeOH$ (2Ln, where Ln = Dy, Ho, Er and Yb), with overlap between the two series found Abstract: Two series of new lanthanoid complexes containing 2-in the cases of Dy and Ho. Magnetic studies reveal that 1Tb, 1Dy and 2Er show distinct slow magnetic relaxation under external DC fields. The magnetic data for 1Gd yielded the *J* value for weak antiferromagnetic coupling and the magnetocaloric – $\Delta S_m$ value of 20 J $kg^{-1}$ $K^{-1}$ at 2 K and $\Delta H$ = 0 - 5 T.

**New homoleptic rare earth 3,5-diphenylpyrazolates and 3,5-di-*tert*-butylpyrazolates and a noteworthy structural discontinuity**

Nazli E. Rad, Peter C. Junk, Glen B. Deacon and Jun Wang

Z.Anorg Allg. Chem. 2019. 645, 887-891

**Abstract**

Direct thermally induced reactions between rare earth metals (Ln = Y,Ce, Dy, Ho and Er) activated by Hg metal and 3,5-diphenylpyrazole ($Ph_2pzH$) or 3,5-di-*tert*-butylpyrazole ($tBu_2pzH$) or yielded either homoleptic complexes $[Ln_n(R_2pz)_{3n}]$ or a heteroleptic complexe $[Ln(Ph_2pz)_3(Ph_2pzH)_2]$ From $Ph_2pzH$, $[Ce_3(Ph_2pz)_9]$, $[Dy_2(Ph_2pz)_6]$, $[Ho_2(Ph_2pz)_6]$, and $[Y(Ph_2pz)_3(Ph_2pzH)_2]$ were isolated. The first has a bowed trinuclear $Ce_3$ backbone with two $\eta^2$ pyrazolate ligands on the terminal metal atoms and one on the middle, and bridging by both $\mu$- $\eta^2$: $\eta^2$ and $\mu$- $\eta^2$: $\eta^5$ ligands between the terminal and the central Ce atoms. Although both the Dy and Ho complexes are dinuclear, the former has the rare $\mu$- $\eta^2$: $\eta^1$ bridging whilst the latter has $\mu$- $\eta^2$: $\eta^2$ bridging. Thus the dysprosium complex is 7-coordinate and the holmium is 8-coordinate, contrary to any correlation with $Ln^{3+}$ ionic radii, and the series has a remarkable structural discontinuity. The heteroleptic Y complex is eight coordinate with three chelating $Ph_2pz$ and two *transoid* unidentate $Ph_2pzH$ ligands. From $tBu_2pzH$, dimeric $[Ln_2(tBu_2pz)_4]$ (Ln = Ce, Er) were isolated and are isomorphous with eight coordinate Ln atoms ligated by two chelating terminal $tBu_2pz$ and two $\mu$- $\eta^2$: $\eta^2$ $tBu_2pz$ donor groups. They are also isomorphous with previously reported La, Nd, Yb and Lu complexes.

# Big Picture of Relativistic Molecular Quantum Mechanics

## by Wenjian Liu, Member EUAS

Short Biography

*Education Background:*

1. *Sept., 1992-July, 1995, Ph. D, Peking University, Beijing*
2. *Sept., 1989-July, 1992, M. Sc., Shandong University, Jinan*
3. *Sept., 1985-July, 1989, B. Sc., Shandong University, Jinan*

*Work Experience:*

1. *Dec., 2018-present, Shandong University, Chair Professor, inaugural director of Qingdao Institute for Theoretical and Computational Sciences*
2. *Dec., 2001-Dec., 2018, Cheung Kong Professor, Peking University*
3. *Jan., 1998-Dec., 2001, postdoc, Ruhr-Universität Bochum, Germany*
4. *Sept., 1995-Dec., 1997, postdoc, Max-Planck-Institut für Physik komplexer Systeme, Germany*

*Academic Distinctions:*

1. *Fellow of Royal Society of Chemistry (2019)*
2. *Member of EU Academy of Sciences (2019)*
3. *Fellow of Asia-Pacific Association of Theoretical and Computational Chemists (2017)*
4. *Fukui Medal of Asia-Pacific Association of Theoretical and Computational Chemists (2017)*
5. *Member of International Academy of Quantum Molecular Science (2014)*
6. *Bessel Award of the Humboldt Foundation (2007)*
7. *Annual Medal of International Academy of Quantum Molecular Science (2006)*
8. *Pople Medal of Asia-Pacific Association of Theoretical and Computational Chemists (2006)*
9. *Outstanding Young Scientist Award of National Natural Science Foundation (2006)*
10. *Cheung Kong Scholarship, State Education Ministry of China (2001)*
11. *QSCP (Quantum Systems in Chemistry and Physics) Promising Scientist Prize of CMOA (Centre de Mécanique Ondulatoire Appliquée), Europe, 2001*

*Academic Distinctions:*

1. *Member of board of directors of International Society of Theoretical Chemical Physics (2019.7-present)*
2. *Associate editor, Molecular Physics (Taylor & Francis; 2016.6-present)*
3. *Advisory editorial board member, Journal of Chemical Theory and Computation (ACS; 2015.1-present)*
4. *National representative of International Society of Theoretical Chemical Physics (2013.8-2019.7)*
5. *Advisory editorial board member, Molecular Physics (Taylor & Francis; 2013.1-2016.6)*
6. *Advisory editorial board member, International Journal of Quantum Chemistry (Wiley; 2013.1-present)*
7. *Editorial board member, Chemical Physics (Elsevier; 2010.7-present)*
8. *Editorial board member, Acta Physico-Chimica Sinica (2009.10-2015.6)*
9. *Editorial board member, Interdisciplinary Sciences: Computational Life Sciences (Springer; 2009.3-present)*
10. *Scientific board member, Asia-Pacific Association of Theoretical and Computational Chemists (2007.6-present)*
11. *Editorial board member, Journal of Theoretical and Computational Chemistry (World Scientific, Singapore; 2007.3-present)*

*Specializations*
*quantum electrodynamics, relativistic quantum chemistry, relativistic electronic structure theory, relativistic many-electron Hamiltonians, relativistic many-electron wave functions, relativistic time-dependent density functional theory, relativistic theories of magnetic properties, relativistic energy band theory, time-dependent density functional theory for nonadiabatic couplings between excited states, many-body theory for strongly correlated electrons, solvers for exterior/interior solutions of large eigenvalue problems*

**Scientific Achievements**

Dr. Liu has long been working in the field of relativistic quantum chemistry, focusing mainly on methodological developments and programming. His achievements include (1) a series of relativistic many-electron Hamiltonians (eQED, Q4C, X2C, spf-X2C+soc-DKHn/BSSn/X2Cn) for electronic structure calculations of heavy elements; (2) a body-fixed four-component relativistic molecular Hamiltonian for spectroscopies involving the nuclear degrees of freedom; (3) four-component and exact two-component relativistic theories of nuclear magnetic shieldings (4C/X2C-NMR) that capture naturally the diamagnetism missed in the standard relativistic linear response theory; (4) several variants of time-dependent density functional theory (4C/X2C-TD-DFT, spin-adapted open-shell TD-DFT, linear scaling TD-DFT, NAC-TD-DFT for nonadiabatic couplings between excited states); (5) a series of novel wave function-based correlation methods (SDSPT2, SDSCI, iCI, iCIPT2) for strongly correlated electrons; (6) an exact two-component relativistic energy band theory that provides absolute positions of energy bands; (7) a very efficient and robust solver for exterior or interior solutions of large eigenvalue problems; (8) the BDF program package for relativistic electronic structure calculations.

The mathematical structure of the many-electron Schrödinger equation (SEQ) has long been known, viz., the Schrödinger-Coulomb (SC) Hamiltonian is self-adjoint and bounded from below, while the wave function is continuous and satisfies the SEQ locally everywhere. As such, what one needs to do is just to design various Ansätze (methods) to model the wave function, so as to solve the SEQ as accurately and efficiently as possible. However, the situation changes dramatically when we come back to the real world where light travels at a constant, finite speed (ca.137 a.u. or 300,000 km/s). The central questions are:

What equation is to be solved? How to solve it?

More specifically, the following questions must be addressed properly:

1. What is the appropriate (most accurate) relativistic many-electron Hamiltonian?
2. Is the Hamiltonian self-adjoint? Does it have bound states? But, are these relevant? That is, even if the Hamiltonian is self-adjoint and does have bound states, can the resulting equation be solved in the same way as the SEQ?
3. When is the no-pair approximation safe? If so, is it possible to make no-pair four- and two-component relativistic theories completely equivalent?
4. How to fuse relativistic quantum chemistry (RQC) and quantum electrodynamics (QED), the as yet two mutually exclusive subfields for electronic structure, so as to establish a continuous and complete field of relativistic molecular quantum mechanics

(RMQM)?

5. How to derive a body-fixed relativistic molecular Hamiltonian for spectroscopies involving nuclear degrees of freedom?
6. How does the relativistic wave function behave at the coalescence of two electrons? How to do relativistic explicit correlation?
7. How to formulate relativistic properties that sample the electronic wave function in the vicinity of a nucleus?

These are the most general and fundamental issues concerning the three components (i.e., Hamiltonian H (Q1 to Q5), wave function Ψ (Q6), and energy/property E(λ) (Q7) of the relativistic quantum mechanical equation HΨ =EΨ. Due to shortage of space, we can only summarize the essentials here.

(1) Relativistic Hamiltonians

Quantum electrodynamics (QED) is undoubtedly the highest level of theory for electromagnetic interactions between charged particles (nuclei, electrons, positrons). However, full QED can nowadays be applied only to single ions of at most 5 electrons. To extend QED to many-electron atoms and molecules, in which correlation effects dominate over QED effects, we introduced an effective QED (eQED) approach[1-3] in a bottom-up fashion, i.e., without recourse to QED itself at all. For the same second order energy, eQED requires only three Goldstone diagrams but the standard formulation of QED has to take 28 Feynman diagrams. The former can readily go to higher orders whereas the latter suffers from too numerous diagrams. In short, eQED not only extends the applicability of QED from few- to many-electron systems, but also paves a seamless bridge between relativistic quantum chemistry and full QED[2-5]. Starting from eQED, various simplified no-pair relativistic Hamiltonians [quasi-4-component (Q4C)[4], exact two-component (X2C)[5-7], spin-separated X2C (sf-X2C+soc-DKHn/BSSn/X2Cn)[8,9], etc.] can be derived based solely on physical arguments. Together with other nonrelativistic and relativistic Hamiltonians, they form a complete and continuous "Hamiltonian Ladder"[10,11], from which one can pick up the right Hamiltonian according to the target physics and accuracy. In essence, relativistic Hamiltonians can only be formed in Fock space, whereas all first-quantized Hamiltonians suffer from the contamination of negative energy states[12], such that the corresponding QM equations cannot be solved in the same way as the SEQ. Instead, the no-pair approximation to first-quantized relativistic QM equations must be adopted from the outset. On the other hand, no-pair four- and two-component relativistic calculations can be and have been made completely equivalent in all aspects of simplicity, accuracy and efficiency[4]. For more thorough discussions see the comprehensive reviews[10,11,13,14].

(2) Relativistic Wave Functions

It has long been known that the exact wave function of the many-electron SEQ has cusps at the coalescence of two electrons, which cannot be modeled by orbital products (Slater determinants). As a direct consequence, electron correlation energies calculated by orbital-based methods converge extremely slowly with respect to the basis set size. The situation can only be improved by using explicitly correlated trial wave functions that depend explicitly on the interelectronic distances. Due to the interplay between relativity and correlation, electron correlation energies converge even slower in the relativistic regime. To resolve this issue, we analyzed in depth the structure of

relativistic wave functions by making full use of the internal symmetry of reduced two-electron relativistic Hamiltonians[15] and thereby established the general framework for relativistic explicitly correlated wave function methods[14,15].

(3) Relativistic Properties

Among others, nuclear magnetic shielding is a prototypical all-electron, relativistic property since it samples the electronic wave function in the vicinity of the nuclear position. Due to the fact that the Dirac operator is only linear with respect to magnetic fields, the standard four-component relativistic linear response theory of NMR shielding has only one term, the so-called paramagnetic term. That is, the familiar diamagnetic term known from nonrelativistic NMR theory[16] is `missing'. This is not only a conceptual problem but also a computational problem: The computation is extremely demanding due to the requirement of basis functions of high angular momenta. The way out of these conceptual and computational difficulties is to explicitly build in the magnetic balance (MB) condition between the small and large components of the Dirac bispinors. However, a successful formulation that captures naturally the `missing' diamagnetism and meanwhile is free of numerical instabilities has not been achieved until 2007[17]. Now it is clear that there exist many equivalent ways[18,19] to incorporate the MB condition, in conjunction with a proper treatment of the distributed gauge origins[20]. For more details, we refer the reader to the comprehensive reviews[14,21].

Albeit a physical observable, absolute NMR shieldings cannot be measured accurately. Instead, they are usually translated from the nuclear spin-rotation (NSR) coupling constants that can be determined accurately through hyperfine splittings of molecular rotational spectra. However, the mapping relationship[16] between NSR coupling constants and NMR shieldings holds only in the nonrelativistic limit. Therefore, the so-obtained "experimental NMR shielding" is nonrelativistic in nature. In other words, a fully relativistic experimental measurement is translated into a nonrelativistic value, which necessarily breaks down for heavy atoms (even for atoms like C to F bonded to light ligands, relativistic effects are already sizable, ca. 2–5 ppm). To establish a "relativistic mapping" between NSR and NMR, we have to (1) formulate a body-fixed relativistic molecular Hamiltonian for spectroscopies involving nuclear degrees of freedom, (2) formulate a rigorous theory of NSR coupling constants, and (3) find a connection between NSR coupling constants and NMR shieldings. All these have been achieved[22-24]. With this new relativistic mapping, that goes back to the nonrelativistic one in the limit of an infinite speed of light, new experimental shielding scales can be established[25].

It is believed that all the fundamentals pertinent to relativistic Hamiltonians, relativistic wave functions and relativistic properties have well been understood, such that the big picture of RMQM has been established. However, this does not imply that RMQM has come to an end. Rather, it implies that RMQM has entered a new era.

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# Functionalized Cellulose Nanocrystals for Advanced Material Applications

**by Qinglin Wu, Member EUAS**

Short Biography

***A. EDUCATION***

| | |
|---|---|
| *1993* | *Ph.D. in Wood Science & Engineering, Oregon State Univ, Corvallis, Oregon.* |
| *1989* | *Master Eng. Sci. in Mechanical Engineering, University of Tasmania, Australia.* |
| *1983* | *BS in Agricultural Engineering, Henan Agricultural University, PR China* |

***B. HONORS***

| | |
|---|---|
| *2019* | *Endowed Gordon D Cain Chair Professor, LSU College of Agriculture* |
| *2009* | *LSU AgCenter Rogers Research Excellence Award* |
| *2008* | *LSU Chapter Sigma Delta Gamma Honor Society Research Award* |
| *2008* | *Elected to be an International Academy of Wood Science (IAWS) Fellow* |
| *2007* | *Awarded JSPS Fellow, Shizuoka University, Shizuoka, Japan* |
| *2005* | *Forest Products Society Markwardt Wood Engineering Award, Madison, WI* |
| *2004* | *Endowed Professorship - Roy O Martin Sr. Professor, LSU AgCenter* |
| *1993* | *Wood Award, Forest Products Society Madison, WI* |

***C. POSITIONS HELD***

| | |
|---|---|
| *7/2009-present* | *Adjunct Professor, LSU Chemistry* |
| *7/2004-present* | *Professor, Renewable Natural Resources, LSU AgCenter* |
| *7/2000-6/2004* | *Associate Professor, Renewable Natural Resources, LSU AgCenter* |
| *1/1996-6/2000* | *Assistant Professor, Renewable Natural Resources, LSU AgCenter* |
| *7/1994-12/1995* | *Research Associate, Forestry, Michigan State Univ, East Lansing, MI* |
| *7/1993-6/1994* | *Research Associate, Forest Products, Oregon State Univ, Corvallis, OR* |
| *8/1989-6/1993* | *Research Assistant, Forest Products, Oregon State Univ, Corvallis, OR* |
| *1987-7/1989* | *Research Assistant, Mechanical Engineering, Univ of Tasmania, Australia* |

***D. SYNERGISTIC ACTIVITIES***

1. *Fellow, EU Academy of Science, International Academy of Wood Science (IAWS)*
2. *Served as Panel Member for NSF SBIR, NSF SIM, USDA 1890 teaching/extension/capacity building; USDA HSI; Chinese NSF, USDA SBIR, and CSREES NRI; and as proposal reviewer for USDA NRI/SBIR/NIFA, Canadian NSRP, Swiss NSF, Chinese NSF*
3. *Member of ISO, FPS, SWST, ACS, AWPA, and IRG;*
4. *Editorial Boards: Cellulose and Wood/Fiber Science; Editor for International Journal of Polymer Science, and reviewer for 20 journals including Science, Advanced Material, Biomacromolecules, Macromolecules, NanoScale, ACS AMI, Cellulose, ACS SCE*

## Introduction

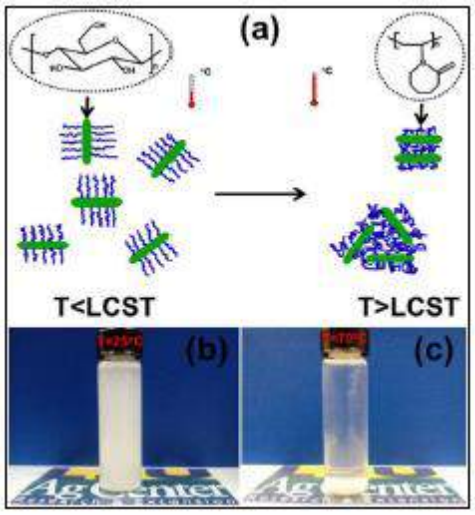
Cellulose is one of the most abundant sustainable biopolymers on the earth. Cellulose fibrils consist of disordered (amorphous) regions and highly ordered (crystalline) regions. In the crystalline regions, cellulose chains are closely packed together with high order (in both parallel and perpendicular to the direction of the fibril length), dictated by the intricate intra- and intermolecular hydrogen bonding; whereas in the amorphous regions, cellulose chains stacking is less ordered and are not as closely packed. Therefore, the amorphous regions are more vulnerable to both physical disintegration and chemical hydrolysis in comparison with crystalline regions, producing nanofibrillar domains broadly referred to as cellulose nanomaterials (CNMs). CNMs include both cellulose nanofibers (CNFs) and cellulose nanocrystals (CNCs). The following material summarizes our recent work in developing functionalized cellulose nanocrystals for their use in composites, gels and responsive materials.

## Thermoresponsive hydrogel from block copolymer poly(n-vinylcarprolactam) grated cellulose nanocrystals: synthesis, structure and liquid-to gel transition behavior.

Zhang, J; **Wu, Q**; Li, M; Song, K; Sun, X; Lee, S; Lei, T. 2017. ACS Sustainable Chemistry & Engineering 5, 7439-7447.

**Abstract:** A novel thermo-responsive copolymer poly(N-vinylcaprolactam) grafted cellulose nanocrystals (PVCL-g-CNCs) was synthesized by using surface-initiated atom transfer radical polymerization, and its temperature responsive behavior was studied in this work. The chemical structure characterization by Fourier transform infrared spectroscopy, solid-state CP/MAS 13C NMR spectroscopy and X-ray photoelectron spectroscopy confirmed the presence of covalently grafting PVCL chains on the CNC surface. The crystalline structure and nanorod-shaped morphology of CNCs were well preserved after polymerization. Transmission electron microscope results indicated that the surface of CNCs was covered with grafted PVCL brushes. The viscoelastic properties of PVCL-g-CNCs aqueous suspensions (1.0 wt%) by dynamic rheology measurements confirmed the thermally induced phase transition behavior. The work presented herein paves a way to design CNC-based advanced functional materials benefiting both from the intrinsic characteristics of CNCs and the new properties imparted by the temperature sensitive grafted polymer chains.

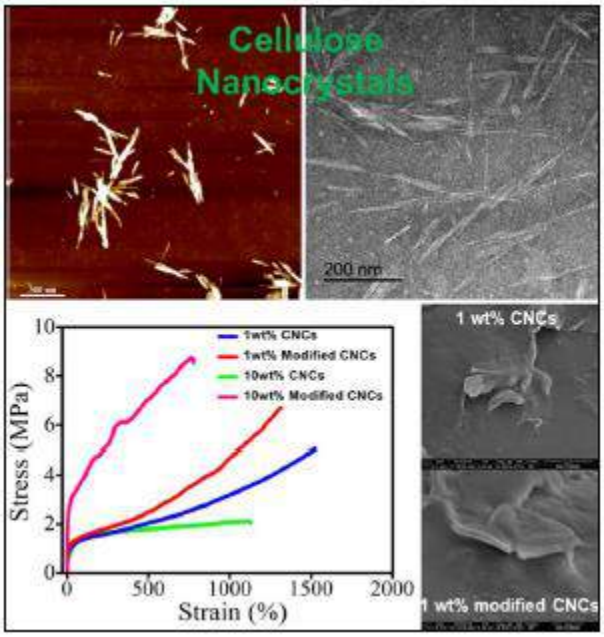
At temperature below the $T_{liquid\text{-}to\text{-}gel}$, the PVCL chains were extended due to their hydrophilic nature. Entropic repulsive interactions between particles made the aggregation or connection between particles unfavorable below the $T_{liquid\text{-}to\text{-}gel}$ of PVCL chains, resulting in liquid-like features. Therefore, they had low G′ and G″ as confirmed by the dynamic rheology measurement. Upon heating above the $T_{liquid\text{-}to\text{-}gel}$, PVCL chains collapsed into a thin hydrophobic layer on the surface of CNCs. The hydrophobic nature of the PVCL globules dominated the inter-particle attractions among CNC particles, and the absence of any electrostatic repulsion formed coagulation of PVCL-g-CNCs, resulting in gel-like features supported by the larger G′ and G″ in the dynamic rheology measurement.




**Surface Modified Cellulose Nanocrystals for Tailoring Interfacial Miscibility and Microphase Separation of Polymer Nanocomposites.**

Zhang J, M Li, X Zhang, X Zhang, S Ren, L Dong, S. Lee, H.N. Cheng, T Lei, and **Q Wu***. 2019. Cellulose 26 (7), 4301-4312.

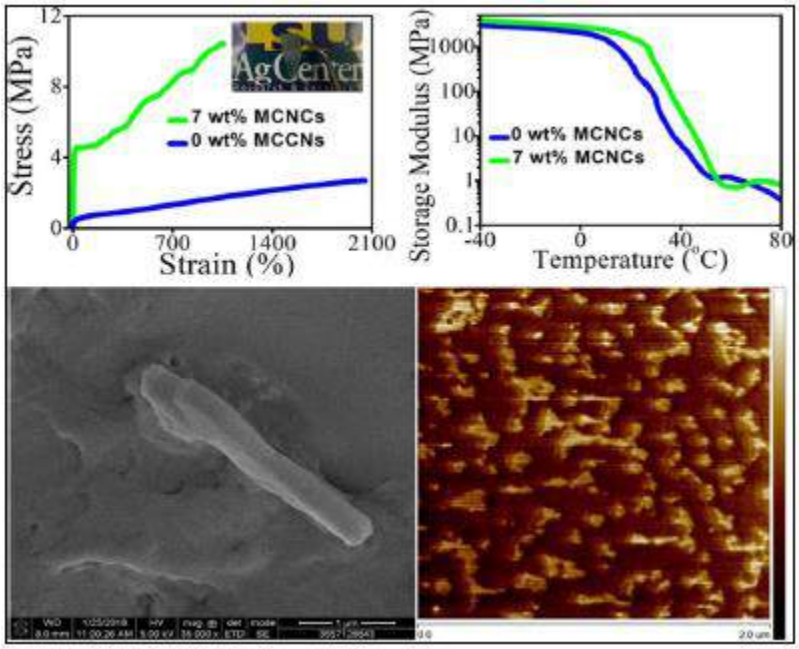
**Abstract:** High performance nanocomposites with a homogeneous dispersion of nanoparticle inclusion and phase separated morphology has received a great attention. Cellulose nanocrystals (CNCs) was first grafted with hydrophobic poly(methyl methacrylate)-PMMA chains to produce modified CNCs (PMCNCs) with an increased thermal stability and hydrophobic surface. Such surface tailored CNCs effectively influenced the phase morphology and consequently altered mechanical properties of the poly(butyl acrylate)-co-PMMA (PBA-co-PMMA) nanocomposites. Morphological analysis indicated a nanoscale phase separation behavior of PMCNCs/PBA-co-PMMA nanocomposites with PBA as the soft domain and PMMA as well as CNCs as hard domain. The nanocomposites with 10 wt% PMCNCs/PBA-co-PMMA had an increase in Young's modulus of more than 20-fold and in tensile strength at about 3 times compared to that of neat PBA-co-PMMA copolymer. Therefore, the PMCNCs played a crucial role for controlling their dispersion and tuning the phase morphology of composites. It is of primary importance for such micro-phase separation to delineate potential paths for nano scaled morphological control and to subsequently tune resultant composite properties.




**Cellulose Nanocrystal Driven Microphase Separated Nanocomposites: Enhanced Mechanical Performance and Nanostructured Morphology.**

Zhang J, X Zhang, M Li, J Dong, SY Lee, H.N. Cheng, T Lei, and Q Wu*. 2019. Inter J. Biomacromelcules. 130: 685-694.

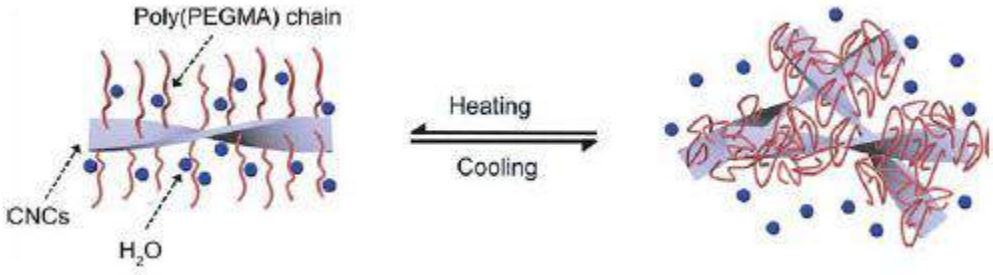
**Abstract:** The interest of modification of cellulose nanocrystals (CNCs) lies in its potential to homogenously disperse CNCs in hydrophobic polymer matrices and to promote interfacial adhesion. In this work, poly(methyl methacrylate) (PMMA) as well as poly(butyl acrylate) (PBA) was grafted with CNCs, imparting their hydrophobic traits. The successful grafting modification led to an increased thermal stability of modified CNCs (MCNCs), and hydrophobic surface modification was integrated with crystalline structure and morphology of CNCs. The nanocomposites with 7 wt% MCNCs/PBA-co-PMMA had an increase in Young's modulus of more than 25-fold and in tensile strength at about 3 times compared to these of neat PBA-co-PMMA copolymer. In addition, a micro-phase separated morphology (PBA- soft domains, and PMMA- as well as CNCs- hard domains) of MCNCs/PBA-co-PMMA nanocomposites was observed. The large increase in the storage moduli (glass transition temperatures) and organized morphology of MCNCs/PBA-co-PMMA nanocomposites also elucidated the relationship of mechanical properties and micro-phase separated morphology. Therefore, the modified MCNCs are effective reinforcing agents for the PBA-co-PMMA thermoplastic elastomers, opening up opportunities for their wide-spread applications in polymer composites.




**Thermoresponsive Poly(poly( Ethylene Glycol) Methylacrylate)s Grafted Cellulose Nanocrystals Through SI-ATRP Polymerization.**

Zhang, X., J. Zhang, L. Dong, S Ren, **Q. Wu**, T. Lei. 2017Cellulose 24(10), 4189-4203.

**Abstract:** A new kind of hybrid poly(PEGMA)s grafted CNCs with tunable thermoresponsive properties was demonstrated in this work. They were efficiently synthesized with well-defined structures by SI-ATRP polymerization of two comonomers, di(ethylene glycol) methyl ether methacrylate and oligo (ethylene glycol) methyl ether methacrylate. Poly(PEGMA)-g-CNCs retain typical rod-like nanostructures just as the native CNCs, but display enhanced dispersity in various solvents due to grafting of well-soluble OEG-based polymers. Furthermore, they exhibit characteristic thermoresponsive behavior in aqueous solution, and the LCSTs can be tuned in the range of 34–66 C by varying the feed ratios of comonomers. The dependence of LCSTs on comonomer ratios was revealed to follow a linear formula of first order, which gives a facile way to design LCSTs on-demand for real applications. AFM was first used to study the morphologies of thermally induced aggregations of poly(PEGMA)-g-CNCs in aqueous solution. It can be found that poly(PEGMA)-g-CNCs dispersed homogeneously as individual rod-like nanostructures at room temperature, but aggregated into large sphere nanoparticles composed of loose and dense packing of CNC nano-rods with diameters of 200–500 nm above LCSTs. This thermally induced aggregation was fully reversible, as the morphology returned to nano-rod form upon cooling. These PEGlyated CNC hybrids would open a new opportunity for the development of cellulose-based ‘‘smart’’ materials, such as switchable film filters, biosensors and smart surfaces.




At room temperature, hydrogen bonding is formed between the ether oxygen of PEG and hydrogen atoms of water, promoting the solubility of the polymer chains in water, which leads to the stable aqueous dispersion of CNC nano-rods. After the temperature is increased above the LCSTs, the hydrophilic-hydrophobic balance is broken due to the decrease of the number of hydrogen bonds, and the polymer–polymer interactions become more thermodynamically favorable compared to polymer-water interactions, leading to the dehydration and collapse of the poly(PEGMA) chains. The individual CNC nano-rods surrounded by hydrophobic shells are further assembled into large aggregates by dense packing due to hydrophobic interaction, which also decreases the transmittance of the suspension. After cooling the solution below the LCST, the dissolution of poly(PEGMA)s promotes CNCs to redisperse into the individual nano-rods again.

**Conclusions**

CNCs with surface functionalization have a distinct advantage for improving performance properties of nanocomposites and gels. The obviously effect of modified CNCs in these materials could help facilitate the potential applications of CNC-filled nanocompsite as advanced function materials.

# New Trends at the Institute of Nanotechnology (INT) of the Karlsruhe Institute of Technology (KIT)

## by Herbert Gleiter, Member EUAS

Short Biography

***Professional Career***

*Since 2015* ***Senior Fellow*** *(jointly with the Nobel and Fields Medal Laureates Haroche, Lehn and Small) of the Institute of Advanced Studies,* ***City University of Hong Kong.***

*Since 2012* ***Founding Director*** *of the* ***Herbert Gleiter Institute of Nanoscience*** *of* ***Nanjing University*** *of Science and Technology, Nanjing, P.R.China*

*Since 2006* ***Institute Professor*** *and* ***Distinguished Fellow*** *of the* ***Institute of Nanotechnology****, Karlsruhe Institute of Technology (KIT), Germany*

*2007 - 2010* ***Distinguished Professor, Arizona State University****, Phoenix, USA*

*2005* ***Distinguished Scholar*** *of the* ***Korean Research Foundation,*** *Seoul, Korea*

*2004 - 2007* ***Kuang-pui Chair Professor, Zhejiang University****, Hangzhou, PR China*

*1998 - 2004* ***Director*** *of the* ***Institute of Nanotechnology****, Research Center Karlsruhe, Germany*

*1998* ***Founding Director*** *(jointly with Profs. J M Lehn and D. Fenske) of the* ***Institute of Nanotechnology****, Research Center Karlsruhe, Germany*

*1994 - 1998* ***Member*** *of the* ***Executive Board*** *of the* ***Research Center Karlsruhe****, Germany*

*1987 - 1994* ***Founding Director*** *of the* ***Institute*** *of* ***New Materials****, Saarbruecken, Germany*

*1982* *Call to the* ***Federal Institute of Technology (ETH****) Zurich, Switzerland*

*1980* *Call to the* ***University of Hamburg****-Harburg, Germany*

*1973 -1994* ***Professor/Director*** *of the* ***Institute*** *of* ***Material Science****, University of the Saarland, Germany*

*1972* ***Professo****r, Institute of Materials Science,* ***University Bochum****, Germany*

*1971* ***Visiting Scientist*** *of the* ***Massachusetts Institute of Technology (MIT),*** *Cambridge, USA*

*1970* *D. Sc. (Habilitation)* ***in Material Science*** *at the University of Bochum, Germany*

*1966 - 1969* ***Research Fellow*** *at* ***Harvard University*** *Cambridge, USA*

*1966* *Ph.D. in* ***Physics*** *at the Technical University of Stuttgart, Germany*

*1959-1965* *Student of* ***Mechanical Engineering and Physics*** *at the Technical University of Stuttgart*

***Honours and Awards (selection)***

*2018* ***Jan Czochralski Medal and Award,*** *Polish Academy of Science, Warsaw University,*

*2016* ***Friendship Award*** *and* ***Medal of Merit*** *of Chinese Government, Jianzu, China*

*2015* ***Cothenius Medal*** *of the German National Academy of Sciences - Leopoldina*

*2015* ***Honorary Doctor*** *of the City University of Hong Kong*

*2014* ***2014 Distinguished Lecturer****, University of Hong Kong*

*2012* ***Zijin Chair Professor Award*** *of the Herbert Gleiter Institute of Nanoscience of the Nanjing University of Science and Technology, Nanjing, China*

*2012* ***Nanomaterials Award 2012***

*2012* ***Edward DeMille Campbell Award****, American Society for Metals (ASM)*

*2009* ***R.F. Mehl Award*** *of the Minerals, Metals, Materials Society, USA*

*2009* ***Blaise Pascal Medal*** *of the European Academy of Sciences, Belgium*

*2009* ***NANO Today Award*** *of the Agency for Science, Technology Research, Singapore*

*2008* ***Honorary Doctor*** *of the University of Muenster, Germany*

*2008* ***Honorary Doctor*** *of the Federal Institute of Technology (ETH) Zurich, Switzerland*

*2008* ***Achievement Award NANOSPD*** *Int. Steering Committee*

*2008* ***Staudinger-Durrer Award*** *of the Federal Institute of Technology (ETH) Zurich, Switzerland*

*2008* ***Honorary Member*** *of the German Materials Society DGM*

*2008* ***Von Hippel Award*** *of the Materials Research Society, USA*

*2007* ***Gold Medal*** *of Acta Materialia*

*2006* ***Humboldt Medal*** *of the Alexander von Humboldt Foundation, Germany*

*2005* ***Distinguished Scholar*** *of the Korean Research Foundation*
*2004* ***Honorary Professor*** *of Lanzhou University, PR China*
*2004* ***H. Lee Lecture Award*** *of Chinese Academy of Science*
*2004* ***Honorary Professor*** *at Zhejiang University, Hangzhou, PR China*
*2003* ***Nanomaterials Award*** *of the Deutsche Bank, Germany*
*2002* ***Honorary Doctor*** *of the Technical University of Darmstadt, Germany*
*2000* ***Van Horn Award*** *of Case Western University Cleveland, USA*
*1999* ***Werner Heisenberg Medal*** *of the Alexander von Humboldt Foundation, Germany*
*1998* ***Heyn Medal*** *of the German Society for Materials Science*
*1995* ***Gold Medal*** *of the Federation of European Material Societies (FEMS), Belgium*
*1993* ***Vinci of Excellence Award*** *of the Hennessy-Vuitton Foundation, France*
*1993* ***Max-Planck-Research Prize*** *of the Humboldt Foundation and the Max Planck-Society, Germany*
*1992* ***Member of the President's Council*** *of the University of Illinois, USA*
*1992* ***TMS Lecture Award*** *of the US Minerals, Metals and Materials Society*
*1991* ***Order of Merit*** *of Saarland, Germany*
*1988* ***Leibniz Prize*** *of the German National Science Foundation (DFG)*
*1984* ***Alcoa Prize*** *of the Alcoa Foundation, USA*
*1979* ***Karl-Schurz Award*** *of the University of Wisconsin, USA*
*1972* ***Masing Prize*** *of the German Society for Metals*

***Memberships in National Academies***

*1998 Member of the* ***German National Academy of Sciences*** *– Leopoldia, Germany,*
*2004 Member of the* ***US National Academy of Engineering***
*2004 Member of the* ***American Academy of Arts and Sciences***
*2006 Member of the* ***Indian National Academy of Engineering***
*2007-12* ***Vice President*** *of the* ***German National Academy*** *of Sciences*
*2009 Member of the* ***European Academy of Sciences***
*2009 Member of the* ***Indian Academy of Sciences***
*2011 Member of the* ***Indian Science Academy***
*2014 Member of the* ***Academia Europaea***
*2014 Member of the* ***European Academy of Sciences and Arts***
*2015 Member of the* ***EU Academy*** *of* ***Sciences***
*2016 Member of the* ***US National Academy of Inventors***

***Founding of a New Research Institute***

*Founding of the "****Herbert Gleiter Institute of Nanoscience****" in 2012 at Nanjing University of Science and Technology. This Institute is planned to have a size and a structure of a Max Planck Institute in Germany.*

Herbert Gleiter received in 1966 his Ph.D. in Physics at the University of Stuttgart. Between 1966 and 1971 he joined Harvard University, MIT and Bell Laboratories as a Post Doctoral Fellow or Visiting Scientist, cooperating with B. Chalmers, D. Turnbull, E. Orowan and A. Argon. In 1970 he was awarded a D.Sc. Degree by the University of Bochum and in 1971, he was appointed to the Chair Professorship in Materials Science at this University. In 1973 he was offered and accepted a position as a Professor and of the Director of the Institute of Materials Science of the University of Saarbuecken, Germany. In 1987 he became the Founding Director of the Institute of New Materials (INM) at the same University. This institute is today one of the most productive and successful research centers in the area of Material Science in Germany. In 1994 he accepted the position of the

President of the Research Center of Karlsruhe (FZK), Germany's largest National Laboratory. In this function, he founded the Synchrotron Facility (ANKA) of the FZK, expanded the neutrino research activities to a large international cooperation and founded - in 1998 - the Institute of Nanotechnology (INT) of the Research Center Karlsruhe. At present he is one of the Institute Professors of the INT. Since 2012 he is also the Director of the "Herbert Gleiter Institute of Nanoscience" at the Nanjing University of Science and Technology.

Professor Herbert Gleiter is considered today to be one of the scientists who initiated and pioneered nanotechnology. By the end of the 70's he and his research group opened the way to a new kind of materials, called today nano-crystalline materials. In fact, today more than 800 papers are published annually in this new area of Materials Science and about 6 to 8 international conferences on nano-materials are organized every year. The field nano-materials keeps expanding at a remarkable rate: In 2011 more than 80 000 publications in this field were retrieved by the Web of Science, and according to a recent study of the German Government, the annual value of the products based on nano-materials is beyond 2 billion US$ with a growth rate of about 15 to 20% per year.

In recent years, Herbert Gleiter expanded this field of Materials Science by developing nanostructured non-crystalline materials that are called today nano-glasses. It is the attractive perspective of these nano-glasses that they have the potential to open the way to a world of new technologies. These new technologies – based on nano-glasses – differ from today's technologies that are primarily based on crystalline materials such as metals, semiconductors or ceramics. The reason why nano-glasses permit the development of a new world of technologies is that their properties differ from the properties of the crystalline materials available today because nano-glasses can be produced with atomic structures and with chemical compositions that cannot be generated in the form of the crystalline materials or in the form of the glassy materials we have today. The new properties of nano-glasses result from their novel atomic structures and/or their novel chemical compositions. The utilization of these new properties permits the development of technologies that

could not be developed in the past by utilizing crystalline materials. In other words, nano-glasses may open the way into a “glass age. The new technologies of this “glass age” would be based on the new properties of nano-glasses, similar to the bronze or iron age that were based on the new properties of bronze or iron when they were discovered.

Very recently, Herbert Gleiter and his group have started to apply methods of nanotechnology to probe conceivable application limits of today’s Quantum Physics to systems of macroscopic size e.g. to viruses or to clusters consisting of many thousand atoms.

During his career he received more than forty prizes and awards among them are the Leibniz Prize, the Max Planck Prize, the Helmholtz Medal, the Cothenius Medal, which is the highest award of the German National Academy of Sciences, six Honorary Doctor Degrees and several Honorary Professorships. Since 1998 he is a member of the German National Academy of Science, Leopoldina. Between 2007 and 2015 he served as one of the Members of the Presidium of this Academy. In addition to this functions in the Leopoldina, he is an elected member of ten National Academies of Science and/or Engineering in Europe and world-wide e.g. of the American Academy of Arts and Sciences, the US National Academy of Engineering, the US National Academy of Inventors. the EU Academy of Sciences. the Indian National Academy of Sciences, the Indian National Academy of Engineering, the European Academy of Science and Arts and the Academia Europaea,

In 2012 he became the Founding Director of the Herbert Gleiter Institute of Nanoscience of Nanjing University of Science and Technology, Nanjing, China. Recently he has been asked by the Chinese Academy of Science (CAS) to set up a new research laboratory of the CAS at Sheyang , the Herbert Gleiter Research Laboratory (HGIL). This laboratory will be officially opened in 2021.

# Experiments on Continuous Unbonded Post-Tensioned Beams

## by Thomas Kang, Member EUAS

Short Biography

*Dr. Thomas Kang is a Professor of structural engineering in the Department of Architecture & Architectural Engineering and the Director for Engineering Education Innovation Center & GECE (Global Education Center for Engineers) at Seoul National University (SNU), Korea, and served as a part of the Vice-Deans' group of the College of Engineering at SNU. Before that, he was an Assistant Professor in the School of Civil Engineering and Environmental Science at the University of Oklahoma, Norman, OK, USA. He has held various affiliated positions in the U.S. and Japan, including Adjunct Professor at the University of Oklahoma, Adjunct Professor at the University of Illinois at Urbana-Champaign, and Lecturer at UCLA, the University of Hawaii at Manoa and the University of Tokyo. Prof. Kang received his PhD from UCLA, his MS from Michigan State University, and his BS from Seoul National University.*

*Prof. Kang is a Fellow of Post-Tensioning Institute (PTI) and a Fellow of American Concrete Institute (ACI). Prof. Kang received the Kenneth B. Bondy Award for Most Meritorious Technical Paper as Lead Author from PTI in 2012, and the Wason Medal for Most Meritorious Paper as Lead Author from ACI in 2009 with the subject of post-tensioned concrete. He regularly teaches the course of Post-Tensioned Concrete Structures at the University of Illinois at Urbana-Champaign every other summer (both on campus and online) and at the University of Hawaii at Manoa every fall (real-time online lectures). Prof. Kang is an Editor-in-Chief for three journals: International Journal of Concrete Structures and Materials, Journal of Structural Integrity and Maintenance, and Advances in Computational Design; and Associate Editor for PTI Journal of Post-Tensioning Institute. He is one of the founding and voting members of PTI DC-20 Committee, Building Design, and has been a voting member for ACI Committees 318L, Structural Concrete Building Code – International; 320, Post-Tensioned Concrete Building Code; and 369, Seismic Repair and Rehabilitation; and Joint ACI-ASCE Committees 335, Composite and Hybrid Structures, 352 Joints and Connections in Monolithic Concrete Structures, and Joint ACI-ASCE Committee 423, Prestressed Concrete; as well as Joint ACI-ASME Committee 359, Concrete Containments for Nuclear Reactors. Not to mention that he has contributed to various committees and societies in Korea.*

*Prof. Kang published more than 130 international journal papers (as of Dec. 2019), including over 40 in ACI Structural Journal and over 10 in PTI Journal, and more than 100 international conference proceedings. He has chaired numerous sessions/symposiums of structural engineering; delivered many plenary/keynote/invited speeches; and organized several international conferences/workshops as a Chair.*

*Additionally, Dr. Kang has done a lot of practices as a consulting engineer in Korea and the U.S. Prior to joining the academia, he had a working experience in California, USA (e.g., John A. Martin & Associates), and was a licensed Professor Engineer (PE) in California. He is currently working on the smart stressing system as a Consultant with EVEHX, a world-leading company in the area of post-tensioning headquartered in Brazil. Prof. Kang has also been working on the adoption of newer technologies such as artificial intelligence (AI) for the performance-based design in wind engineering, and holds a patent titled "Automatic Detection Method and System of Design Wind Speed based on Artificial Intelligence."*

**Abstracts of Selected Recent Papers and Patent**

**Experiments on Continuous Unbonded Post-Tensioned Beams with 2400 MPa Strands**

K. Kim and T. H.-K. Kang

ACI Structural Journal, V. 116, No. 5, Sept.-Oct. 2019

Experiments on seven two-span unbonded post-tensioned beams were conducted under four-point static loading conditions. Variables considered included: strand type (nominal tensile strength); tendon drape (height of tendon profile); and magnitude of prestress. Experimental emphasis was placed on the applicability of using higher-strength 2400 MPa strands instead of ordinary 1860 MPa strands in unbonded post-tensioned beam members. Observed results revealed that specimens with 2400 MPa tensile strength 15.2 mm diameter strands developed equivalent tendon stress increment, load-carrying capacity, and flexural ductility while at the ultimate limit state having earlier and wider plastic hinge.

**Comparative Study on Performance of Corrosion Protective Systems for post-Tensioned Concrete Members**

I.-S. Yoon, H. Shin, and T. H.-K. Kang

ACI Structural Journal, V. 116, No. 3, May-June 2019

Prestressing strands subjected to high tensile stresses are likely to become vulnerable to hydrogen embrittlement due to stress corrosion. Corrosion protection should be selected for safety and durability of the post-tensioned concrete structure. In this study, performances of corrosion protective systems used in post-tensioning construction were evaluated by the electrochemical and weight loss measurement methods. Test specimens represented the bonded strand and unbonded strand with plastic sheathing in grouted multi-strand tendons, as well as unbonded single-strand tendon and bare-strand. Corrosion tests were carried out in accordance with PTI M55.1-12 with slight modifications. Tests conducted included: corrosion by chloride ion (Cl–) solution and corrosion by chloride ion and dissolved oxygen (Cl– + DO) solution. Test results indicated that the specimens using plastic sheathing showed 0.03 to 0.07 $\mu A/cm^2$ average corrosion current densities, which can be regarded as insignificant corrosion condition in comparison with the average value of critical corrosion current densities of 0.15 or 0.17 $\mu A/cm^2$ for strand-corrosion testing due to only chloride ion or both chloride ion and dissolved oxygen. Therefore, the plastic sheathing had the best protective performance among the tested specimens; even significant sheath damage was considered during the installation process. The corrosion resistances of specimens protected by cement grout and grease coating, respectively, were similar to each other. This study is expected to contribute to the selection of effective corrosion protective systems for construction of post-tensioned concrete structures requiring high durability.

**System for Monitoring Tension Force of Tendon in Post-Tensioning**

T. H.-K. Kang and K. N. Jeong

United States Patent Application Publication, Dec. 2018

A system for monitoring tension forces of tendons disposed inside a concrete structure in post-tensioning includes a hydraulic jack coupled to one tendon at one end of the concrete structure to apply the tension force to the tendon by means of the forward movement of a piston; a hydraulic pump connected to the hydraulic jack by means of a hydraulic pressure supply pipe to supply a hydraulic pressure to the hydraulic jack; a digital elongation length measurement sensor disposed on the hydraulic jack to measure the elongation length of the piston; a measurement unit having a data logger adapted to receive and store the elongation length data measured by the digital elongation length measurement sensor and to send the elongation length data to a main server; a digital pressure measurement sensor disposed on the hydraulic pressure supply pipe of the hydraulic pump; and a control module adapted to receive the elongation length data from the data logger or the main server, calculate the tension force, compensate for the coefficient of elasticity of the tendon according to the ratio of the real-time elongation length data to the pressure data, and compensate for the tension force calculated.

**Modeling of Sliding Behavior of Unbonded Tendons in Post-Tensioned Concrete Members**

Y. Huang and T. H.-K. Kang

ACI Structural Journal, V. 115, No. 4, July-Aug. 2018

This paper discusses a nonlinear finite element formulation comprising contact and engineering elements in modeling post-tensioned concrete members. The study focuses on modeling of the sliding behavior observed in post-tensioned tendons. Detailed discussion is presented for the modified node-to-segment contact formulation, by which the bonding interface is discretized and physically modeled. Perfectly unbonded, partially bonded, and fully bonded conditions are considered by introducing frictionless and frictional contact. Post-tensioned tendons are modeled by the nonlinear truss element and are embedded into the nonlinear reinforced concrete beam element. The embedding element comprises elastic Euler beam element with very large stiffness. The nonlinear anchorage element and the prestressing procedure are also proposed to simplify and to properly model the complex jacking process. The proposed formulations were implemented in a nonlinear finite element code developed in MATLAB. Validation of the proposed formulations and implementations were carried out in several numerical studies. The proposed formulation performed with a reasonably good accuracy in reproducing global flexural behavior as well as predicting localized prestress loss and redistribution.

# Epigenetics Drug Discovery for Cancer

## by William Nelson, Member EUAS

Short Biography

*Dr. Nelson remains the Marion I. Knott Professor of Oncology and Director of the Sidney Kimmel Comprehensive Cancer Center at Johns Hopkins. He arrived at Johns Hopkins after completing undergraduate studies in Chemistry at Yale University, and earned Doctor of Philosophy (Pharmacology) and Doctor of Medicine degrees from the Johns Hopkins University School of Medicine, He subsequently undertook Internship and Residency training in Internal Medicine and Fellowship training in Medical Oncology at the Johns Hopkins Hospital. Dr. Nelson joined the Johns Hopkins faculty and rose through the ranks to Professor of Oncology, Medicine, Pharmacology, Pathology, Radiation Oncology, Urology, and Environmental Health Sciences.*

*Dr. Nelson's research has focused on cancer epigenetics and on prostate cancer development. He has now authored more than 280 journal article and book chapters, attracting >35,000 citations with an h-index of 98. He also has 11 issued patents from the US Patent and Trade Office. He currently serves on the Board and as Scientific Director of the V Foundation, as a Scientific Co-Chair for Stand Up 2 Cancer, and on the Scientific Advisory Board for the Prostate Cancer Foundation. He is also the Executive Editor of Cancer Today, a Senior Editor of Cancer Research, and on the Editorial Board of the Journal of Clinical Investigation.*

### Targeting Somatic Epigenome Defects in Cancer Cells as Cancer Treatment

Of all the somatic changes in genes and gene function that characterize human cancers, only the so-called 'epigenetic' alterations occur consistently (virtually all cases), arise early (first appearing in pre-neoplastic lesions), and are potentially reversible (the DNA sequence remains intact)[1]. The best studied such change, increased CpG dinucleotide methylation at CpG islands, leads to the transcriptional silencing of critical cancer genes, creating a heterochromatin state that can be passed through mitosis to daughter cells. The ubiquitin-like protein containing PHD and ring finger domains 1 (UHRF1) allows the coordinated reproduction of epigenetic 'marks' on DNA and chromatin proteins during genome replication [2]. CpG island hypermethylation prevents gene transcription by interfering with the binding and/or function of transcriptional *trans*-activators, by attracting histone

deacetylases (HDACs), or by recruiting $^{5\text{-me}}$CpG-binding domain (MBD) epigenetic "reader" proteins directing the formation of heterochromatin [3]. Accumulating evidence indicates that CpG island hypermethylation-associated gene silencing in human cancers is, as has long been suspected, functionally equivalent to somatic loss of function mutations/deletions [4]. Using genome-wide DNA methylation profiling tools for a study of life-threatening prostate cancer at autopsy, CpG island hypermethylation changes driving changes in gene expression were found to be consistently present in *all* metastatic cancer deposits, suggesting that these epigenome alterations were subject to selection during metastatic cancer dissemination [4].

CpG island hypermethylation triggers silencing of ~400 genes or more in most human cancers, though some cancers exhibit more extensive epigenome corruption as part of a 'CpG island methylator phenotype (CIMP)' [5-7]. $^{5\text{-me}}$CpG marks are established and maintained by DNA methyltransferases (DNMTs), which catalyze the transfer of a methyl group from *S*-adenosyl-methionine to cytosine bases in CpG islands, and removed by Ten Eleven Transformation (TET) enzymes, which catalyze the conversion of 5-methylcytosine to 5-hyrodroxymethylcytosine [8]. Provocatively, CpG island profiling of cancers with somatic gene defects affecting the maintenance of $^{5\text{-me}}$CpG marks has provided a plausible genetic basis for CIMP. Among the TET enzymes (TET1, TET2, and TET3), epigenetic silencing of *TET1* has been associated with CIMP in colorectal cancers and with non-Hodgkin lymphomas, and inactivating *TET2* mutations serve as drivers of clonal hematopoiesis, myelodysplasia, and leukemia [9-11]. TET enzymes function as α-ketoglutarate (αKG)-dependent dioxygenases [12]. By producing 2-hydroxyglutarate (2HG) to compete with αKG, mutant isocitrate dehydrogenases (IDHs) can effectively inhibit TET enzymes [13]. A variety of human cancers, including some brain tumors and leukemias, carry missense *IDH1* and *IDH2* mutations permitting 2HG production [14]. *IDH* and *TET2* mutations are mutually exclusive in acute myeloid leukemias (AMLs), consistent with enzyme function in the same pathway, and both somatic gene changes tend to drive CIMP in AML cells [14].

Early attempts to target epigenetic gene silencing attributable to somatic CpG island hypermethylation have only really gained a significant foothold in the treatment of myelodysplasia, a premalignant syndrome often associated with *TET2* mutations and CIMP, and in the treatment of AML [11,14]. The initial epigenetic treatment strategies have focused on DNMT inhibitors, such as azacitidine (Vidaza®) and decitabine (Dacogen®), given as single agents to reduce $^{5\text{-m}}$CpG density at CpG island sequences in dividing cancer cells [15,16]. Another approach, now in clinical development for treatment of AML, has been to target mutant TET enzymes directly [17-20]. The performance of single agent DNMT inhibitors for the more common solid organ cancers, even ones showing CIMP, has been abysmal [21].

Working with longtime collaborator Srinivasan Yegnasubramanian, M.D., Ph.D., we have been exploring two compelling new candidate epigenetic drug targets:

MBD2 and UHRF1. The MBD family protein MBD2, a 'reader' of the $^{5\text{-me}}$CpG mark in CpG island, acts to direct the assembly of repressive chromatin at sites of $^{5\text{-me}}$CpG serves hypermethylation [22]. MBD2 presents an attractive anti-cancer drug target, as siRNAs targeting MBD2 antagonize repression of epigenetically silenced genes in cancer cells, *Mbd2*$^{-/-}$ cells fail to repress reporter gene expression in transient transfection assays using $^{5\text{-me}}$CpG-containing promoter constructs, and *Mbd2*$^{-/-}$ mice, which are otherwise viable and healthy, show marked reductions in intestinal neoplasia when crossed to *Apc*$^{Min/+}$ mice [23-26]. UHRF1 contains a SET- and RING-associated (SRA) domain of UHRF1 that can bind hemimethylated DNA, directing the recruitment of DNMTs to copy the methylation patterns on daughter DNA strand during replication. Loss of UHRF1 function can lead to demethylation and re-expression of epigenetically silenced tumor suppressor genes and can reduce cancer cell growth and survival. We have built high-throughput screening (HTS) for agents interfering with both MBD2 and UHRF1 interactions with $^{5\text{-me}}$CpG-comtaining DNA, revealing promising inhibitors comprising 'toolbox' compounds and 'leads' for drug discovery [27,28]. One of the MBD2 inhibitors has already been successfully used in preclinical models of medulloblastoma [29].

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# Fatigue and Fracture Mechanisms of Metallic Materials

## by Zhe Feng Zhang, Member EUAS

Short Biography

***Education***

- *09/1995 – 07/1998, Institute of Metal Research, Chinese Academy of Sciences (IMR CAS), PhD in Engineering, Major in Material Science, Research Focus: Fatigue cracking mechanisms of Cu bicrystals.*
- *09/1992 – 07/1995, Xi'an Jiaotong University, Master in Engineering, Major in Material Science, Research Focus: Fatigue of metallic materials.*
- *09/1988 – 07/1992, Xi'an Jiaotong University, Bachelor in Engineering, Major in Material Science.*

***Work Experience***

- *07/1998 - 08/1999: IMR CAS, Shenyang, China, **Research Associate**;*
- *09/1999 - 12/2003: IMR CAS, Shenyang, China, **Associate professor**;*
- *09/2000 - 09/2001: Advanced Institute of Science and Technology (AIST), Sendai, Japan, **JSPS fellow**;*
- *10/2001 - 01/2003: IFW-Dresden, Germany, **Research Fellow** of Alexander von Humboldt Foundation;*
- *01/2003 - 12/2003: Max-Planck Institute for Metal Research, Stuttgart, Germany, **Visiting Scientist**;*
- *01/2004 - Present: IMR CAS, Shenyang, China, **Full Professor**;*
- *01/2005 - Present: Shenyang National Laboratory for Materials Science (SYNL), IMR CAS, Shenyang, China, **Head** of Materials Fatigue and Fracture Division;*
- *03/2006 - Present: IMR CAS, Shenyang, China, **Supervisor of PhD students**;*
- *04/2009 - Present: SYNL, IMR CAS, Shenyang, China, **Director** of Materials Failure Evaluation Center;*
- *05/2009 – 07/2012: IMR CAS, Shenyang, China, **Director Assistant**;*
- *07/2012 – 12/2018 : IMR CAS, Shenyang, China, **Deputy Director**.*
- *01/2019 – present : Dvision head of Laboratory of Fatigue and Fracture for Materials, IMR, CAS*

***Memberships***

- *06/2006 - Present: **Member**, Youth Committee, Chinese Materials Research Society;*
- *06/2006 - Present: **Secretary-General** and **Member**, Fatigue Division, Chinese Materials Research Society;*
- *11/2007 - Present: **Member**, Chinese Materials Research Society;*
- *12/2007 - Present: **Member**, "Hundred and Thousand of Talent Project" of Liaoning Province;*
- *08/2009 – Present: **Member**, the International Scientific Advisory Committee of ICSMA.*
- *01/2011 – Present: **Editorial Broad member**, International Journal of Fatigue.*
- *01/2012 – Present: **Editorial Broad member**, Materials Science Engineering A.*
- *01/2012 – Present: **Editorial Broad member**, Advanced Engineering Materials.*

***Research areas and publications:***

*Dr. Zhe Feng Zhang mainly studies the mechanical behaviors, fatigue and fracture mechanisms of metallic materials. He has published more than 480 papers in international SCI journals, including Nature Mater.,*

*Prog. Mater. Sci., Phys. Rev. Lett., Adv. Mater., Acta Biomater., Acta Mater. etc. His research has been cited more than 12000 times by SCI papers with H-index of 52.*

**Abstract**

The fatigue properties and fracture mechanisms of various metallic materials are significantly important for structural materials and components. Firstly, the evolution of dislocations in face-centered cubic metals (Cu, Al, Ag, Ni) and Cu-Al, Cu-Zn alloys were investigated during cyclic deformation. Some criteria were proposed to explain the formation mechanisms of persistent slip bands (PSBs), cells, labyrinth by considering a unified factor, which may further demonstrate the evolution of dislocations, stacking faults and deformation twinning. Secondly, the fatigue cracking mechanisms of various large-angle grain boundaries (GBs), including twin boundaries (TBs) were investigated under low-cycle fatigue. It is found that all the random large-angle GBs are preferential sites for the fatigue cracking; however, some TBs have higher resistance to fatigue cracking, which depends on the orientation difference and stacking fault energy (SFE) of the alloys. Thirdly, a low-cycle fatigue life prediction model was proposed by taking the hysteresis energy of metallic materials into account. Fourthly, the fatigue strength of metallic materials including Al alloys, Cu alloys, high-strength steels and Ti alloys were systematically investigated under high-cycle fatigue. A fatigue strength prediction model was proposed, and the fatigue strength displays an increasing trend then becomes decreasing with the increase of tensile strength. Finally, the asymmetry between strength and fracture angle of metallic glasses under tension and compressive loadings was observed and based on the large number of experimental results, an ellipse criterion was proposed which can unify the four classical criteria including the maximum normal stress criterion, Tresca criterion, Mohr-Coulomb criterion and von Mises criterion and apply it to exemplarily describe the tensile fracture behavior of BMGs as well as a variety of other materials.

## 1. Evolution Principle of Dislocations During Cyclic Deformation

This study systematically summarized the cyclic deformation behaviors of different kinds of face-centered cubic (fcc) single crystals, including Cu, Ni, Ag, Au, Al, as well as Cu-Al, Cu-Zn and Cu-Ni alloys in attempt to provide a historical perspective of the developments over the last several decades [1-4]. Combined with plenty of previous research results, the influencing factors of cyclic deformation behaviors can be listed as follows: temperature, frequency, orientations and stacking fault energy (SFE). Among them, the orientation and SFE are the core factors. Firstly, it is confirmed that at low strain amplitudes the effect of SFE on the cyclic deformation behavior of fcc single crystals is decisive. And then a new criterion is proposed to judge if regular saturation dislocation patterns could form or not in various fcc single crystals and the physical nature of the formation mechanism of ladder-like PSBs could be explained[3]. Secondly, with increasing strain amplitudes, the orientation gradually replaces SFE to become a new decisive factor affecting the cyclic deformation behavior of fcc single crystals because the formation of the complex dislocation patterns depends on the activating secondary slip system[4]. Finally, compared with the above two factors, temperature and frequency can be regarded as the extrinsic factors. As the testing temperature increases, the plateau of the cyclic stress-strain (CSS) curves gradually disappears and the saturation resolved shear stress decreases distinctly at low strain amplitudes. However, the increase in frequency does not affect the appearance of the plateau behavior, but the corresponding plateau stress slightly increases.

## 2. Fatigue Cracking Mechanisms of Grain Boundaries and Twin Boundaries

As one of model materials, single crystals have been widely investigated to reveal the fundamental fatigue damage mechanism and cyclic deformation features by taking the crystallographic orientations into account. However, there is still a big gap between single crystals and polycrystals. One of the most elements is different GBs or TBs, which often play a very important role in the properties of polycrystals and are possible to establish the connection between the well known features obtained in single crystals and the active polycrystalline materials.

On the one hand, it is found that for all the random large-angle GBs in copper bicrystals, fatigue cracks always prefer to nucleate at the GBs, rather than along PSBs [5,6]. The GB cracking is independent of the interaction angles between the GB plane and the stress axis. The intergranular fatigue cracking can be well explained by the PSB-GB damage (or piling-up of dislocations) mechanism. Therefore, the large-angle GBs play a weakening effect on the bicrystals or polycrystals during cyclic deformation although they often strengthen polycrystals under unaxial loading conditions. It is suggested that intergranular fatigue cracking strongly depends on the interactions of PSBs with GBs, rather than the GB structure itself. The nucleation of fatigue cracks along a PSB or a GB is a competitive process, depending on the movement processes of dislocations carried by PSB. The fatigue damage of the ductile f.c.c. crystals originates from the activation of dislocations carried by slip bands. When the dislocations can be freely transported to the surface by slip bands, the gradual surface toughness will become the origin of fatigue crack, in most case, resulting in PSB cracking. When dislocations carried by PSBs cannot transfer through a GB, they will pile-up at the GB; furthermore result in the intergranular fatigue cracking due to the accumulation of the residual dislocations.

On the other hand, TBs are key factors influencing the mechanical properties of crystalline materials. We have investigated the intrinsic fatigue cracking mechanisms of TBs during the past decade[7-9]. The effects of TB orientations on the fatigue cracking mechanisms were revealed via cyclic deformation of a series of grown Cu bicrystals with a sole TB. Furthermore, the combined effects of crystallographic orientation and stacking fault energy (SFE) on the fatigue cracking mechanisms were clarified through cyclic deformation of polycrystalline Cu and Cu alloys. Combining with the previous studies on the fatigue cracking behaviors of various types of GBs, i.e. HAGB and low-angle GB (LAGB), it can be concluded that LAGB is the strongest in resisting fatigue cracking but the weakest in strengthening materials, HAGB is the strongest in improving material strength but the weakest in resisting fatigue cracking. However, TB is the only boundary that can serve as effective strengthening phase and meanwhile inhibit fatigue cracking. To be specifically, the fatigue cracking behaviors of TBs are controllable and can be tuned through proper alloying tactics and texture adjustments. Therefore, an optimized combination of both strength and endurance may be achieved in materials by incorporation of TBs. This is beneficial to the interfacial design of high-performance materials with optimal mechanical properties.

## 3. Low-Cycle Fatigue Life Prediction Model of Metallic Materials

The extremely-low-cycle fatigue (ELCF) behaviors of pure Cu and Cu–Al alloys are comprehensively studied following the cyclic push–pull loading tests with extremely high strain amplitudes (up to ±9.5%). Compared with the common low-cycle fatigue (LCF) region, several unique features in the ELCF regime can be noticed, including the deviations of fatigue life from the Coffin–Manson law, the non-negligible proportion

occupied by the cyclic hardening stage of the whole fatigue life, special microstructures formed by cyclic loading containing deformation twins, shear bands and ultra-fine grains and the transformation of fatigue cracking modes. All these characteristics indicate the existence of special interior fatigue damage mechanisms of ELCF. To help discover the new damage mechanisms under ELCF, a model of fatigue life prediction with a hysteresis energy-based criterion is proposed [10]. Based on the analysis of the experimental and modeling results, two intrinsic factors determining the ELCF properties were concluded: the capacity of ELCF damage, and the defusing and dispersion ability of the external mechanical work. The former can be evaluated by a parameter of the model called the intrinsic fatigue toughness $W_0$, which is related to the microstructure evolution condition, the cyclic hardening ability, the deformation homogeneity and possibly the static toughness. The latter can be represented by the damage transition exponent $\beta$, which can be enhanced by improving the planarity, reversibility and uniformity of plastic deformation, reflecting the decline in the degree of surface damage and the dispersion of fatigue cracks. For Cu–Al alloys with increasing Al content, cooperation between an increasing damage capacity and a decreasing damage accumulation rate leads to a comprehensive improvement in the ELCF properties. Furthermore, the model had been applied to predict the high-temperature LCF lifetime and thermo-mech fatigue lifetime of metallic materials.

## 4. High-Cycle Fatigue Strength Prediction Model of Metallic Materials

For the anti-fatigue design of metallic materials, the exploration of the possible correlations between static and dynamic mechanical behaviors could be of great theoretical and practical significances. In this study, a brief Y-T-F model was proposed for the first time, which built up the relationship among the Yield strength, Tensile strength and Fatigue strength [10]. Different from common empirical relationship, the Y-T-F model is built based on the clear mechanism (the restriction between the overall and localized fatigue damage resistance), and successfully considered the influences of compositions, microstructures, defects and loading conditions via parameters (the *damage capacity C*, *damage weight coefficient* $\omega$ and *yield ratio*). Moreover, according to a large amount of experimental data, this model is verified to be applicable to various metallic materials (including steels, copper alloys, aluminum alloys and magnesium alloys), even no matter whether they obey the Wöhler's rule or not. Through this Y-T-F model, it would be promising to conduct the prediction and improvement of fatigue strength much more efficient, thus attribute to the anti-fatigue design of metallic materials.

## 5. Fracture Mechanisms and Strength Theory of Metallic Glasses

The compressive and tensile deformation, as well as the fracture behavior of a $Zr_{59}Cu_{20}Al_{10}Ni_8Ti_3$ bulk metallic glass were investigated. It was found that under compressive loading, the metallic glass displays some plasticity before fracture. The fracture is mainly localized on one major shear band and the compressive fracture angle $\theta_C$ between the stress axis and the fracture plane is always smaller than 45°. Under tensile loading, the material always displays brittle fracture without yielding, and the tensile fracture angle $\theta_T$ between the stress axis and the fracture plane is often higher than 45°. Therefore, both $\theta_C$ and $\theta_T$ deviate from the maximum shear stress plane (45°), indicating that the fracture behavior of the metallic glass under compressive and tensile load does not follow the von Mises criterion [12-14]. Furthermore, we find that the classical failure criteria,

i.e. maximum normal stress criterion, Tresca criterion, Mohr-Coulomb criterion and von Mises criterion, cannot satisfactorily explain the tensile fracture behavior of the bulk metallic glass (BMG) materials. For a better description, we propose an ellipse criterion as a new failure criterion to unify the four classical criteria above and apply it to exemplarily describe the tensile fracture behavior of BMGs as well as a variety of other materials [15]. It is suggested that each of the classical failure criteria can be unified by the present ellipse criterion depending on the difference of the ratio $\alpha=\tau_0/\sigma_0$. Based on the analysis of substantial experimental observations of fracture behaviors of metallic glasses and other high-strength materials, here we developed a new fracture criterion and proved it effective in predicting the critical fracture conditions under complex stress states[16]. The new criterion is not only a unified one which unifies the three classical failure criteria, i.e., the maximum normal stress criterion, the Tresca criterion and the Mohr-Coulomb criterion, but also a universal criterion which has the ability to describe the fracture mechanisms of a variety of different high-strength materials under various external loading conditions.

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12. Zhang, Z. F., Eckert, J., and Schultz, L., Difference in compressive and tensile fracture mechanisms of $Zr_{59}Cu_{20}Al_{10}Ni_8Ti_3$ bulk metallic glass, *Acta Mater.*, 51 (2003) 1167-1179.
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# Mechano - Electrochemical Effect of Pipeline Corrosion

## by Y. Frank Cheng, Member of EUAS

Short Biography

*Professor and Canada Research Chair in Pipeline Engineering, University of Calgary*
*An internationally recognized researcher in Oil/Gas Pipeline Corrosion and Integrity*
*Ph.D. in Materials Engineering at the University of Alberta in Canada*

***Professional Experiences***

| | |
|---|---|
| *2012 – present* | *Professor, Canada Research Chair in Pipeline Engineering University of Calgary, Canada* |
| *2009 – 2012* | *Associate Professor, Canada Research Chair in Pipeline Engineering University of Calgary, Canada* |
| *2005 – 2009* | *Assistant Professor, Canada Research Chair in Pipeline Engineering University of Calgary, Canada* |
| *2002 – 2005* | *Research Scientist, Centre for Nuclear Energy Research, University of New Brunswick, Canada* |
| *2000 – 2002* | *Postdoctoral Industrial Research Fellow, Natural Science and Engineering Research Council of Canada* |

***Prestigious Awards***

*2019 Distinguished Materials Scientist Award, Canadian Metallurgy and Materials Society*
*2018 Member of EU Academy of Sciences (EUAS)*
*2018 Changjiang Scholar Professor, Ministry of Education, China*
*2018 Engineering Research Achievement Award, University of Calgary, Canada*
*2017 Metal Chemistry Award, Canadian Metallurgy and Materials Society*
*2017 Engineering Research Achievement Award, University of Calgary, Canada*
*2017 Supervision Excellence Award, China Scholarship Council (CSC)*
*2016 Fellow, NACE International, the Corrosion Society, U.S.A.*
*2015 Shi Chang-Xu Award, Chinese Society for Corrosion and Protection*
*2014 Herbert H. Uhlig Award, NACE International, the Corrosion Society*

***Publications***

*Over 220 papers in peer-reviewed journals, including 1 commentary article published in Nature. The total citations exceed 8,500, with the H-index of 59.*

Pipelines have been the most effective, safest and more economic means for transportation of oil, natural gas and petrochemical products over a long distance from the production sites to processing plants and consumers. Pipelines have attracted public's keen attentions in recent years due to some widely reported leaking and ruptures incidents, causing huge energy loss, serious environmental impact, and even death. With

continuously increasing energy demands, pipelines activities have been booming in most territories in the world, contributing to significant economic development. At the same time, pipelines are being criticized as one of the key contributors the increased greenhouse gas emission and adverse climate change, and thus facing intense resistance in countries such as Canada.

To balance the industry and economy development with the reduced environmental footprint, the maintenance of integrity and safety of the pipeline system is critical to its sustainability.

Corrosion has been identified as one of the major mechanisms causing pipeline failures. At the same time, buried pipelines are under a complex stressing condition, where the internal pressure results in hoop stress and the soil movement can generate longitudinal stress or strain on the steel pipeline. Thus, pipeline corrosion progresses under the synergism of mechanical and electrochemical factors, resulting in the mechano-electrochemical effect of pipeline corrosion.

**Pipeline Corrosion under Elastic Stress**.

According to stress-based design, the pipeline must operate at a safe stressing level, which is below the specified minimum yield stress (SMYS), by a safety factor. As a result, the maximum allowable operating pressure (MAOP) can be calculated for the pipeline during it design life. It is thus seen that, when a pipeline operates at a pressure that is below or at the MAOP, the pipeline steel is under an elastic stress condition.

In elastic stress region, the change of the potential, $\Delta\varphi^0_e$, of a steel by the applied stress is calculated by:

$$\Delta\varphi_e^0 = -\frac{\Delta P V_m}{zF} \quad (1)$$

where $\Delta P$ is the excess pressure (Pa), $V_m$ is the molar volume of the steel ($m^3$/mol), $z$ is the charge number, and $F$ is Faraday's constant (96,485 C/mol). Therefore, an external stress ($\Delta P > 0$) would cause a decreased potential of the steel, and thus, an enhanced electrochemical corrosion activity. When a uniaxial stress ($\sigma$) is applied on the steel, and $\Delta P$, as the hydrostatic pressure, equals to 1/3 of the applied stress. Take the relevant parameters for an X100 pipeline steel and the maximum uniaxial stress of 600 MPa into Eq. (1), it is calculated that the theoretical change of the equilibrium potential is $\Delta\varphi_0$=7.4 mV. Fig. 1 shows the potential of X100 steel in a diluted bicarbonate solution under stress from 0 to tensile-600 MPa or compressive-600 MPa, which is applied at the 300$^{th}$ s. The potential jumps upon the application of the tensile stress, and then recovers gradually to its initial value. There is no apparent change of the potential when the compressive stress is applied. Moreover, the measured steady-state potential in Fig. 1 is a compromise potential of both anodic and cathodic reactions. The potential change can be less than the theoretical value of 7.4 mV.

With several millivolts of potential difference between a stress-free and the stressed steels, the corrosion activity of the latter would be slightly higher than the former. The minor difference may be offset the corrosion products covering the steel specimen. As a result, the effect of elastic stress on the steel corrosion is usually not obvious, and even undetectable, as shown in Fig. 2, where electrochemical Nyquist diagrams are measured on the steel specimen which is at 0, tensile 600 MPa and compressive 600 MPa, respectively, in the bicarbonate solution. The measured curves copy each other.

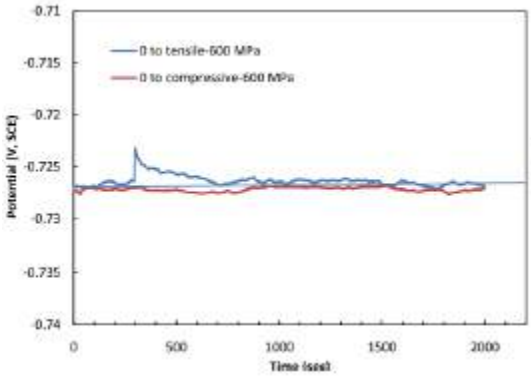


**Fig. 1.** Potential of X100 steel in a bicarbonate solution under stress from 0 to tensile-600 MPa or compressive-600 MPa.

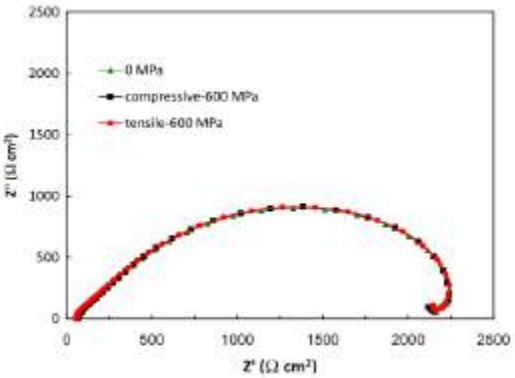


**Fig. 2.** Nyquist diagrams of the steel at 0, tensile 600 MPa and compressive 600 MPa in the bicarbonate solution.

**Pipeline Corrosion under Plastic Strain.**

In addition to the hoop stress, large longitudinal strain can result rom ground movement when a pipeline is in service due to seismic activity, slope instability, frost heave, thaw settlement or mine subsidence. During plastic deformation, the density of mobile dislocations increases remarkably. The dislocation density, $\Delta N$, is calculated:

$$\Delta N = N_0\left[\exp\left(\frac{n\Delta\tau}{\alpha k N_{\max} T}\right)-1\right] \quad (2)$$

where $N_0$ is the initial density of dislocations prior to plastic deformation, $\Delta\tau$ is the hardening intensity, $n$ is the number of dislocations in a dislocation pile-up, $\alpha$ is coefficient ($10^9$-$10^{11}$ cm$^{-2}$), $k$ is Boltzmann constant, $N_{\max}$ is the maximum dislocation density, and $T$ is temperature. The plastic strain at the hardening stage can be expressed by:

$$\varepsilon_p = \frac{N_0}{\alpha\nu}\left[\exp\left(\frac{n\Delta\tau}{\alpha k N_{\max} T}\right)-1\right] \quad (3)$$

where $\upsilon$ is the orientation-dependent factor, equalling to 0.4-0.5 for tensile deformation. The change of the potential, $\Delta\varphi^0_p$, in plastic deformation is:

$$\Delta\varphi_p^0 = -\frac{n\Delta\tau R}{\alpha k N_{\max} zF} \quad (4)$$

where $R$ is the gas constant 8.314 (J/K mol). Substitute Eq. (3) into Eq. (4) to eliminate parameters $n$, $\Delta\tau$, $k$ and $N_{\max}$, the shift of the potential as a function of plastic strain, $\varepsilon_p$, is established:

$$\Delta\varphi_p^0 = -\frac{TR}{zF}\ln\left(\frac{\upsilon\alpha}{N_0}\varepsilon_p + 1\right) \quad (5)$$

To calculate of the theoretical potential shift by Eq. (5), it is assumed that $T$ = 295 K, $z$ = 2 for steels, $\upsilon$ = 0.45, and $\alpha$ = 1.67×10$^{11}$ /cm$^2$. The theoretical calculation of the electrochemical corrosion potential shift is shown in Fig. 3. It is apparent that the shift of the potential increases negatively with plastic strain, indicating an enhanced electrochemical activity of the steel. The calculated result is well consistent with the measurement results in Fig. 4.

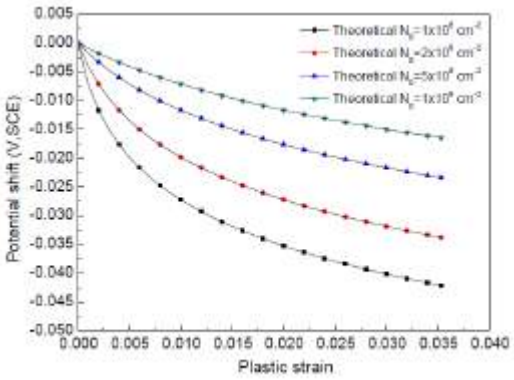


**Fig. 3.** Theoretical calculation of the potential shift as a function of plastic strain.

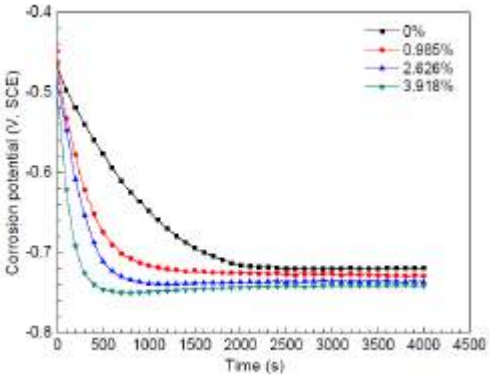


**Fig. 4.** Time dependence of potential of the steel under various pre-strains.

## Pipeline Corrosion under Mechano-Electrochemical Interaction.

With consideration of the synergism of mechanical and electrochemical factors on pipeline corrosion, a finite element-based multi-physics filed coupling model was developed to simulate and predict the effect of stress/strain on electrochemical corrosion of the steel. Figs. 5 and 6 show the dependences of electrochemical potential and anodic/cathodic current densities on the mechanical stress applied on the steel in a bicarbonate solution, respectively. Clearly, the modelling results are well consistent with the experimental data, indicating the validity and reliability of the model in prediction of pipeline corrosion. As the increase in mechanical stress, the potential of the steel shifts negatively, indicating the increasing corrosion activity. In the elastic deformation region, with the increase of von Mises stress, the absolute values of both anodic and cathodic current densities increase slightly. When the stress exceeds the yield strength of the steel, i.e., plastic deformation starts, both anodic and cathodic current densities increase significantly. The knee points of both curves are consistent with the yielding point of the steel. The results show that, while the elastic deformation affects the steel corrosion slightly, sometimes, at an undetectable level, the plastic deformation would increase corrosion of the steel remarkably. This is of great importance for pipelines operating in the geologically instable regions.

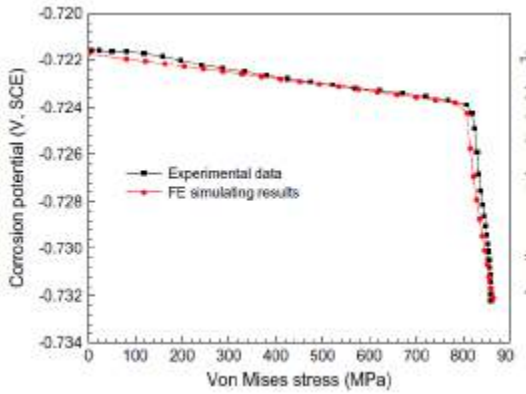


**Fig. 5.** Comparison of the experimental and modelling corrosion potential of the steel as a function of von Mises stress.

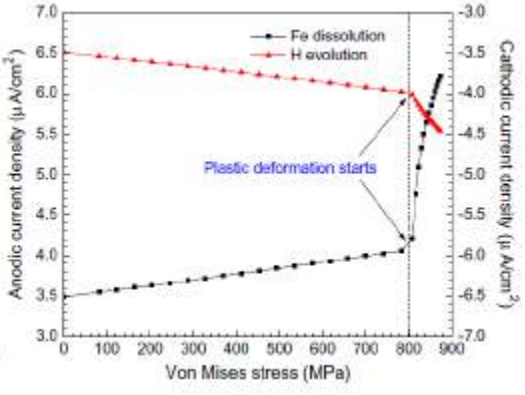


**Fig. 6.** Anodic and cathodic current densities of the steel as a function of von Mises stress.

# Optoelectronic Materials and Applications

## by Henry Radamson, Member EUAS

Short Biography

*Henry H. Radamson is manager of Optoelectronics Innovation Center in Chinese Academy of Sciences. In 2016, he became full professor in Chinese Academy of Science in Beijing. In 2018, he received 1000-talent foreign expert in China. His research field is nanomaterials, nanophotonics and nanosensors.*

*He received Ph.D. degree in semiconductor materials from Linköping University in Sweden in 1996. He joined KTH Royal Institute of Technology in Stockholm in 1997 as senior scientist.*

*Henry Radamson has contributed to various national and European projects in total of ~15M EURO. He has been project coordinator of national projects in photonics and electronics as well as four Semiconductor Research Corporation (SRC) with Texas Instruments (2005-2014).*

*Henry Radamson is the author or co-author of more than 230 publications in reviewed journals and conference proceedings and eight book-chapters. He is co-author of books "Monolithic Nanoscale Photonics-Electronics Integration in Silicon and Other Group IV Elements, Elsevier 2014 and CMOS, Past, Present, and Future, Elsevier in 2018.*

*Henry Radamson is a member of delegates in European Material Research Society (EMRS) where has also organized several symposiums*

*Henry Radamson is Editorial Board of Journal of Materials in Electronics, Springer-Nature and he has been Guest Editor in several conference proceedings.*

**Research Activity**

**I. Infrared Detectors:** Silicon-based photonics has been developing rapidly with the increasing demand for information capacity and transmission rate. Because of its compatibility with CMOS technology, high photon transmission rate and strong anti-interference, silicon photonics has brought great hopes for the new direction of Moore's Law. Therefore, silicon photonics technology has been a focus of attention in recent years. Ge has high absorption coefficient and high carrier mobility in the near-infrared region (NIR), making it widely used in silicon-based photonics integration. In order to achieve high-quality Ge or GeSi PDs with low dark current and high responsivity, a series of research activities have been presented in this field employing different methods.

The research presents the impact of epitaxial quality, contact resistance and profile of Ge PIN photodetectors (PDs) on dark current and responsivity. The PD structures were

processed with either selectively grown Ge with integrated waveguides on SOI wafer or globally grown Ge on the entire wafer. The contact resistance was lowered by introducing NiGe layer prior to the metallization. The n-type doped Ge PIN structure was formed by ion implantation and the contact resistivity was estimated to $2.6\times10^{-4}$ Ω•$cm^2$. This value is rather high and it is believed to be due to fomation of defects during implantation.

The results show a minor difference in dark currents for selectively and globally grown PDs but in both types, it depends on detector area and the epitaxial quality of Ge. For example, the threading dislocation density (TDD) in non-selectively grown PDs with thickness of 1 micrometer was estimated to be $10^6$ $cm^{-2}$ yielding relatively low dark currents while it dramatically changes for PDs with thinner Ge layers where TDD increases to $10^8$ $cm^{-2}$ and the dark current levels increase almost by 1.5 magnitude. Surprisingly, for selectively grown PDs with Ge thickness of 500 nm, TDD was still low resulting in low dark currents.

The dark current densities at -1V bias of non-selectively and selectively grown PDs with optimized profile measured to be 5mA/$cm^2$ and 47mA/$cm^2$, respectively, while the responsivity of these detectors were 0.17A/W and 0.46A/W at λ~1.55μm, respectively.

**II. Full Photonic Integration**: The research presents a full integrated hybrid consisting laser, detector, modulator, and high mobility transistor with nitride (or Si) waveguide integrated inside GOI (photonic-electronic circuit or PEC) operating 2-3 μm. The nitride waveguide provides low energy loss in this PEC. Strain modulation technique may provide high possibility to demonstrate GeSn laser operating at room temperature since the strain is modulated mechanically and not by mismatch in Ge/GeSn heterostructure in meta-stable region. The research provides the opportunity for monolithic integration of photonics and electronics in near future.

**Material Growth Activity**

**I. GeSnSiC growth:** GeSn materials have attracted attention in recent photonic and electronic research due to its properties of indirect-to-direct transition as well high carrier mobility in CMOS. Both MBE and CVD techniques have applied to grow GeSn materials. The fundamental issue for the growth is the large mismatch of almost 15% between Sn and Ge which leads to large segregation of Sn during the growth. One way to tackle this problem is the growth at low temperatures (<300 °C) to impede the Sn segregation. Meanwhile at low temperatures the growth rate is low and practically to deposit detector or laser structures containing many multilayers is practically difficult.

This research presents the growth of GeSn material with Sn content >18% using SnCl4, and Ge2H6 as precursors in RPCVD. The content of Sn has been estimated by HRXRD and RBS tools. The main focus of this study is to demonstrate photoluminescence at room temperature. In our process the growth rate is relatively high excellent the epitaxial quality.

**II. III-V material growth on Si:**: The monolithic hetero-integration of III/V materials on Si substrates could enable a multitude of new Optical device applications and functionalities which would benefit from both the excellent optoelectronic properties of III/V compound materials and the well-established and highly mature Si manufacturing technologies. Obtaining high-quality III-V epitaxial layer of semiconductor materials on Si substrate directly determines the performance of semiconductor optoelectronic devices. Due to the lattice mismatch between most III/V compound semiconductors and Si substrates, monolithic growth inevitably leads to the formation of strain releasing defects

which degrade the final device performance and reliability. This research activity performs the growth of GaAs, InGaP and InP on Ge buffer layer (with special treatment) on 8-inch Si wafers. The high epitaxial quality of III V material with outstanding photoluminescence inaugurates the possibility to use such advanced substrates for the laser and detector structure for industrial application in near future.

**III. Selective epitaxy of SiGe:** Approaching the end of technology roadmap, it becomes more difficult to apply the traditional processes and structures in down-scaling CMOS transistors. In fact, the down-scaling action inherits an increase of power density and off-leakage current, together with carrier mobility degradation. Then, due to these problems, various technical solutions have to be implemented to improve transistor performance. One of the most important technical solutions is using strain technology to compensate the mobility degradation due to the scaling-down of transistor dimensions.

The FinFETs' structure is specially designed by parameters such as the height and width of the fin, doping level and geometry of sidewalls. The last parameter is controlled by an anisotropic over-etch when trapezoid or triangular fins are processed.

In FinFETs process, the epitaxy of SiGe on Si-fins is a very sensitive task since the layer quality may degrade due to any undesired residual species (for example after the etch step) or native oxide. In this case, the ex- and in-situ cleaning are important steps prior to the epitaxy.

One of the concerns about SEG of SiGe is that the profile of the grown layer depends on the variation of chip layout (shape, size and density of the openings). This layout dependency stems from lateral diffusion of gas molecules above the wafer and species on the oxide surface. Several methods have been proposed to improve uniformity of SiGe growth but none of these could effectively eliminate the layout dependency of the SEG. In this research, the integration of selective epitaxy of SiGe films with high Ge content for 10 nm node FinFETs is performed. Moreover, a kinetic model is presented to predict the SiGe profile on Si-fins with sharp triangular shape. The model considers the gas kinetics and diffusion of the formed/dissociated molecules on the Si-fins for a certain layout.

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8. Physically Based Evaluation of Effect of Buried Oxide on Surface Roughness Scattering Limited Hole Mobility in Ultrathin GeOI MOSFETs, X. Wang, …., and H. H. Radamson,***IEEE Transactions on Electron Devices***, 64, 2611-2616 (2017).

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# Bata Quay Wall Design and Ground Characterization

## by Pedro Pinto, Member EUAS

Short Biography

● *Licenciated in Civil Engineer (6 years course,1965-1971)(with honors);*
*- Industry from 1971 to 1975;*
*- Master of Engineering 1975 – 1977 (with high honors);*
*- Specialist in Geotechnique (Ph.D Degree) 1979 - 1983 (with high honors);*
*- Director of Research (Full Professor degree) (with high honors), since 1992.*
● *Related with ISSMGE (International Society for Soil Mechanics and Geotechnical Engineering)*
*- Appointed Board member (2017-2021)*
*- Immediate Past President (2009-2013)*
*- President (2005-2009),*
*- Vice President for Europe (2001-2005),*
*- Chairman of TC4 "Earthquake Geotechnical Engineer Committee" (1994-2000).*
● *Full Professor of Geotechnical Engineering of University of Coimbra*
*- World Bank Consulting for Dams Safety (2013-2015),*
*- Invited Professor of Master Courses "Soil Mechanics" and "Engineering Geology" of New University of Lisbon (1983-1995),*
*- United Nations Consulting for Design and Instrumentation for Dams (1988-1992).*
*- Invited Guest Lecturer of University of California, USA (1992-1994).*
*- President of Portuguese Society for Geotechnique (1996- 2000).*
● *Pedro Sêco e Pinto is a Consulting Engineer and has participated in more than 450 major projects in Dams, Power plants, Bridges, Tunnels, Landslides and Quay Walls, in Portugal, Angola, Argelie, Brazil, Cabo Verde, China, Dominican Republic, Ecuador, Guine- Bissau, Guine Ecuatorial, India, Lebanon, Malawi, Morocco, Mozambique, Senegal, Syria, Tunisie, Uganda, Venezuela and Zambia, covering field and laboratory testing, dynamic analyses, earthquake engineering, numerical analyses, ground improvement, slopes, special foundations, instrumentation and safety evaluation.*
● *He has presented more than 350 State-of-the Art Lectures and Special Lectures in 80 countries of the 5 Continents.*
● *Pedro Sêco e Pinto has organized, under the umbrella of the International Society for Soil Mechanics and Geotechnical Engineering (ISSMGE), more than 50 International Seminars, since 2006, in Africa (Ghana, Mozambique, Nigeria, South Africa, Sudan), in Asia (Bangladesh, Cambodia, China, India, Indonesia, Kazakhistan, Laos, Malasya, Mynamar, Nepal, Pakistan, South Korya, Sri Lanka, Vietnam), in Australasia (Australia and New Zealand) in Europe (Albania, Belarus, Croatia, Germany, Hungary, Lithuania, Slovenia, Ukranie), North America (Mexico), South America (Argentine, Bolivia, Dominican Republic, Haiti, Ecuador, Panama, Paraguai, Peru, Venezuela).*
● *Pedro Sêco e Pinto has received more than 50 international Awards including American Biographical Institute USA, "Special Volume for the Contributors of Earthquake Engineering, Nagadi Lecture by Indian Geotechnical Society, Széchy Lecture by Hungarian S M Society and Hungarian Academy of Sciences, Nonveiller Lecture by Croatia Geotechnical Society, Sukle Lecture by Slovenia Soil Mechanics Society, Chin Lecture by Huanzhou University (China), Qian Jia Huan Lecture by Hohai University (China) and Chin Fung Kee Memorial Lecture*

*by Institute of Engineers of Malasia, 3rd Victor de Mello Lecture by Indian Geotechnical Society and 3rd Braja Das Lecture, GeoMeast 2019, International Congress and Exhibition, Cairo, Egypt.*
*● Related his role with Editorial Boards and Reviewer he acted as:*
*- Associate Editor of International Journal of Earthquake Engineering (since 2017)*
*- Editor in Chief of International Journal of Case Histories (2011-2017)*
*- Co-Editor of Geotechnical and Geological Engineering Journal, Springer Publisher (2005-2011)*
*- Member of Editorial Board of several Journals, namely: "Geotecnia", "Bulletin of Earthquake Engineering", "Acta de Geotecnia", "International Journal of Geotechnical Engineering".*
*- Editor of Proceedings of 4 International Conferences.*
*● Pedro Sêco e Pinto is author or co-author of 500 Technical and Scientific Reports, more than 180 papers for National and International Conferences and Journals and has contributed for 10 books.*

## International Activities in 2019

### International Seminar in Lithuania, 11-12 April 2019

### Bata Quay Wall Design - Invited Lecture

Pedro Simão Sêco e Pinto

**Abstract:** Bata quay wall is composed by 30 caissons with size 16.95m x 24,90m and the caissons are founded in rockfill materials of 1/100 Kg with a thickness of 5/6 m, and the foundation soil will be reinforced by vibrocompaction to aurre and admissible stress of 300 KPa. The caissons are divided into cells with size of 4.50m x 3.50m, filled by granular material (ballast). The bottom level of the caisson is –10,55m (ZH) and the caissons with a total height of 13,25m, will give a work platform at level 2.70m, for the construction of the superstructure.

After an evaluation of the results of the field tests and the laboratory tests, the geotechnical characteristics were defined. The static design of quay wall has followed the Eurocode 7 and so ultimate limit states as well serviceability limit states were analyzed. The SLOPE W code was used to define the minimum safety factor for different scenarios of water level and so to analyze by pseudo-static methods different levels of seismic actions. To verify serviceability limit states stress-strain analyses by SIGMA code were performed. In these analyses all the steps of construction phase were simulated. Due to the low degree of compaction of foundations sandy materials and the risk of liquefaction, a treatment by vibroflotation was performed. The caissons of the quay wall were monitored to compare the observed displacements with the predicted values by analyses.

### GROUND CHARACTERIZATION - Invited Lecture

Pedro Sêco e Pinto

**Abstract:** The general basis of Eurocode 7, the limit states and the design approaches are introduced. The ground characterization and particularly the planning of ground characterization, the location of investigations points for different structures, the recommendations for depth of investigations and the quality of soil samples are addressed. The static and dynamic characterization of ground materials by field and laboratory tests are discussed. Ground investigation report with the components of presentation of geotechnical information and evaluation of geotechnical information is presented. The derived values, the characteristiques values, the design values and the link between design, laboratory and field tests are addressed. The general principles of statistical distributions namely reliability index and the consequence classes versus reliability index, as well the

statistical and probabilistic distributions are presented. The physical and mathematical modelling and the most popular computer codes, using finite element and finite difference methods are analysed. The interaction with other codes is addressed. Some final conclusions are presented.

**3rd Victor de Mello Lecture- India- Goa, 20 thSeptember 2019**

**Static and Seismic Pile Foundaton Design by Load Tests and Calculation Models**

Pedro S. Sêco e Pinto,

**Abstract**. In this paper geotechnical design is addressed and particularly Static and Seismic Pile Foundatin Design by Load Tests and Calculation Models. Within this framework Eurocode 7 - *Geotechnical Design* and Eurocode 8 - *Design of Structures for Earthquake Resistance* are introduced. The ultimate limit states and the serviceability limit states are discussed. Potential liquefiable soils and remedial measures are addressed. Two case histories related with pile design, namely the New Tagus bridge foundation design and the pile design and liquefaction potential evaluation of Leziria bridge foundations based in Eurocodes 7 and 8, are presented. Some conclusions are drawn.

**ISSMGE International Seminar in Mozambique- 2nd October 2019**

**Lessons Learned from Two Landslides Case Histories - Key Note Lecture**

**Pedro Simão Sêco e Pinto - João Barradas & Arlindo Sousa**

**Abstract:** In this paper the triggering mechanics, the prevention and mitigation methods and the risk analysis of landslides are addressed. Two case histories are described. The first case history deals with the stabilization works of a landslide in Portugal. The anchored retaining walls founded on micropiles to stabilize the hills are described. The field and laboratory tests are referred, as well as the geological-geotechnical model. The design of the retaining walls was based in Eurocode 7 and in Eurocode 8. The results of anchorages tests and micropiles to calibrate the design values are presented.

The second case history is related with La Josefina site in Ecuador, where a huge failure has occurred with around 30 cubic millions of rock materials killing more than 100 persons. The canyon of the valley was blocked creating a lake with a volume of water higher than 200 cubic millions putting in great risk the cities of Cuenca and Azuogues.

**ISSMGE Board Meeting, in Capetown, 5th October 2019**

**ISSMGE Council meeting, in Capetown, 6th October**

**17th African Regional Conference, in Capetown, 7-10 October 2019**

**3RD Braja Das Lecture - Cairo, 11 th November 2019**

## UNDERSTANDING PILE FOUNDATIONS DESIGN TROUGH CASE HISTORIES OF NEW TAGUS BRIDGE AND LEZIRIA BRIDGE

Pedro S. Sêco e Pinto - Ricardo Oliveira & Alexandre Portugal

**Abstact:** In this paper pile foundation design and soil-structure interaction are referred. The ultimate limit states and serviceability limit states are introduced. The potentially liquefiable soils and remedial measures are addressed. Two case studies related with pile design of New Tagus bridge based in pile load tests and the pile design and liquefaction potential evaluation of Leziria bridge foundations are presented. Some conclusions are drawn.

# Materials Science, Novel Materials for Environmental Responsive Applications

## by Shu Yin, Member EUAS

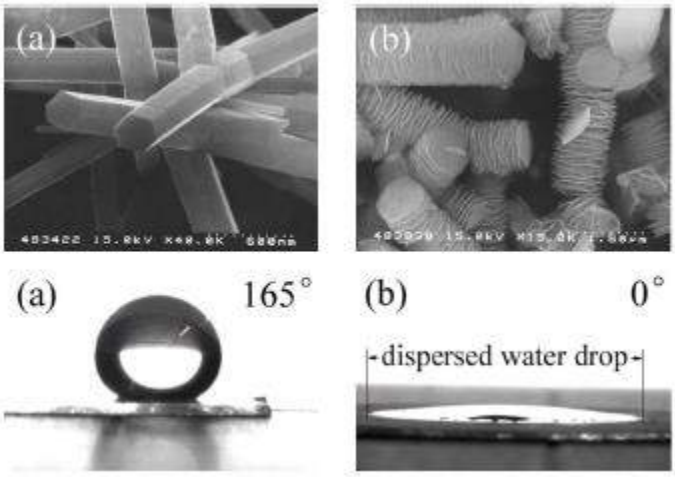
Short Biography

*Shu YIN is a full professor in the Lab. of Environmental Inorganic Materials Chemistry, Center for Exploration of New Inorganic Materials (CENIM), Institute of Multidisciplinary Research for Advanced Materials, Tohoku University, Japan. He received a B. S. degree in inorganic chemical engineering from the Dalian University of Technology in 1987, then received a M. S. degree in chemical metallurgy from the Institute of Chemical Metallurgy (ICM, latterly Institute of Process and Engineering, IPE), Chinese Academy of Science in 1990, then worked as a research associate for 2 years at ICM. He moved to Japan and worked as a research fellow in the Hydrothermal Chemistry Research Laboratory, Kochi University in 1992, then became a research assistant at the Institute for Chemical Reaction Science (ICRS), Tohoku University during 1995-1997. He received a Ph.D. degree in applied chemistry from Tohoku University (research period shortened) in 1999. He had been a research assistant at the ICRS in 1999, then a lecture and associate professor at the Institute of Multidisciplinary Research for Advanced Materials (IMRAM), Tohoku University in 2005, and then a full-time professor in 2016 (http://www2.tagen.tohoku.ac.jp/lab/yin/). He is also an affiliate professor of nine Chinese Universities / Institutes (Lanzhou University; Dalian University of Technology; Guangxi Research Institute of Chemical Industry, Huaqiao University, Taiyuan University of Technology, Sichuan University, Beijing University of Technology, University of Science and Technology Beijing / State Key Laboratory of Rare Earth Resource Utilization). He is the Chair of Japan Chapter, Functional Materials Society. He also acted as the symposium chair of some international conferences such as ISFM2011, ISHA2018 etc.. He is editor of some scientific journals such as Ceram. Int., Funct. Mater.Lett., Nanoscience, Tungsten, and Rare Metal etc. He has authored more than 460 original research papers, contributed 30 book chapters/ review papers and 23 patents. His research papers were cited more than 12455 times and showed a citation h-index = 62, i10 = 233 (Google Scholar, 2019.12). His research interests include morphological control of nanostructured oxides / oxynitrides/ nitrides, photocatalytic materials, UV/IR-shielding materials, gas sensing materials, hydrothermal / solvothermal process, soft chemical synthesis etc.. His outstanding contributions have been recognized by various awards and honors, including "Functional Materials Scientist Award(2009)", "Excellent Academic Photograph Award(2005)", "The 40th Harada Award(2000)". "The 59th Academic Award of the Society of Inorganic Materials Japan (2015)", and "The 69th CerSJ Awards for Academic Achievements in Ceramic Science* and Technology (2015)", The 2018 Best Paper Award, JACERAS(2018), The Chinese Society of Rare Earths , Academic Achievements Award (2019), and member of EUAS (2019).

**Typical Researches and Abstracts**

**Mild solution synthesis of zinc oxide films with superhydrophobicity and superhydrophilicity.**

Journal of Materials Chemistry, 15 (43), 4584-4587,2005.




Superhydrophobic and superhydrophilic surface of ZnO thin film superstructures

A novel and simple approach to the formation of ZnO films with nanorod, nanoscrew and nanodisk superstructures was successfully synthesized by heating 1 mM of a $Zn^{2+}$–hexamethylenetetramine mixed solution at temperatures as low as 95 $^{o}$C for a desired time. Low concentrations and long aging times preferentially formed developed nanoscrew, nanodisk and other superstructures in the mild solution reaction process. Films with different superstructures showed quite different contact angles of water drops.

**Preparation of nitrogen-doped titania with high visible light induced photocatalytic activity by mechanochemical reaction of titania and hexamethylenetetramine.**

Journal of Materials Chemistry, 13 (12), 2996-3001, 2003

Nitrogen-doped yellowish rutile titania was successfully prepared by a mechanochemical method. The samples were prepared by high-energy ball milling of a P-25 titania powder with various amounts of hexamethylenetetramine (HMT) under different milling conditions at around room temperature. The effects of the reaction conditions on the phase composition, particle size, specific surface area, amount of nitrogen-doping, microstructure and photocatalysis of nitrogen monoxide destruction were investigated in detail. The high mechanical energy accelerated the transformation of the phase from anatase to rutile, while the presence of HMT decreased the phase transformation. Residual HMT and by-products could be removed by post-milling calcination in air at 400 $^{o}$C. The nitrogen-doped yellowish titania possessed two absorption edges at around 400 and 550 nm and showed excellent photocatalytic ability for nitrogen monoxide oxidation under visible light irradiation. Irradiation with visible light of wavelength > 510 nm allowed nearly 37% nitrogen monoxide to be continuously removed by the nitrogen-doped titania prepared by planetary ball milling of a P-25 titania–10 wt% HMT mixture at 700 rpm for 120 min followed by calcination in air at 400 $^{o}$C.

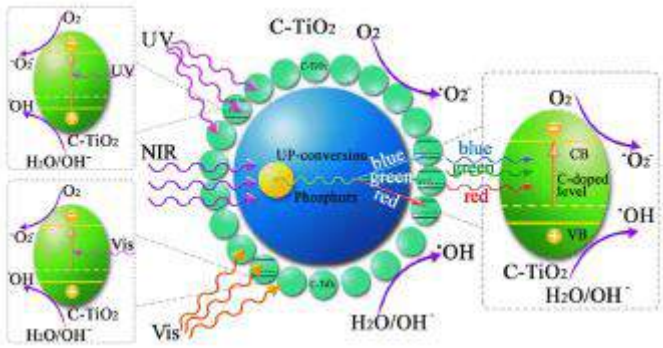
**Synthesis of excellent visible-light responsive TiO2−xNy photocatalyst by a homogeneous precipitation-solvothermal process.**

Journal of Materials Chemistry, 15 (6), 674-682, 2005

Anatase, brookite and rutile type nitrogen-doped titania nanocrystals ($TiO_{2-x}N_y$) which are beige in color were successfully prepared by a 'Homogeneous Precipitation–Solvothermal Process'(HPSP) in $TiCl_3$–hexamethylenetetramine ($C_6H_{12}N_4$) aqueous and alcohol solutions. The phase composition, crystallinity, microstructure, specific surface area, nitrogen doping amount and photocatalytic activity of titania powders greatly changed depending on pH, temperature and the type of treatment alcohols. The $TiO_{2-x}N_y$ powders showed excellent visible-light absorption and photocatalytic activity for nitrogen monoxide destruction under irradiation by both visible-light and UV-light. The beige titania powders prepared in $TiCl_3$–hexamethylenetetramine alcohol solutions at 190 $^oC$ for 2h possessed higher specific surface areas than those in aqueous solution. About 39 and 83% nitrogen monoxide could be continuously removed by the anatase $TiO_{2-x}N_y$ photocatalyst under irradiation of visible-light ($\lambda$>510 nm) and UV-light ($\lambda$>290 nm), respectively.

**Creation of advanced optical responsive functionality of ceramics by green processes**

Journal of the Ceramic Society of Japan 123 [9] 823-834 2015




Possible mechanism of UV, visible and NIR lights induced photocatalysis

Various kinds of optical responsive ceramic nanomaterials and films were successfully synthesized by environmental friendly green processes, such as hydrothermal/solvothermal process, mechanochemical doping process, oxygen plasma treatment process and a water molecular controlled-release solvothermal process (WCRSP). The composites combined the high-sensitive anion doped photocatalysts with up-conversion or long afterglow phosphors showed excellent deNOx photocatalytic activity under UV/ visible/NIR light irradiation, or even after turning off light irradiation. The mixed valence state tungsten based homogeneous nanomaterials possessed excellent IR light responsive properties, implied their potential applications as smart window materials and photothermal ablation cancer therapy materials. Significant contributions are expected for the development of optical responsive functional materials by green processes.

**Recent progress on mixed-anion type visible-light induced photocatalysts**

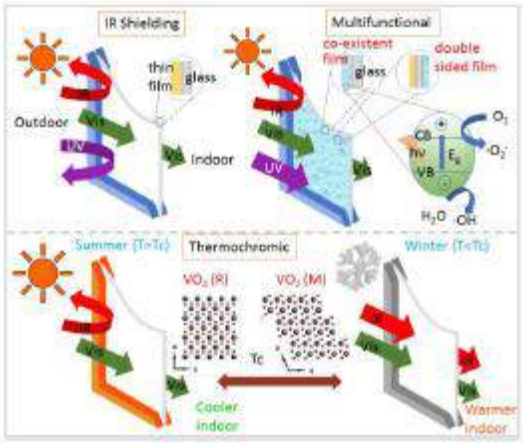
SCIENCE CHINA Technological Sciences 60 (10), 1447-1457, 2017

Environmentally friendly soft chemical processes, including solvothermal/hydrothermal process and mechanochemical process, for the synthesis of mixed anion type visible-light

induced photocatalysts are introduced in this review paper. Titania and strontium titanate based anion doped photocatalysts can be effectively prepared at such low-temperature as below 200 °C. Especially, the mechanochemical process is a useful method for the synthesis of various mixed ions doping functional materials at low temperatures. The mixed anion type photocatalytic compounds consisted of N/O, N/F/O, S/O, N/C/O, show excellent visible light absorption ability and photocatalytic activities, indicating the potential applications in environmental purifications. Full-spectra active long wavelength light induced photocatalyst, full-time active photocatalyst system and infrared radiation (IR) shielding multifunctional photocatalysts are introduced also.

**Nanomaterials for Infrared Shielding Smart Coatings**

Functional Materials Letters 11 (5), 1830004, 2018




Working models for IR shielding smart windows

Synthesis and characterization of functional nanoparticles and their applications for smart window are introduced. Various kinds of nanomaterials and their composites are successfully synthesized by solvothermal process. Thin films on glass substrate can be fabricated by doctor blade method using nanoparticles as starting materials. The mixed valence state tungsten based homogeneous nanomaterials $M_xWO_3$ and $W_{18}O_{49}$ possess excellent infrared (IR) light shielding properties, implies their potential applications for the heat ray shielding and indoor energy saving effect in summer. On the other hand, $VO_2$ monoclinic based nanoparticles possess smart and excellent thermochromic properties, show excellent heat ray shielding effect in summer and heating effect of winter indoors. Also, multifunctionality of thin films can be realized by fabricating the composites with various functional components, implying their potential applications for IR shielding, photocatalysis and self-cleaning at the same time. The design of composites and structure of thin films might result to the properties enhancement for practice applications on window materials.

# Climate Change & Variability, Climate Forecasting & Hydrometeorology

## by Chris Folland, Member EUAS

Short Biography

*Chris K. Folland, Retired UK Met Office Science Fellow, and Universities of East Anglia, UK, Gothenburg , Sweden, and Southern Queensland, Australia*

*The author has had a varied career in meteorology since 1968, mostly at the UK Met Office, after becoming a Fellow of the Royal Meteorological Society in 1967. He joined the Operational Instrumentation Branch in 1969 and took charge of a small group researching the development of surface meteorological instruments, particularly those measuring temperature and humidity on land and at sea. This included probably the first successful automated measurements of atmospheric humidity on a buoy. The author became involved with the World Meteorological Organisation (WMO), providing scientific input to the WMO Working Group on Reference Psychrometry. An instrumental background was to prove valuable for later research on correcting time-varying observed sea surface temperature (SST) biases, important for accurate climate change estimates.*

*The author joined the Met Office branch involved in climate change and UK monthly forecasting, Here, he co-authored a Nature paper in 1974 on the emerging Sahel drought. From 1976-1980, the author led a group working on hydrometeorological research and commercial consultancy. A key activity was working with hydrologists, hydraulics experts and prominent civil engineers to provide meteorological, mainly extreme rainfall statistics, input to a pioneering computerised model and manual for the hydraulic design of storm sewers, an activity sponsored by the UK National Water Council and its Department of the Environment (DOE). Another activity involved research for the WMO Working Group on Precipitation Evaporation and Soil Moisture to develop a physical model to quantitatively explain the long-standing problem of the systematic losses of rainfall from conventional raingauges and to test these ideas in the field. This included working with hydrologists at the UK Institute of Hydrology and led to a new raingauge design to minimise systematic rainfall and snowfall losses from conventional raingauges. This design was initially marketed as the Folland Sevruk Strangeways (FSS)100 tipping bucket raingauge in the late 1980s and is made today as the ARG100 raingauge marketed by several companies. This activity was helped by membership of the Royal Society sub-group on Hydrology (1979-82). For both research activities the author was awarded the Royal Meteorological Society's Hugh Robert Mill Medal and Prize in 1985. The author was also involved with hydrologists in the Institute of Civil Engineers on follow up research to the landmark 1975 UK Flood Studies Report and carried out hydrometeorological consultancy jobs for clients as part of the commercial consultancy work of his group. His most recent scientific work in hydrometeorology published in 2015, (in the Met Office Hadley Centre, see below) was a paper identifying the climatic causes of winter half year (October-March) meteorological and hydrological droughts in southern UK.*

The author then re-joined the Met Office branch concerned with UK monthly forecasting, climate data and climate change where he was in charge of global climate data set development, UK monthly forecasting and aspects of climate change research. The author published probably the first paper describing a partly dynamical monthly weather forecasting system, the remaining methods being statistical, using weather forecasting and climate models in 1986. Another key task was developing the emerging global SST data set. This was extended to include night marine air temperature (NMAT) as a check on the problems with historical SST data. This led in 1984 to the publication of the first global SST data set starting in the mid nineteenth century in *Nature,* and what it showed about

climate variability and change. This paper was the first to identify interhemispheric variations in SST and NMAT, later mainly identified with the Atlantic Multidecadal Oscillation marine mode that particularly affects the Atlantic Ocean. The global SST data set soon allowed the identification of several influences of SST on Sahel rainfall (Fig 1), changing the then dominant paradigm that the key influence was regional soil moisture variations, though this was confirmed as a smaller factor partly related to SST influences. The work, including dynamical climate modelling, was published in *Nature* in 1986 and led to the first, successful, forecast of Sahel rainfall in

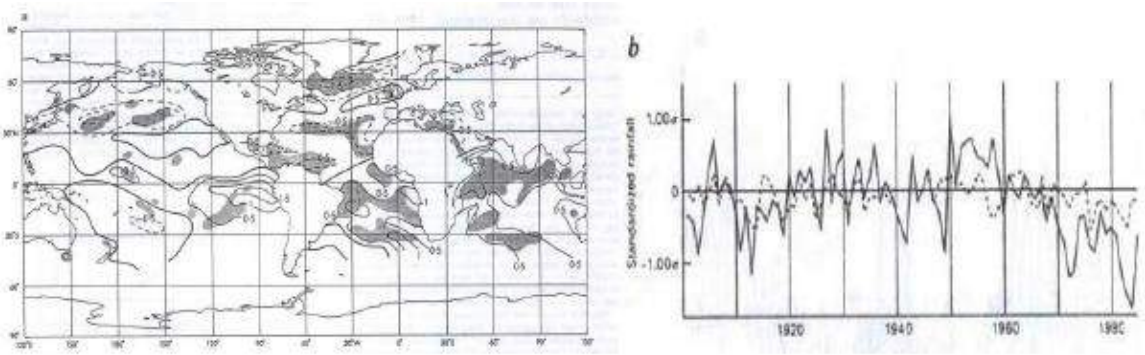



**Fig 1**. (left, a). SST, July to September: average of (1972-73, 1982-84) (Sahel dry) minus )1950, 1952-54, 1958) (Sahel wet). Contours every 0.5°C. Shaded areas are differences from zero at the 90% level of significance according to a t test. (right, b) Observed (solid line) and simulated (dashed line) Sahel rainfall. From Folland et al, 1986, *Nature*, 320, 602-607. 1986 for which the author was awarded a special UK Ministry of Defence prize. These seasonal rainfall forecasts were extended to several regions of West Africa and to North East Brazil in 1987, a region also dominated by SST variations. In this way the author introduced real-time tropical seasonal forecasting into the Met Office which continues to this day on a regular basis. The work was also helped to influence research internationally through the author's membership of the WMO Working Group on Long Range Forecasting Research (1986-90). The author's first involvement with politicians occurred in August 1984 when a Minister for Drought was created after the onset of a severe UK drought when his advice was sought (fortunately correct!) on whether the drought might soon end. This reflected some, if modest, real skill in monthly forecasting (published in 1986) which had been developed, temperature skill being partly due to the persistence of SST anomalies around and upstream of the UK that were now being continuously monitored.

A further key task was the development of the first physically based SST bias corrections, accelerated by a short spell as a visiting scientist at the Massachusetts Institute of Technology (MIT). This led to a joint publication with MIT of a 300 page SST and NMAT Atlas largely funded by the UK DOE as a major background document for the 1990 IPCC Report where Met Office SST data were the chief SST data used. This physically based approach, improved later in the 1990s, has been successfully tested in publications by oceanographers in recent years. Full publication occurred in 1995. Due to changes in observational practices over the last century, unadjusted data show too much climate change since the late nineteenth and early twentieth centuries (Fig 2). SST is a key component of the global surface temperature series as the oceans cover about 70% of the globe. Consequently, contrary to assertions by some climate sceptics, the current adjusted global mean surface temperature data sets (combined land air temperature and ocean surface temperature) show less climate change than unadjusted data, though different SST adjustment methods are now used by some other international groups that give similar

results.

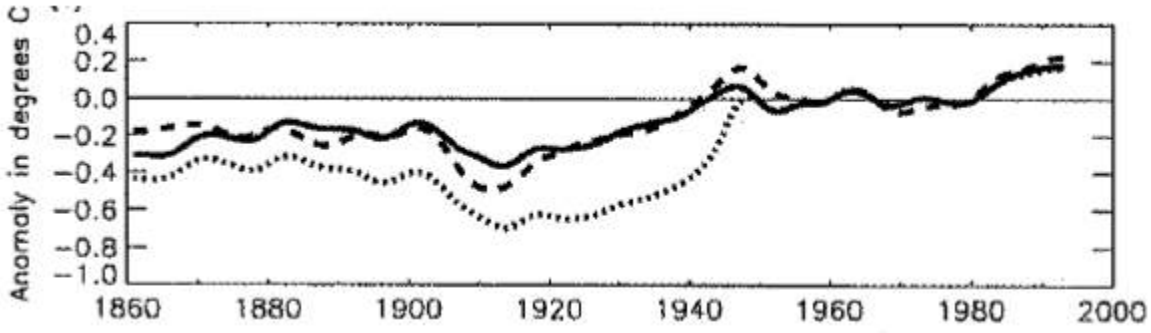



**Fig 2.** Annual marine surface temperature anomalies from a 1951-80 average smoothed by approximately 10year low pass filtered for the globe. Adjusted SST (solid line), unadjusted SST (dotted line) and adjusted NMAT (thick dashed line). From Folland and Parker, 1995, *Quarterly Journal of the Royal Meteorological Society*, 121, 319-367. Note that the term anomalies here and elsewhere means differences from a long-term average.

The author spent a year at the then NOAA Climate Analysis Center (CAC) in Washington DC (1988-89), becoming a Convening Lead Author on Observed Climate Variability and Change for the first,1990, IPCC Report, and organising in USA an early IPCC Workshop. He also co-authored two *Nature* papers involving progress and problems with monitoring temperature changes,and was commissioned by the CAC Director to write a paper on its future strategy. Soon after returning to the Met Office, the author became what is now known as a Met Office Science Fellow. In April 1990 the Met Office Hadley Centre for Climate Prediction and Research (as it then was called) was created, and the author also became the Head of the Climate Variability group, later Climate Variability and Forecasting (1990-2008). Soon afterwards, the author shared the main Met Office scientific prize for his SST research, the 1991 L.G. Groves Memorial Prize for Meteorology. His key responsibility in the Hadley Centre was to lead development of a wide range of global data sets ranging from SST, NMAT and sea ice, radiosonde temperatures of the atmosphere, to pressure at mean sea level and later, extremes in global temperature and rainfall. These data were then used to understand and monitor climate variability as well as develop seasonal to interannual forecasting, all partly using climate models. They also provided a prominent input to the IPCC Science Reports. Consequently, the group gained a reputation as a leading world developer and user of global climate data sets as well as creating the first daily Central England temperature data set, the longest daily temperature set in the world starting in 1772. A flagship global marine data set was published in 2003, the HadISST SST and sea ice data set, together with what it showed about marine climate change. This paper was identified by the Carbon Brief blog in 2015 as the fifth most cited paper in climate change science. Now with over 5,500 citations in Web of Science and nearly 7,000 in Google Scholar, it is believed to be the most cited Met Office lead authored paper in its history. For this, the author shared a Met Office Achievement Award in 2008.

The physical basis of the tropical seasonal forecasts for West Africa and North east Brazil was increasingly improved in the late 1980s and early 1990s. Dynamical forecasts were introduced, initially using observed SST forcing but nowadays a fully coupled climate model is used for tropical seasonal forecasting, though statistical methods remain

competitive in North East Brazil, As a result, the author shared with colleagues the 1996 WMO Norbert Gerbier-Mumm International Award (Medal and Prize) for tropical seasonal forecasting. Another development was the creation of real-time forecasts a year ahead of global mean surface temperature. Initially these were purely statistical, but since 2008 a climate model has been given equal weight and both have comparable skill with high skill overall (Fig 3). Twenty one forecasts have been issued since 2000, the latest being for 2020 issued in December 2019 and similar to the 2019 forecast.

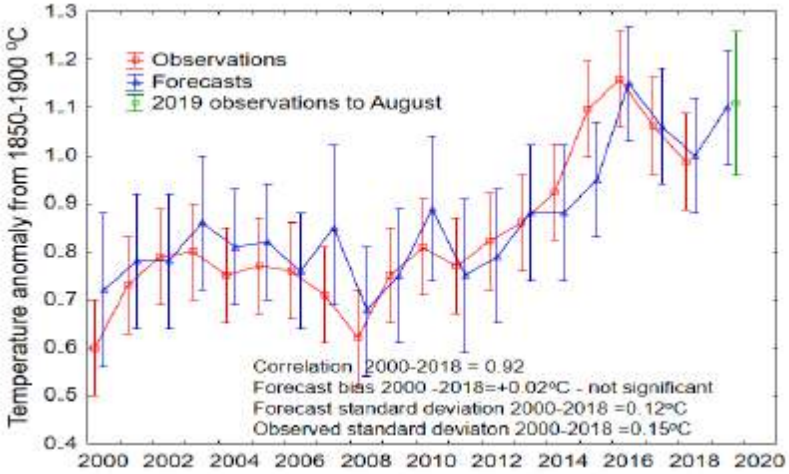



**Fig 3** Performance of forecasts of annual mean global mean surface temperature one year ahead. Vertical bars are 95% confidence ranges: observations (red) and forecasts (blue). Updated from Folland et al, 2013, *Geophysical Research Letters*, 40, 761–767, doi:10.1002/grl.50169.

The need to test the developing flagship SST data sets in more remote regions like the South Pacific and Southern Ocean led to the author becoming a Meteorological Fellow of the Link Foundation of New Zealand in 1993. The foundation gave him visiting scientist awards in 1994 and 2000 to work at the New Zealand National Institute of Water and Atmospheric Research. This led to successful, published, tests of the SST data in the Southern Ocean region. Related published work also led to the identification of the Interdecadal Pacific Oscillation SST and NMAT patterns in 1999 and influences of the IPO on South Pacific and Australian climate. The IPO (a Pacific wide marine mode on decadal to interdecadal time scales) has been identified widely as a key mode of climatic variability that can affect the global climate.

The author's international involvement in climate change and variability continued after the creation of the Met Office Hadley Centre, partly through positions as a Convening Lead Author of Climate Variability and Change Chapters in the 1992 Supplementary and 2001 Reports and as Lead Author of the Climate Models - Evaluation Chapter in the 1996 Report as well as contributions to several teports as a Contributing Author, and a reviewer in recent IPCC reports. The author also shared in the 2007 Nobel Peace Prize given to IPCC Lead authors. In addition, the author initiated and co-chaired the CLIVAR Climate of the Twentieth Century (C20C) Project (1999-2014) which has published a number of papers and continues, as planned, as the C20C+ Detection and Attribution project which published its progress in 2019. He also became Deputy Chair of the WMO Working Group on Climate Change Detection and Indices which led to key Met Office papers on changing temperature and rainfall extremes in the 2001 and 2007 IPCC Reports. He also led the Met

Office contributions involving climate variability and change research to four European Union Projects over the period 1990-2008.

A key development, started in the mid-1990s, was to work towards an operational dynamical monthly and seasonal forecasting system, especially for UK, using improved dynamical climate models and to extend seasonal predictions throughout the globe. This activity is now a monthly routine forecast conference. Through a number of dynamical and observational papers, most prominently in *Nature* in 1999, it became clear that there was particular predictability for the North Atlantic Oscillation atmospheric mode of winter climate variability mentioned above. This strongly affects European winters, opening the way for potentially useful winter forecasting for UK especially. The first operational winter season forecast using dynamical methods was published for winter 2005-6. These forecasts are now entirely dynamical, probabilistic in nature, and made during the whole year. They are certainly skilful in winter for UK, with a number of experimental users, and include seasonal forecasts for every inhabited continent updated monthly.

In 2009,the author published the concept and behaviour of the Summer North Atlantic Oscillation (SNAO) (Fig 4 overleaf). The SNAO differs from its winter counterpart in that its pattern is shifted further north and somewhat north east and is a little smaller in scale. Recently this analysis has been extended to the whole summer (June-August) and its mechanisms are being studied, including the causes of some pronounced interdecadal variability.

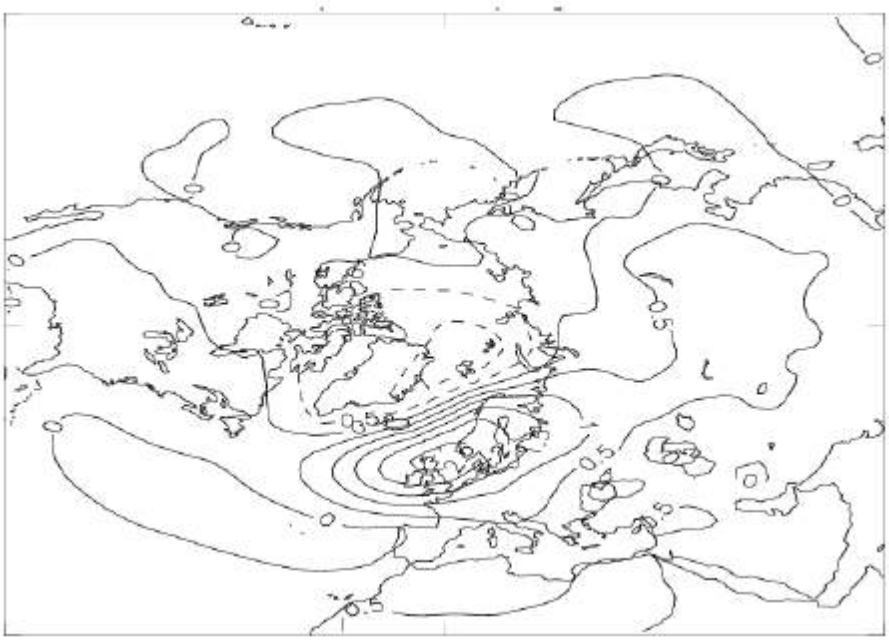


**Fig 4.** The July-August Summer North Atlantic Oscillation pattern in pressure at mean sea level (PMSL). From Folland et al, 2009, *Journal of Climate*, 22, 1082–1103, DOI: 10.1175/2008JCLI2459. Dotted lines show oppositely signed PMSL anomalies from solid lines.

The author was invited to give plenary presentations to WMO Congress in 1999 on the problems of climate data and on observed climate change to the World Climate Congress in Moscow in 2003, opened by President Putin, and which led to Russia signing the Kyoto Protocol. Especially in the 1990s, the Met Office was developing its relationship with UK politicians over climate change issues, so the author gave many presentations to UK politicians during this period, including the then UK Prime Minister, Mrs Thatcher, at the opening of the Hadley Centre in 1990. A recent publication by the author on climate change (in 2018) has, among other results, explained the well-known slowdown in global warming over 1998 to 2013 as being partly due to the influence of an unusually large solar radiation cycle, as well as supporting previous explanations. This highlights the fact that,both globally and regionally. natural climate variability can for a time, offset or enhance longer term climate change. This is now the subject of decadal climate forecasting using climate models. The author was a co-author of the first published decadal forecast of global mean surface temperature in *Science* in 2007.

Besides his academic interests, the author has carried out many media interviews and given outreach talks to local societies on climate change. He has been involved with learned societies additionally to contributions mentioned above, being a member of Council of the Royal Meteorological. Society in 1978-81, its Education Committee (1976-81) and recently its History of Meteorology and Physical Oceanography Committee. As a member of the Climate Variability and Change Committee of the American Meteorological Society. (2010-16), he was given an Outstanding Service Certificate. The author in retirement since 2017 has started mentoring post graduate students studying climate topics at Reading University.

The author's long period as a climate scientist has also been rewarded by Fellowship of the Institute of Physics (1996), Fellowship of the American Meteorological Society (2003), a Met Office Career Achievement Award in 2007, Fellowship of the American Geophysical Union (2011) given to only 0.1% of its members in a specific year, Honorary Professor at the University of East Anglia (2003), Adjunct Professor at the University of Southern Queensland (who also fund Met Office posts) and Guest Professor of Climatology at the University of Gothenburg (2011). The Swedish Research Council partly funded the author in 2013-16 to research Summer North Atlantic Oscillation mechanisms. In 2016 the Korean Meteorological Administration awarded the author an Honorarium as an Expert Scientist to give a lecture course in South Korea on seasonal climate forecasting and climate variability and change. Recently, the author has been given the University of Southern Queensland's 2019 Research Giant Award to present lectures and provide advice at the University on worldwide decadal climate forecasting and climate change.

# Lithium Ion Battery Fire Dynamics & Prevention - Research on Hydrogen Safety

**by Jinhua Sun, Member EUAS**

Short Biography

***Education and Positions***

*2004~ Vice Director of State Key Laboratory of Fire Science of China*
*2002~ Professor, University of Science & Technology of China*
*1999~2002 Research Professor, Japan Science and Technology Agency, Japan*
*1996~1999 Ph.D., The University of Tokyo, JAPAN*
*1988~1996 Associate Professor, Anhui University of Science & Technology, China*
*1986~1988 M. Sc., Nanjing University of Science and Technology, China*
*1983~1986 Assistant Professor, Anhui University of Science & Technology, China*
*1979~1983 B. Sc., Nanjing University of Science and Technology, China*

***Professional Activities***

*Vice-chairman of Asia-Oceania Association for Fire Science and Technology (2007~)*
*Committee Member of the International Association for Fire Safety Science(2008~2017)*
*Committee Member of the National Science and Technology Award (2010~)*
*Academic Committee Member of University of Science and Technology of China (2009~)*
*Safety expert committee Anhui Province, Civil blasting group leader(2009~)*
*Member of Science and Technology Award Committee, Ministry of Public Security (2007~)*
*Member of Academic Committee of urban safety and disaster prevention, Urban Planning Society of China (2005~2015)*
*Evaluation expert in international scientific and technological cooperation program, Ministry of Science and Technology of China (2005~)*
*Executive director of Anhui Fire Protection Association (2005~)*
*Associate Editorial or Editorial Board of five International Journals(2010~)*
*Editorial Board of nine national Journals(2003~)*
*Academic Committee Member of China Fire Protection Association(2003~)*

***Honors and Awards***

*National Science and Technology Progress Award, First-class Award, China (1993)*
*Member of Hundred Talent Program, Chinese Academy of Sciences (2001)*
*Outstanding Member Hundred Talent Program, Chinese Academy of Sciences (2005)*
*National Science and Technology Progress Award, Second-class Award, China (2006)*
*Science and Technology Award for Young Scientist, Anhui Province (2006)*
*Safety Science and Technology Award of State Administration of Work Safety, Second-class Award (2006)*
*Beijing Science and Technology Award, Third-class Award, Beijing (2008)*
*Teaching Award of Anhui Province, First-class Award, Anhui Province (2010)*
*Zhu Li Yuehua excellent teacher Award, Chinese Academy of Sciences (2014)*
*Excellent graduate student supervisor Award, Chinese Academy of Sciences (2014)*
*Zhu Li Yuehua excellent teacher Award, Chinese Academy of Sciences (2017)*
*Excellent graduate student supervisor Award, Chinese Academy of Sciences (2017)*
*Science and Technology Innovation Award, First-class Award, China Fire Protection Association (2018)*

*Special government allowance of the State Council（2019）*

Professor Sun Jinhua has long been devoted to academic research and education in the area of fire science and fire protection. He has made substantial accomplishments in a number of fields in fire safety science and engineering, including fire risk assessment, performance-based fire protection design, building fire safety, industrial fire safety, fire safety in new energies. He led as a PI more than 20 important national research projects, such as the National "973 Program", key projects funded by National Natural Science Foundation of China (NSFC), the "11th Five-Year plan" and the "13th Five-Year Plan" national key R&D program, the sixth Framework Project of the EU International Cooperation Program in Science and Technology, NSFC general projects, and "Outstanding Talents" project funded by the Chinese Academy of Sciences.

Prof. Sun has published more than 300 papers in peer-reviewed journals, including Progress in Energy and Combustion Science, Combustion and Flame, Renewable and Sustainable Energy Reviews, et al, which have been cited more than 9,400 times (Google scholar). Contributions have also been recorded in 11 academic books or book chapters and over 40 keynote or invited talks at national or international conferences. In addition, Dr. Jiang has supervised more than 40 PhD students.

**Major Research Areas**

1. Theories and methods of fire prevention for new energies.
2. Methods for fire risk assessment and safety design of buildings and urban areas.
3. Theory of fire dynamics, fire prevention and control for buildings.
4. Industry fire dynamics and fire prevention.

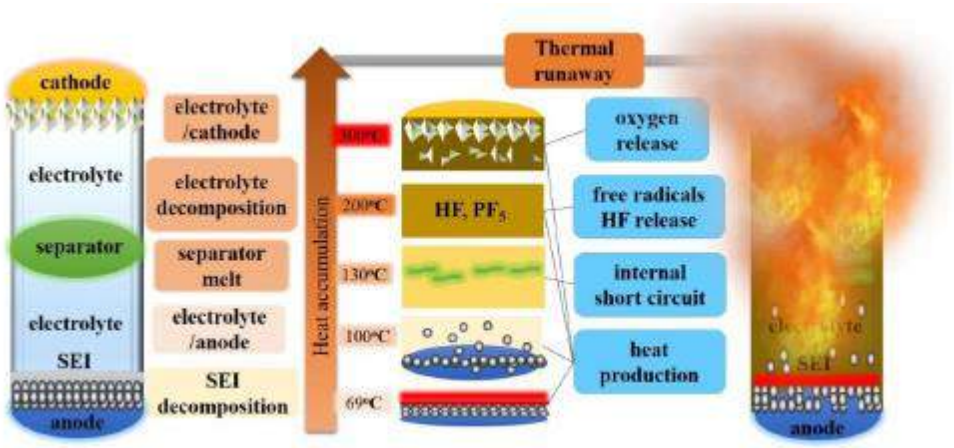
**Some New Research**

**1. Lithium Ion Battery Fire Dynamics & Prevention**

Due to its high voltage, high specific energy, long cycle life, no pollution to the environment and other excellent performance, Li-ion battery has become the dominant power in the field of consumer electronics. Meanwhile, Li-ion battery has been contemplated by energy storage and power supply industry such as photovoltaic energy, nuclear energy, wind energy, (hybrid) electric vehicles and aircraft. However, fire incidents caused by thermal runaway of Li-ion battery have been reported recent years. Safety has become one of the most intractable barriers to the wide application of Li-ion battery in the above industry. Therefore, study on thermal runaway and fire hazard of Li-ion battery and high-safety battery system can improve our understanding on the origins of thermal runaway and fire of the battery, clarify the main unsafe reason, determine the behavior and hazard of thermal runaway and fire quantitatively, and propose the safe battery system to reduce the possibility of the incidents, to provide data base and technical support for the battery safety and fire protection design. The work are summarized as following :

Thermal hazards of some electrolytes based on different lithium salts are studied and compared based on thermodynamic analysis. It is shown that the lithium salt influences the thermal hazard of electrolyte markedly. Deconvolution method is proposed to investigate

the thermal runaway hazard of the full cell system, based on the thermal analysis results of the electrolyte-electrode coexisting system, the detail process of the thermal runaway behavior for the full cell system is clarified. It is shown that the content of electrolyte is related with the thermal reactivity of the system; the decomposition of solid electrolyte interface (SEI) film initiates the thermal reaction of the system; the reactions involved with positive material release much heat, which is the largest part of the overall heat; the Joule heat caused by the short circuit following with the melting of separator increases the hazard of thermal runaway for the system. Full-scale burning test system for the large and high-energy Li-ion battery is established. The fire behavior and hazard of 50Ah LiFePO4/graphite battery is studied systematically, it is shown that the Li-ion battery shows a special fire behavior, the repeated jetting fire, and reveling the influence of state of charge (SOC) and electrode materials. Studying the fire spread behavior between lithium titanate batteries and parallel arrangement, and obtaining the criticality of fire spread by Semenov and Frank-Kamenetskii models; creating the cricality model of battery thermal runaway through revising the classic Semenov and Thomas models; predicting the influence of heat convection coefficient, cell size and shape to critical condition of battery thermal runaway on base of the revised model.




## 2. Research on Hydrogen Safety

As a clean and efficient alternative energy source, hydrogen is attracting more and more attention from all over the world including China because of its wide range of sources, high energy density, pollution-free and renewable properties. At present, high-pressure hydrogen storage is the most ideal hydrogen storage means. However, the chemical properties of high-pressure hydrogen are very active. Under certain conditions, hydrogen can react with various metals and cause hydrogen embrittlement problems. As a result, the hydrogen storage container and the pipeline are broken, which eventually causes release of the entire hydrogen storage system. Once the high-pressure hydrogen gas releases, it is prone to spontaneous ignition in the pipeline, causing combustion and explosion, resulting in unpredictable casualties and property losses. In addition, premixed combustion of the combustible gas mixture is a very fundamental and potential subject for practical application, e.g. accidental explosions. The fundamental understanding of premixed flame propagation phenomena is essential for the development of novel analytical and numerical combustion models. Premixed flame dynamics in confined vessels is of particular importance since it provides understanding of the burning processes taking place in

internal combustion engines, and explains the mechanisms behind flame acceleration that can lead to transition from deflagration to detonation.

**Mechanism of Spontaneous Ignition During High-pressure Hydrogen Release:** current researches on the mechanism, micro-kinetics and related influencing factors of spontaneous ignition of high-pressure hydrogen release is not deep enough. The critical conditions, spontaneous ignition characteristics, critical burst pressure, shock wave generation and propagation characteristics inside the tube, and the formation mechanism and propagation characteristics of the hydrogen jet flame outside the tube have not been fully revealed. We use the experimental method to study the effect of the tube geometry, the opening ratio of the burst disc and the mixing gas in the tube on the spontaneous ignition of high-pressure hydrogen. The numerical simulation method is used as well to simulate the micro-kinetics in the tube and the spontaneous ignition mechanism in detail. A similitude analysis method was used to establish a prediction model of hydrogen spontaneous ignition based on the mechanism of spontaneous ignition of high-pressure hydrogen.

**Dynamics of Premixed Hydrogen-Air Flame Propagating in Ducts:** The experimental study shows that the premixed hydrogen/air flame in ducts undergoes more complex shape changes and exhibits more distinct characteristics than that of other gaseous fuels. One of the outstanding findings is that significant distortions happen to the classical tulip flame front after its full formation when equivalence ratio ranges from 0.84 to 4.22 in the closed duct. A distorted tulip flame is initiated as the distortions or indentations are created very near the leading tips of the tulip lips after a well-pronounced classical tulip flame is produced. The distorted tulip flame develops into a salient “triple tulip” shape as the secondary tulip cusps approach the center of the primary tulip lips and appear comparable to the primary cusp. A second distorted tulip flame appears with a cascade of secondary cusps on the primary tulip lips just before the collapse of the first one. The salient tulip flame distortions are specially scrutinized and distinguished from the classical tulip. The dynamics of distorting tulip flame is different from that of classical tulip flame. The distorting tulip flame undergoes more complex shape changes and more unstable combustion process than the classical tulip flame.

# The "Nanomachine", NhaA Na+/H+ Antiporter

## by Etana Padan, Member EUAS

Short Biography

***CURRENT POSITION/ADDRESS*** *: Professor, Dept. of Biological Chemistry, The Alexander Silberman Inst. of Life Sciences, The Hebrew University of Jerusalem*

***ACADEMIC TRAINING***

| | |
|---|---|
| *1958-1963* | *Received M.Sc. degree with honors, Major subject: Biochemistry. Minor subject: Physiology and Genetics.* |
| *1963-1969* | *Received Ph.D. degree, Ph.D. Thesis: Study of the Properties of Blue-Green Algal Viruses." Worked under the guidance of Prof. M. Shilo, Department of Microbiological Chemistry. Hebrew University Hadassah Medical School.* |

***PROFESSIONAL EXPERIENCE***

| | |
|---|---|
| *1969* | *Appointed Instructor in the Department of Microbiological Chemistry, Hebrew University-Hadassah Medical School.* |
| *1970* | *Appointed Research Fellow (Lecturer) in the Department of Microbiological Chemistry, Hebrew University-Hadassah Medical School.* |
| *1972* | *Research Fellow in the Department of Biochemistry, Weizmann Institute, Rechovot. (Post Doctorate with Prof. M. Avron and Prof. H. Rottenberg).* |
| *1973* | *Visiting Fellow in the Department of Zoology, Rand Afrikaans University, Johannesburg, Republic of South Africa.* |
| *1974* | *Appointed Senior Lecturer in the Department of Microbiological Chemistry, Hebrew University.* |
| *1977* | *Received tenure (Senior Lecturer).* |
| *1978-1979* | *Visiting scientist (Sabbatical) in the Department of H.R. Kaback, Membrane Biochemistry, Roche Institute of Molecular Biology, Nutley, New Jersey, U.S.A.* |
| *1979* | *Appointed Associate Professor in the Department of Microbial and Molecular Ecology, Life Sciences Institute, Hebrew University, Jerusalem.* |
| *1980* | *Appointed the head of the Oceanography programme in the Hebrew University.* |
| *1982* | *Appointed a science advisor in Biochemistry by the Binational Science Foundation.* |
| *1983* | *Member of the organizing committee of the 2nd International Workshop on primary productivity held in April, 1984, Haifa, Israel.* |
| *1985* | *Appointed full professor in the Department of Microbial and Molecular Ecology, Life Sciences Institute, Hebrew University, Jerusalem.* |
| *1985-1986* | *Visiting scientist (Sabbatical) in the Department of H.R. Kaback, Membrane Biochemistry, Roche Institute of Molecular Biology, Nutley, New Jersey, U.S.A.*<br>*Member of the Editorial Board of FEMS Microbiology Reviews.* |
| *1988* | *Member of the organizing committee of the 6th International Symposium on Photosynthetic Prokaryotes, Holland, August, 1988.* |
| *1989* | *Head of Department of Microbial and Molecular Ecology, Life Sciences Institute, Hebrew University, Jerusalem.* |
| *1990* | *Visiting Professor in the Department of Biochemistry, Mount Sinai Medical Center of the University of New York.* |
| *1992-1995* | *Head of Institute of Life Sciences, Hebrew University of Jerusalem, October, 1992.* |
| *1995* | *Awarded M. Launda Prize of the Israeli Payis Institute for "Understanding of Physiology of Microorganisms and Their Adaptations to* |

| | |
|---|---|
| | *Changing Environment."* |
| *1996* | *Awarded EMBO Fellowship, Visiting Professor with Prof. H. Michel, Max-Planck-Institute fur Biophysik, Frankfurt, Germany.* |
| *1998* | *Chairperson of The Second FISEB, Societie of Experimental Biology, Eilat December, 1998.* |
| *1998-2001* | *Prorector of the Hebrew University of Jerusalem.* |
| *1999* | *Awarded EMBO Fellowship, Visiting Professor with Prof. H. Michel, Max-Planck-Institute fur Biophysik, Frankfurt, Germany.* |
| *2000-2006* | *Editor for Biomembrane Section of Biochem. Biophys Acta* |
| *2001* | *Elected to the American Academy of Microbiology* |
| *2002* | *Member of the International Advisory Board of the XIII EBEC, European Bioenergetic Conference, Pisa 2004* |
| *2004* | *President-Elect of the Israeli Society of Biochemistry and Molecular Biology* |
| *2004* | *Advisory Board of E-MeP, The European Membrane Protein Consortium, 2004-2009.* |
| *2005* | *Awarded EMBO Fellowship, Visiting Professor with Prof. H. Michel, Max-Planck-Institute fur Biophysik, Frankfurt, Germany.* |
| *2005* | *Faculty 1000 Biology chosen paper.* |
| *2006* | *Member of Bikura panel. Israel Science Foundation.* |
| *2009* | *Editorial Advisory Panel Member of Molecular Membrane Biology.* |
| *2011* | *Member of the organizing committee of the EBEC, European Bioenergetics Conference* |
| *2012* | *Invited lecture in the EDICT symposium Portugal, Trevira* |
| *2012* | *Invited lecture in the meeting: The Intricate workings of membrane proteins, Jerusalem* |
| *2013* | *Invited lecture in the International Congress of Molecular and Cell Biology, July, Suzhou.* |
| *2013* | *Invited to deliver this years' Lars Ernster Lecture in Bioenergetics at the Department of Biochemistry and Biophysics at Stockholm University, Sweden.* |
| *2014* | *Invited Plenary-lecture in EBEC, European Bioenergetics Conference, Lisbon, July, 2014.* |
| *2014* | *Invited lecture at Membrane Transport and Communication,Riedberg, Germany.* |
| *2015* | *Invited lecture at the Antiporters Structure and Function meeting, Frankfurt, Germany.* |
| *2015* | *Chairperson, Annual Meeting of The Israel Society for Biochemistry and Molecular Biology, Focus on Membrane Proteins. November, Bar-Ilan University, Israel.* |
| *2015* | *Invited lecture at the Workshop on Structural and Functional Dynamics of Na+/H+ Antiporters, November, Frankfurt, Germany.* |
| *2016* | *Invited lecture at the Symposium in Memory of Prof Haim GartyRegulation of Sodium Transport in Health and Disease,January, Weitzmann Institute of Science.* |
| *2016* | *Invited lecture at the 80th Birthday of H.R. Kaback, NIH, Washington DC, USA* |
| *2016* | *Chairperson and organizing commeetee EBEC, European Bioenergetics Conference, Italy.* |
| *2017* | *Awarded the Ilanit- Katzir Prize for outstanding research achievements in the Life Sciences* |
| *2017* | *Elected member of the EU Academy of Sciences* |
| *2018* | *Awarded the Mitchell Prize and medal for outstanding research in bioenergetics and molecular and structural biology of NhaA, the Na+/H+ antiporter. 20th European Bioenergetics Conference (EBEC) Budapest, Hungary 25-30 August, 2018* |

## The "Nanomachine", NhaA $Na^+/H^+$ Antiporter

**Etana Padan**

**Biological Chemistry, Institute of Life Sciences, Hebrew University of Jerusalem, Israel**

$Na^+/H^+$ antiporters are essential for homeostasis of intracellular pH, $Na^+$, and cell-volume. Several antiporters have long been drug targets. Determining the crystal structure of NhaA $Na^+/H^+$ antiporter has been a breakthrough (1). It revealed a unique fold characterising many secondary transporters: two inverted repeats of helices with unwound chain in each repeat cross each other forming a delicately elocrostatic balanced area in the middle of the membrane essential for activity (2).

NhaA is a dynamic "nano-machine"; binding $2H^+$ at one side of the membrane and exchanging them with either 1 $Na^+$ or 1 $Li^+$ on the other side by alternating the protein conformations. We employ interdiciplinary techniques to unravel the mechanism of the conformational changes. Hydrogen-Deuterium Exchange Mass Spectroscopy revealed $Li^+$ induced global coordinated conformational changes in NhaA (3). Comprehensive evolutionary analysis of the present 6,537 $Na^+/H^+$ antiporter sequences revealed a sequence motif that determines the phenotypic characteristics of NhaA (4).

NhaA is a dimer with lipids between its monomers. We revealed that cardiolipin is essential for the NhaA dimeric structure by developing a novel *in-vitro* assay which likely be applicable to future studies of protein–lipid interactions: detergent-delipidation split the dimers into monomers and subsequent exposure to cardiolipin reconstitute the dimers (5). The human NhaA homologues involved in severe pathologies might also require phospholipids so our results open a new direction to drug design.

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# Hydrodynamics of Fluidization & Heat Transfer: Supercomputer Modeling

## by Dimitri Gidaspow, Member EUAS

Short Biography

*Dimitri Gidaspow, Distinguished Professor Emeritus*

***Education:***

*B.Ch.E. (cum laude), the City College of New York, 1956;M.ChE. Polytechnic Institute of Brooklyn, 1959.Ph.D., Illinois Institute of Technology, 1962 ( Surface Combustion of Hydrogen, AIChE J.10,707-716,1964 and ASME 1961 paper )*

***Academic Experience:***

*Distinguished Professor of Chemical Engineering, IIT; 2000-2010; Institute of Gas Technology (IGT), 63-77; Principal Advisor of 65 Ph.D. students and co-advisor to students in Norway, Italy and Thailand .*

***Industrial Experience:***

*Air Products 1956; IGT - 1) fuel cells; dozen refereed papers, patents and NASA 1969 award from the Marshall Space Flight Center,(2)desiccant air conditioning; 12 papers and a patent ,1982.AEC in Idaho- consultant 1972-1974. Consultant to Lawrence Livermore Lab; Energy*

*Research Corp., Argonne National Lab.; Department of Energy (fuel cell survey), UTC, EXXON, Westinghouse, IITRI, MOBIL ,UOP, Polysilicon Corp.*

***Publications and Patents:*** *( Over 15,000 citations )*

*10 US patents; Over 200 refereed publications,*

*Books: 1. Dimitri Gidaspow," Multiphase Flow and Fluidization,Continuum and Kinetic Theory Description ", Academic Press (1994).*

*2.Dimitri Gidaspow & Veeraya Jiradilok, "Computational Techniques" Nova Science Publishers, 2009.*

*3.H. Arastoopour, D. Gidaspow & E. Abbasi, "Computational Transport Phenomena of Fluid-Particle Systems" Springer, 2016.Full text to be published in 2020.*

***Awards:***

*AIChE 1984 Donald Q. Kern Award Lecture: "Hydrodynamics of Fluidization and Heat Transfer: Supercomputer Modeling", in Appl.Mech. Rev. 39, No. 1, 1-23, 1986. NSF 1986 Creativity Award.; Fellow of the American Institute of Chemical Engineers; IIT Alumni awards; AIChE 2002 Flour-Daniel Lectureship Award in Fluidization.; Thiele award,.2005; Sigma Xi award.; 2006 Thomas Baron award. Festschrift, I&EC Research, 49,No.11, June 2, 2010; 2013 PTF award for lifetime*

*Achievements.*

### Research

Over the last 3 decades we developed a kinetic theory- based science of multiphase flow and fluidization, first presented as AIChE 1984 Donald Q. Kern Award Lecture: "Hydrodynamics of Fluidization and Heat Transfer: Supercomputer Modeling", in Appl. Mech. Rev. 39, No. 1, 1-23, 1986.A more recent review is : . "Hydrodynamics of fluidization using kinetic theory: an emerging paradigm. 2002

Flour-Daniel lecture", Dimitri Gidaspow, Jonghwun Jung, Raj K. Singh, Powder Technology, 148, 123-141 (2004)

Traditionally multiphase systems and reactors were built using trial and error and scaled up using scale factors. Such an approach led to nuclear accidents and oil spills. For example, see Dimitri Gidaspow, Fang Li and Jing Huang," A CFD simulator for multiphase flow in reservoirs and pipes " , Powder Technology 242,2-12 ( 2013 ).

The kinetic theory based multiphase flow theory and our computer codes are described in our two books :

1. Dimitri Gidaspow," Multiphase Flow and Fluidization, Continuum and Kinetic Theory Description ", Academic Press (1994).Over 4,000 citations.
2. Dimitri Gidaspow & Veeraya Jiradilok, " COMPUTATIONAL TECHNIQUES. The Multiphase CFD Approach to Fluidization & Green Energy Technologies" Nova Science Publishers, 2009

The kinetic theory based multiphase code also permits a better understanding of blood flow. Traditionally blood flow has been modeled using incompressible Navier - Stokes equations with a viscosity three times that of water. However, it was known since the invention of the microscope that red blood cells in small blood vessels migrate away from the walls. This phenomenon reduces the blood viscosity and hence the pressure drop .Our code and theory predict this and also compute the motion of platelets.
See:

D. Gidaspow and Jing Huang, " Kinetic theory based model for blood flow and its viscosity " Annals of Biomedical Engineering 37, No 8 August ( 2009 ) pp 1534-1545.
The platelet concentration ,n, is given by the simple expression for developed flow, $n/n_{inlet} = 1/ [ 1-(r/R)^4]$ where R is the tube radius and r is the radial coordinate. See Dimitri Gidaspow and Vishak Chandra, " Unequal granular temperature model for motion of platelets to the wall and red blood cells to the center " Chemical Engineering Science 117, 107-113 ( 2014 )

The computational fluid dynamics code can be extended to include the motion of arteries and their inelastic behavior due to the deposit of plaque. This will allow the placement of stents into regions of arteries not permitted to-day, in place of complicated bypass surgery.

Unlike commercial CFD codes our model and code are well-posed as an initial value problem. The commercial codes are only conditionally well posed as an initial value problem and therefore may, sometimes lead to incorrect solutions.
For example, see the code developed by professor Lu Huilin based on the MFIX code of Madhava Syamlal, Fellow of the US Department of Energy:
L.Huilin and D.Gidaspow, Chemical Engineering Science 58(16) 3777-3792.

We have used our code to design a circulating fluidized bed reactor to potentially remove carbon dioxide from air and from fossil energy power plants with only a small energy input compared to that of commercial amine reactors.( CO2 capture in a multistage CFB. parts one and two, Sutthichai Boonprasop, et al ,AIChE Journal,63,No12,5267-5289 (2017)). Circulating fluidized bed reactors, unlike the bubbling reactors used by US Department of Energy, operate essentially isothermally. This allows the conversion in the reactors to be very high leading to innovative designs, such as the removal of pollutants from air for electric cars (Patent, in preparation ).

The reason for isothermal behavior is explained below, as described in Gidaspow's provisional patent application for polymerization reactors.

Multidimensional, multiphase energy balances are derived in Chapter one in Gidaspow's 1994 book . The energy balance for a riser with conversion of monomer $\Delta Y$ and heat of reaction $\Delta H$ can be written as follows:

$$\rho_g v_g \varepsilon_g c_{pg} (T_{bed} - T_{in}) + \rho_s v_s \varepsilon_s c_{ps} (T_{bed} - T_{in}) = \rho_g v_g \varepsilon_g \Delta H \Delta Y \qquad (1)$$

**Net rate of energy outflow + solids outflow = rate of energy generation**

The density, $\rho_s$, is of the order of magnitude of 2 to 3 times larger than the density of gas. Therefore, the first term in the above equation can be neglected. Hence the rise in temperature becomes as follows:

$$T_{bed} - T_{in} = ((\Delta H \Delta Y)/(c_{ps}\varepsilon_s)) (\rho_{g/}\rho_s) (v_g\varepsilon_g/v_s\varepsilon_s) \qquad (.2)$$

**Adiabatic temperature rise= Conventional adiabatic temperature rise x gas to solids density ratio x slip ratio.**

The volume fractions and the velocities of the gas and the particles are of the same order of magnitude. But the ratio of the gas to solids densities is two to three orders of magnitude smaller. Hence the temperature rise in the riser is two to three orders of magnitudes smaller than that in the stirred reactor or in the bubbling bed reactors.

# Novel Synthesis and Property of Inorganic 1D/2D Nanomaterials and Their In-situ TEM Study

**by Yoshio Bando, Member EUAS**

Short Biography

*Prof. Yoshio Bando has been leading the communities of nanomaterials and electron microscopy for many years. Holding a PhD degree from Osaka University, he joined the National Institute for Research in Inorganic Materials (NIRIM) as a researcher in 1975. He was a visiting scientist at the Arizona State University, USA (1979-1981), and in 1992, he became an adjunct professor at the University of Tsukuba until 2003. He was promoted to be a supervising researcher of Advanced Beam Analysis Station of NIRIM in 1996. In 2001, NIRIM was merged with the National Research Institute for Metals to form the National Institute for Materials Science (NIMS), and he was appointed as Director of the Advanced Beam Analysis Group, followed by being appointed Director-General of International Center for Young Scientist (ICYS), NIMS. He became a NIMS Fellow in 2004 and Deputy-Director General of International Center for Materials Nanoarchitectonics (MANA), one of the nine research centers sponsored by Japan's Ministry of Education, Culture, Sports, Science and Technology (MEXT) for the World Premier International Research Center Initiative (WPI) in 2007. From 2008 to March 2017, he was responsible for the operation of MANA with the appointed position of Chief Operating Officer (COO). In addition, he was adjunct professor of University of Tokyo (2009-2012) and guest professor of Waseda University (2008-2016). Since 2017, he is an Executive Advisor of WPI-MANA in NIMS, and a Distinguished Professor at the University of Wollongong, Australia and also a Professor at Tianjin University, China since 2018.*

*Prof. Yoshio Bando has received many prestigious awards and fellowships, including the "Sacred Treasure" given from the Emperor in 2017, The 3rd Thomson Reuters Research Front Award in 2012, The Tsukuba Prize in 2005, Academician, World Academy of Ceramics in 2004, The Commendation Award by the Minister of State for Science and Technology in 1998, The Academic Award of the Ceramic Society of Japan in 1997, The Seto Award of Electron Microscopy Society of Japan in 1994, and The Science and Technology Accomplishment Award by the Minister of State for Science and Technology in 1994. In 2002, he was chosen as one of the "Top Thirty Key Persons in Nanotechnology" in Japan by the scientific journal, "Nikkei Science". He was appointed as adjunct member of the Science Council of Japan in 2006. He is also a Fellow of the American Ceramic Society and the Royal Society of Chemistry. He served as Editor-in-Chief of Journal of Electron Microscopy from 2008-2012, and was an Editorial Board Member of "Small",*

*"Journal of Nanoscience and Nanotechnology", and others. He is now an editorial board in "Nanotechnology", "Nano Energy", "Materials Horizon", "Nanomatials", "Journal of Ceramic Science and Technology" and others.*

Professor Yoshio Bando has been working on the synthesis of 1D/2D inorganic nanomaterials and detailed analysis of their atomic structures and properties using methods of advanced electron microscopy. He discovered many new nanotubes and nanowires, such as those made of BN, MgO, AlN and others. One particular highlight was the discovery of a carbon nanotube-based "nanothermometer", which is listed in the Guinness book of world records as the world's smallest thermometer. Professor Bando's research group is a world pioneer in the large-scale BN nanotube fabrication and clarified many unique properties of BN nanotubes for the first time. In particular, his group has succeeded in producing polymer composite thin films containing BN nanotubes that show excellent mechanical and thermal properties. Recently, he and his colleagues have pursued nano-property measurements inside a Transmission Electron Microscope (TEM) and performed the first ever direct bending and tensile tests on BN nanotubes. All these delicate experiments allowed them to get a clear structure-property relationship down to the nanoscale of the materials dimensions, which is the Holy Grail of the whole Materials Science.

Professor Yoshio Bando has been selected as ISI Highly Cited Researcher in Materials Science in 2012, 2014, 2015, 2016 2017, 2018 and 2019. To date, he has authored 878 original research papers that have been cited more than 50,341 times with h-index of 117 (Web of Science in January 2020). He has been registered 43 foreign patents and 159 Japanese patents.

**1) In situ property study of 1D/2D nanomaterials under TEM**

Abstract

Understanding the mechanical properties of 1D/2D nanomaterials is not only fundamentally interesting but also practically important, because of their broad applications, ranging from energy storage to composite materials, where the mechanical properties will determine the structural reliability and long-time performance. In situ transmission electron microscopy (TEM) attached with STM/AFM holders is unique for probing mechanical/electrical properties at nanometer scale, simultaneously enabling manipulation at sub-nanometer precision, quantitative mechanical measurements and deformation mechanisms at atomic resolution. In this talk, I will present our recent works on the mechanical properties of 1D/2D nanomaterials such as BN and C nanotubes, Si nanowire, $MoS_2$ nanosheet and others by applying the in situ TEM methods. Based on the stress-strain curve of BNNTs, the Young modulus was successfully determined to be about 0.9 TPs, which is comparable with CNTs. In addition to the intrinsic chemical bonding and famous size effects, we investigated the influences of the "microstructures" and external loading conditions. Due to an interlocked joint geometry, the deformation mechanism of bamboo-shaped BNNTs was switched from an interplanar sliding

mode to an in-plane tensile elongation mode, with tensile strength up to 8.0 GPa. The fracture mechanism was well given by MD simulation. Due to the different stress states, Si nanowires showed distinct deformation behaviors under tension and bending. Under tension, Si NWs deformed elastically until brittle fracture. However, under bending, the Si NWs demonstrated considerable plasticity with a crystalline-to-amorphous phase transition. Due to the surface energy, the bending behaviors of $MoS_2$ atomic layers demonstrated strong size dependence, from spontaneous rippling (<5 atomic layers) to homogeneous curving (~10 layers) and to kinking (>20 layers).

Our work has greatly enriched the understanding of mechanical properties of 1D/2D nanomaterials and offers valuable guidelines for the design of mechanically reliable nanodevices.

*(This work was presented at The 12th K.H.KuO Summer School of Electron Microscopy and Crystallography, Beijing, China, June 2019)*

**2) Low-dimensional Boron Nitride Nanomaterials for Energy Applications**

Abstract

Hexagonal boron nitride (h-BN), a layered material with a regular network of BN hexagons, is a structural sister system of famous graphite. Due to such chemical structural similarity, BN nanomaterials undergo a development history closely entangling with the carbon analogs, from fullerenes via nanotubes to nanosheets. Nevertheless, different from near metallic graphite, BN are highly insulating and wide-bandgap in properties, and more stable than graphite in thermology and chemistry. These make BN be a perfect sidekick of graphite nanomaterials, and enable their bright prospects in high thermal conductivity, strong ultraviolet emission, glorious thermal and chemical inertness, rubout insulation and superb lubrication. However the insufficient production of BN nanomaterials greatly hampered their studies and rather limited the full realization of their exciting nanotechnology potentials. Herein an overview insight into mass-synthesis and diverse applications of BN and its low-dimensional nanostructures is presented, including nanosheets, nanoribbons, nanotubes and nanoparticles developed by us. Recent year's novel methods for realizing the high purity mass production of BN nanotubes and nanosheets will be focused, which fundamentally ensures and promotes the studies and applications based on the large quantities of BN nanomaterials. Some BN nanomaterial filled polymeric composites are additionally discussed, which are expected for the heating-release insulting packaging of down-sizing faster electronic devices. In addition, in situ mechanical and electrical properties from individual BN nanomaterials have been successfully studied under the TEMs using STM/AFM-TEM special holders.

*(This work was presented at the 3rd International Conference on Emerging Advanced Nanomaterials, Newcastle, Australia, November 2018)*

# Toward Data Science Computing Model: Interactive Granular Computing (IGrC)

## by Andrzej Skowron, Member EUAS

Short Biography

***Andrzej Skowron,*** *ECCAI and IRSS Fellow, Member EU Academy of Sciences, received the Ph. D. and D. Sci. (habilitation) from the University of Warsaw in Poland. In 1991 he received the Scientific Title of Professor. He is Full Professor in the Systems Research Institute, Polish Academy of Sciences as well as in Digital Research Center of Cardinal Stefan Wyszyński University in Warsaw. He is Emeritus Professor in Faculty of Mathematics, Computer Science and Mechanics at the University of Warsaw. Andrzej Skowron is the (co)author of more than 400 scientific publications and editor of many books and volumes of conference proceedings. His areas of expertise include reasoning with incomplete information, approximate reasoning, soft computing methods and applications, rough sets, rough mereology, granular computing, intelligent systems, knowledge discovery and data mining, decision support systems, adaptive and autonomous systems, perception based computing, and interactive computational systems. He was the supervisor of more than 20 PhD Theses. In the period 1995-2009 he was the Editor-in-Chief of* Fundamenta Informaticae *journal. He is on Editorial Boards of many others international journals. Andrzej Skowron was the President of the International Rough Set Society from 1996 to 2000. He has delivered numerous invited talks at international conferences including a plenary talk at the 16th IFIP World Computer Congress (Beijing, 2000), a keynote talk at the 8th Joint Conference on Information Sciences (JCIS 2005) (encompassing 12 individual conferences and workshops) (USA, 2005), an invited talk at the 2006 IEEE/WIC/ACM International Conference on Intelligent Agent Technology (IAT 2006) and on Web Intelligence (WI 2006) (Hong Kong, 2006), and a plenary talk at the 2nd World Congress on Biologically Inspired Computing (Japan, 2010). He was serving as (co-)program chair or PC member of more than 200 international conferences. He was involved in numerous research and commercial projects including dialog-based search engine (Nutech), fraud detection for Bank of America (Nutech), logistic project for General Motors (Nutech), algorithmic trading (Adgam), control of UAV (Linköping University), and medical decision support (e.g., in Polish-American Pediatric Clinic in Cracow). Andrzej Skowron was on the ICI Thomson Reuters/ Clarivate Analytics lists of the most cited researchers in Computer Science (globally) in 2012, 2016, 2017.*

**EXTENDED ABSTRACT**[1]

The problem of understanding intelligence is treated, by some prominent researchers, as the greatest problem of this century. In one of the recent issues of *ERCIM News*, there is an explanation of the title of the issue *Smart Things Everywhere* emphasizing that it is more than Internet of Things or Industrial Internet of Things because it encompasses in

particular intelligence, cognitive systems and technology, machine learning and AI. In our research we assume that to justify a decision support systems to be intelligent there is a need for developing new reasoning tools which can also take into account the significance of sensory measurement, experience and perception of situations (i.e., understanding of situations in the physical world to a satisfactory degree for making relevant decisions). We research how such reasoning, called adaptive judgment, can be performed over objects interacting in the physical world using Interactive Granular Computing Model (IGrC). The basic objects in IGrC are called the complex granules. They make it possible to link the abstract and physical worlds, and help to realize the paths of judgments starting from sensory measurement and experience to perception. The IGrC model, which creates the foundation of Wisdom Technology for Intelligent Systems, is very much needed in different domains of applications. Some details are discussed below.

Rough sets, introduced by Zdzisław Pawlak [1], play a crucial role in the develop-ment of Granular Computing (GrC) [2–4]. The extension of GrC to IGrC (initiated by Skowron and co-workers [5–7][2]), requires generalization of the basic concepts of rough sets and GrC. For instance, it is needed to shift from granules to complex granules (including both physical and abstract parts), information (decision) systems to interactive information (decision) systems as well as methods of inducing hierarchical structures of information (decision) systems to methods of inducing hierarchical structures of interactive information (decision) systems. IGrC takes into account the granularity of information as used by humans in problem solving, as well as interactions with (and within) the real physical world. The computations in this IGrC model are realized on the interactive complex granules and that must be based on the consequences of the interactions occurring in the physical world. It is worthwhile to cite here the following opinion [8]:

It seems that we have no choice but to recognize the dependence of our mathematical knowledge (...) on physics, and that being so, it is time to aban-don the classical view of computation as a purely logical notion independent of that of computation as a physical process.

Consequently, the computational models in IGrC related to the complex phenomena cannot be constructed solely in an abstract mathematical space. They must also take into account continuous interactions with and within the real physical space. In particular, the computational models cannot ignore the laws of physics. It is worthwhile to cite here the opinion of Immanuel Kant (see [9], p. 4):

[...] cognition is the result of the interaction of two independent agents, the mind and the real object.

With the interaction rules learned from the acquired data through computations an agent can approximate complex vague concepts related to the expectations of the agent. This agent itself can be regarded as a complex granule. The objective of IGrC is also in line with the proposition of Fredrick Brooks (a recipient of the Turing Award). According to him [10]:

Mathematics and the physical sciences made great strides for three cen-turies by constructing simplified models of complex phenomena, deriving, properties from the models, and verifying those properties experimentally. This worked because the complexities ignored in the models were not the essential properties of the phenomena. It does not work when the complexities are the essence.

The IGrC models, in the form of complex networks of complex granules, have to be created adaptively and autonomously through a process of continuous interaction with real world. Due to the uncertainty in the perception of situations different local models, which are discovered, can be inconsistent with each other; but their relevant aggregation should

lead to the discovery of a new knowledge about the perceived situation. It should be noted that models created in the abstract space must be also able to adapt to the changes perceived in the external physical reality. The main aim of the current research in IGrC is to develop the IGrC models over complex granules. More compound granules are represented by networks of interacting simpler granules changing with time. Any IGrC model must also be able to direct the attention of complex granules (e.g., agents) to focus on the significant fragments of the reality that are measured by the sensors and explored by the actuators used in performing the actions or plans. Results of interactions are collected in information systems (data tables), which constitute some fragments of the complex granules.

Following another Turing Award winner, Leslie Valiant, these tables are then aggregated to create new complex granules as computational building blocks for cognition[3].

There are many challenges related to IGrC. Some of them are related to reasoning, called adaptive judgment [11, 12], about properties of complex granules and interactive computations over them. One of the main aim of adaptive judgment performed by complex granules (e.g., agents) is to derive conclusions regarding selection of action(s) that should be currently initiated (or terminated). The actions are activated on the basis of the satisfiability of some complex vague concepts labelled by actions. It should be noted that these concepts are drifting with time. Adaptive learning of such concepts based on judgment is a great challenge[4]. The whole process towards inducing approximation of these vague concepts labelled by actions may be treated as a process of discovery of a complex game. In such a game, the concepts (along with their respective associated judgement mechanism) can be treated as the players. These players using their judgement mechanism can derive arguments for and against the satisfiability of the concepts on the basis of the information about the perceived situation. Furthemore, there are other judgment mechanisms, in the hands of a judge, that can be used to resolve conflicts among the collected arguments to select the winning player (concept). Then actions labelling the winning concepts are initiated.

It should be also noted that approximation of the complex vague concept should be based on a notion of adaptive judgment rather than only on the basis of partial inclusion of sets which is widely used in the rough set approach. The former approach is much more general than the latter one. The approach based on judgment is especially relevant when in data analysis it is required to have a deeper judgment about the perceived complex situation related to the classification of complex vague concepts. The approach based on partial containment of sets alone is not satisfactory for dealing with many real-life applications, where more advanced judgment should be made to identify the perceived situation, to classify it relative to the complex vague concepts or to reason about risk for supporting the decision making. In particular, it is needed to develop new logical tools for reasoning based on judgment toward approximation of complex vague concepts, i.e., the rough set approach based on adaptive judgment performed over computations on complex granules. This, in particular, creates a room for extensions of rough sets to adaptive rough sets and rough sets over distributed networks of granules changing with time.

Another challenging research direction is related to self-organization in synthesis of complex granules and their networks.

Finally, it is worthwhile mentioning that IGrC is also in agreement with the recently raised discussions about the Turing test for intelligence. In addition to linguistic as-pects and reasoning, it incorporates perception and actions, and it follows what Leslie Valiant's calls ecorithms [14, 15].

The proposed model of computation based on complex granules seems to be of fundamental importance for developing intelligent systems dealing with complex phenomena, in particular in such areas as Data Science, Internet of Things, Wisdom Web of Things, Cyber Physical Systems, Complex Adaptive Systems, Natural Computing, Software Engineering, applications based on Blockchain Technology, etc (see, e.g., the first works using IGrC related to some of these domains [16, 7, 17]).

## Notes

1 This is the extended abstract of the keynote talk of Andrzej Skowron delivered at the CS&P 2019 workshop and prepared in cooperation with Dr Soma Dutta and Professor Andrzej

2 see also publications about IGrC listed at https://dblp.uni-trier.de/pers/hd/s/ Skowron:Andrzej

3 see https://people.seas.harvard.edu/~valiant/researchinterests.htm

4 Some progress in this direction was made using reinforcement learning but much more work should be done when we deal with complex real-life applications (see, e.g., [13].

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16. Skowron, A., Jankowski, A.: Interactive computations: Toward risk management in interac-tive intelligent systems. Natural Computing 15(3) (2016) 465 – 476
17. Dutta, S., Jankowski, A., Rozenberg, G., Skowron, A.: Linking reaction systems with rough sets. Fundamenta Informaticae 165 (2019) 283–302

# Progress in Nanomagnetism

## by Hartmut Zabel, Member EUAS

Short Biography

***Education/Degrees:***

*1969 Bachelor in Physics, University of Bonn*
*1973 Master in Physics, Technical University of Munich*
*1978 Ph.D. in Physics, University of Munich*

***Academic Positions:***

*1978 - 1979 Postdoctoral Fellow, Department of Physics, University of Houston, Texas*
*1979 - 1983 Assistant Professor of Physics, University of Illinois at Urbana - Champaign*
*1983 - 1986 Associate Professor of Physics, University of Illinois at U - C*
*1986 - 1989 Professor of Physics, University of Illinois at U - C*
*1989 - 2013 Chair, Prof. of Experimental Physics/Solid State Physics, Ruhr-Univ. Bochum*
*2013 – 2018 Visiting Senior Research Professor, University of Mainz*
*since 4/1989 Adjunct Professor of Physics, University of Illinois at U - C*

***Guest positions:***

*Summer Guest Scientist, Brookhaven National Laboratory, 1985 and 1988; Guest Scientist, Risø National Laboratory, Denmark, 1986; Guest Scientist of the NIST, Reactor Division, Gaithersburg, USA, 1993; Guest Scientist of the Institut Laue-Langevin, Grenoble, France, 1997; Guest Scientist and Lecturer, University of Uppsala and KTH Stockholm, Sweden, 1998/99; Senior Guest Research Professor, University of Mainz, Germany, 2013-2018.*

***Fellowships/Awards:***

*Fellow of the Cusanus Fellowship Program for Superior Students, 1971 – 1973; Fellow of the Institute for Advanced Studies, University of Illinois at Urbana-Champaign, 1982; Fellow of the JSPS, 1989; Fellow of the Volkswagenstiftung, 1993 and 1997; Election to Fellow of the APS, 1996; Honorary Doctor of the KTH Stockholm, 2001; Elected "Outstanding Referee" of the APS, 2010; MAINZ Research Award, J G University Mainz, 2013; Elected Member, European Academy of Sciences, 2017.*

***Professional activities:***

*Advisor and Co-advisor of 51 PhD students with successful thesis completion, referee work for more than 25 journals, referee for more than 15 funding agencies, member of numerous national and international PhD disputation panels, organization of 4 international conferences and 4 summer schools, member of numerous advisory boards of national and international conferences, Chief Editor of the Elsevier Journal: Superlattices and Microstructures, Elsevier (2003-2013);Member and Chair of the scientific councils at the Hahn-Meitner Institute Berlin, Institut Laue-Langevin, Grenoble, Materials Research Laboratory, University of Illinois at U – C.*

***Publications:***

*More than 500 refereed scientific publications in technical journals, 36 review papers and book chapters, editor of five books , author of the textbook "Physik" , Thieme publisher, 2nd edition 2016, Textbook "Medical Physics", de Gruyter publisher, 1st edition 2017.*

***Research activities:***
*Physical properties of hydrogen in metals; structure, dynamics, and magnetism of graphite intercalation compounds; strain state and strain relaxation in semiconductor heterostructures; order and disorder in metal superlattices and heterostructures; oxidation of epitaxial metal films; magnetic phase transitions in rare earth films and superlattices, phonons in layered compounds; magnetism of thin films and heterostructures; proximity effects between superconductors and ferromagnets; tuning of magnetism in spintronic materials; shear behavior of polymer chains; shear induced order of micellar polymer solutions; relaxation rates of polymer micelles; sliding and depletion lengths of Newtonian fluids at the solid-liquid interface; magnetic x-ray and neutron scattering, magneto-optics; magnetic nanostructures with spin-ice properties; magnetic nanoclusters, odd-triplett superconductivity; time-resolved magnetization precession and magnetization reversal processes, antiferromagnetic spintronics.*
***Teaching activities:***
*Introductory Physics Course; Modern Physics; Condensed Matter Physics; X-ray and neutron scattering; Exploring Condensed Matter at Large Scale Facilities; Physical Properties of Hydrogen in Metals; Condensed Matter Magnetism; Medical Physics. Numerous Lectures at National and International Summer Schools.*

# Selection of publications in the years 2018 – 2019

## Experimental determination of exchange constants in antiferromagnetic $Mn_2Au$

A. A. Sapozhnik, C. Luo, H. Ryll, F. Radu, M. Jourdan, **H. Zabel**, and Hans-Joachim Elmers, Physical Review B **97**, 184416 (2018),
DOI: 10.1103/PhysRevB.97.184416

Abstract

$Mn_2Au$ is an important antiferromagnetic (AF) material for spintronics applications. Due to its very high Néel temperature of about 1500 K, some of the basic properties are difficult to explore, such as theAF susceptibility and the exchange constants. Experimental determination of these parameters is further hampered in thin films by the unavoidable presence of uncompensated and quasiloose spins on antisites and at interfaces. Using x-ray magnetic circular dichroism (XMCD), we measured induced perpendicular spin and orbital moments for a $Mn_2Au$(001) film in fields up to ±8 T. By performing these measurements at a low temperature of 7 K and at room temperature (RT), we were able to separate the loose spin contribution from the susceptibility of AF coupled spins. The value of the AF exchange constant obtained with this method for a 10-nm-thick $Mn_2Au$(001) film is (22 ± 5) meV.

## Gilbert damping in NiFeGd compounds: Ferromagnetic resonance versus time-resolved spectroscopy

R. Salikhov, A. Alekhin, T. Parpiiev, T. Pezeril, D. Makarov, R. Abrudan, R. Meckenstock, F. Radu, M. Farle, **H. Zabel**, and V. V. Temnov
Physical Review B **99**, 104412 (2019), DOI: 10.1103/PhysRevB.99.104412

Abstract

Engineering the magnetic properties (Gilbert damping, saturation magnetization, exchange stiffness, and magnetic anisotropy) of multicomponent magnetic compounds plays a key role in fundamental magnetism and its applications. Here, we perform a systematic study of (Ni81Fe19 )100−*x*Gd*x* films with $x = 0\%$, 5%, 9%, and 13% using ferromagnetic resonance (FMR), element-specific time-resolved x-ray magnetic resonance, and femtosecond time-resolved magneto-optical pump-probe techniques. The comparative analysis of field and time domain FMR methods, with complimentary information extracted from the dynamics of high-frequency exchange magnons in ferromagnetic thin films, is used to investigate the dependence of Gilbert damping on the Gd concentration.

**Exchange bias in epitaxial $Mn_2Au$(001)/Fe(001) bilayers**
A A Sapozhnik, M Jourdan, **H Zabel**, M Kläui and H-J Elmers
J. Phys. D: Appl. Phys. **52,** 465003 (2019),
https://doi.org/10.1088/1361-6463/ab3966

Abstract

A major step to implement antiferromagnetic $Mn_2Au$ in spintronics is to understand the exchange bias (EB) mechanism in $Mn_2Au$/ferromagnet bilayers, which can provide an opportunity for reading the magnetic state of $Mn_2Au$ via TMR. A very high bulk Néel temperature of $Mn_2Au$ (>1500 K) renders its magnetic structure very robust. For this reason, generating an EB by field cooling (FC) in high-quality epitaxial $Mn_2Au$/ferromagnet bilayers is a challenging task. We succeeded in inducing an EB in such systems by tuning the growth conditions of $Mn_2Au$. Our results indicate that the EB effect increases with decreasing atomic order of the $Mn_2Au$ films and can reach EB fields up to 200 Oe. This large EB effect reveals the importance of disorder and interfacial pinning in $Mn_2Au$ for its appearance.

**Ultrafast negative thermal expansion driven by spin disorder**
J. Pudell, A. von Reppert, D. Schick, F. Zamponi, M. Rössle, M. Herzog, **H. Zabel**, and M. Bargheer
Physical Review B **99**, 094304 (2019);
https://doi.org/10.1103/PhysRevB.99.094304

Abstract

We measure the transient strain profile in a nanoscale multilayer system composed of yttrium, holmium, and niobium after laser excitation using ultrafast x-ray diffraction. The strain propagation through each layer is determined by transient

changes in the material-specific Bragg angles. We experimentally derive the exponentially decreasing stress profile driving the strain wave and show that it closely matches the optical penetration depth. Below the Néel temperature of Ho, the optical excitation triggers negative thermal expansion, which is induced by a quasi-instantaneous contractive stress and a second contractive stress contribution increasing on a 12-ps timescale. These two timescales were recently measured for the spin disordering in Ho [Rettig *et al.*, Phys. Rev. Lett. **116**, 257202 (2016)]. As a consequence, we observe an unconventional bipolar strain pulse with an inverted sign traveling through the heterostructure.

# Disorder and Interface Dominated Architected Metastable Materials

## by Jürgen Eckert, Member EUAS

Short Biography

*Jürgen Eckert obtained his Ph.D. (German: Dr.-Ing.) in Materials Science and Engineering at the Friedrich-Alexander-University Erlangen-Nuremberg, Germany in 1990. During collaborative research work with the Siemens Research Laboratories in Erlangen, he started research on the formation of amorphous and quasicrystalline alloys through interdiffusion, and subsequently extended it during a two and a half year postdoctoral stay at the California Institute of Technology. There he worked on the formation of nanocrystalline alloys via mechanical alloying. After a short break in industry, he moved to the Leibniz-Institute for Solid State and Materials Research (IFW) Dresden, one of the leading Materials Research Science Centers in Germany. From 1996 until 2003 he was the Head of the Department Metastable and Nanostructured Materials at IFW Dresden, before he became Full Professor for Physical Metallurgy at TU Darmstadt. In 2006 he was appointed Director of the Institute for Complex Materials at IFW Dresden, and concurrently held the Chair for Synthesis and Analysis of Materials at Dresden University of Technology (TU) Dresden. In 2013/2014 he served as the Scientific Director of IFW Dresden. In 2015 he moved to Austria as Chair Professor of Materials Physics at Montanuniversität Leoben, and Director of the Erich Schmid Institute of Materials Science of the Austrian Academy of Sciences. He also held an Adjunct Professor Position at Michigan Technological University, Houghton, USA between 2002 and 2005, and was a Visiting Professor at University of Vienna, Austria at the Institute of Physics, Physics of Nanostructured Materials (2009 / 2010 / 2012).*

*He is an international expert in the field of metastable materials and has published more than 1150 papers in archival journals (h-index: 79 (WoS), more than 32.000 citations). He also published more than 150 conference papers, 18 book chapters, edited 6 books, conference proceedings and journal issues, holds more than 20 patents, and delivered so far 220 plenary, keynote and invited presentations.*

*Jürgen Eckert was honored as Dr. honoris causa (Dr. h.c.) by the Slovak University of Technology in Bratislava, Slovak Republic (2012), and received the prestigious Gottfried Wilhelm Leibniz Award of the German Research Foundation (2009), the highest Science Prize and scientific honor in Germany. Other honors include the DGM-Prize 2014 of the German Materials Research Society, an ERC Advanced Grant of the European Research Council (2013), the ISMANAM Senior Scientist Award (2012), the Hsun Lee Lecture Award of the Chinese Academy of Sciences (2006), the Georg-Sachs-Prize of the German Materials Research Society and the Austrian Metal Industry (1997), and the FEMS Materials Science and Technology Prize of the Federation of European Materials Science Societies (FEMS) in 1997. In addition, he received the Young Scientist Award of the German Materials Research Society (1994), and the ISMANAM Young Scientist Award (1997). He is a corresponding Member of the Section Mathematics-Natural Sciences of the Austrian Academy of Sciences (2017), a Member of the EU Academy of Sciences (2018) and has been elected to the class of 2018 MRS Fellows of the Materials Research Society, USA (2018). Most recently, he was awarded an ERC-Proof of Conept Grant of the European Research Council (2019) for his work on thin film metallic glasses for tribological applications.*

Jürgen Eckert's research fields and scientific interests include phase formation, processing and structure-property correlations of metastable materials processed under non-equilibrium conditions; processing of materials by mechanical alloying/milling; structural and functional materials and metal matrix composites with particular emphasis on solidification fundamentals; rapid solidification

processing; additive manufacturing techniques; biocompatible, magnetic and superconducting materials, and materials for energy applications and energy harvesting (e.g. next generation batteries, supercapacitors, carbon materials, materials for hydrogen storage) and thin film systems for flexible electronics; solidification of metal matrix composites; mechanical and electrochemical properties of bulk materials, coatings and surfaces; biologically inspired far-from-equilibrium materials and architected structures; mathematical modelling of advanced materials and processes.

Over the years, Jürgen Eckert and his team have provided sustained contributions to research on metastable advanced high performance materials. Early work was devoted to work in the field of glass and quasicrystal formation in metallic systems, and fundamental observations on the development of nanoscale grain sizes in metallic materials. Later on the focus shifted to the development and property optimization of (Zr-, Ti-, Al-, Fe-, Mg-base) bulk metallic glasses (to mention a few) and their composites. In this field the work concentrated on developing plastically deformable bulk metallic glasses and composites through a synergistic approach by understanding how atomic scale structures, microstructural features and stress, plus processing-induced heterogeneities determine the mechanisms of plastic deformation on different length scales such as to overcome the otherwise unavoidable brittleness of glassy materials. Subsequently, this work developed into areas beyond metallic glasses creating new strategies for the design, synthesis and characterization of intrinsic length-scale modulation and phase transformations under highly non-equilibrium conditions. This concept defined new routes for creation of tailored nanostructured or ultrafine-grained structural and functional materials based on scale-bridging intelligent hybrid structures. Accordingly, this work expanded into high-strength lightweight applications, hard and soft magnetic materials, porous bulk materials and hybrid structures for biomedical applications, materials for energy applications (metals, oxides, hierarchical carbon structures), and also touched on surface modification and development of architected gradient structures.

Jürgen Eckert's recent research activities focus on the development and application of methods for in-depth *in situ* and in operando investigation of phase transformations and structure-property correlations using local probes and high resolution techniques for structure characterization and imaging of local structures, chemical compositions and interaction of nanoscale objects with external fields and stimuli (e.g. mechanical, thermal, electrical, magnetic fields). The vision behind this approach is to create and test tailored biologically inspired far-from-equilibrium materials, hierarchical structures and correlated systems *in situ*, for example in a microscope or through flash annealing at extreme heating and cooling rates. This allows controlling the desired material structure and additionally enables direct observation of the effect of structure on physical or mechanical properties. An example for such an attempt is the *in situ* design and testing of glassy metallic structures containing heterogeneities on different length-scales to overcome their

intrinsic brittleness. These heterogeneities can be induced through different stimuli, for example a heat source, a laser, an ion or an electron beam. To study the deformation at the nanoscale, *in situ* tests are carried out within a transmission electron microscope or by using highly focused local probes at synchrotron beamlines. The concept of *in situ* design and testing is applicable to bulk structures and thin film systems and to a wide range of materials, and is therefore expected to open a new research avenue for creating materials with unique properties by design. Some of the key publications in this area include


- B. Sarac, Y.P. Ivanov, T. Karazehir, M. Mühlbacher, B. Kaynak, A.L. Greer, A.S. Sarac, J. Eckert, "Ultrahigh Hydrogen-sorbing Palladium Metallic-Glass Nanostructures", Mater. Horizons 6, 11481 (2019).
- O. Glushko, M. Mühlbacher, C. Gammer, M.J. Cordill, C. Mitterer, J. Eckert, "Exceptional Fracture Resistance of Ultrathin Metallic Glass Thin Films due to an Intrinsic Size Effect", Sci. Reports 9, 8281 (2019).
- B. Sarac, Y.P. Ivanov, A. Chuvilin, T. Schöberl, M. Stoica, Z. Zhang, J. Eckert, "Origin of Large Plasticity and Multiscale Effects in Iron-Based Metallic Glasses", Nature Commun. 9, 1333 (2018).
- C. Gammer, C. Ophus, T.C. Pekin, J. Eckert, A. Minor, "Local Nanoscale Strain Mapping of a Metallic Glass During In-Situ Testing", Appl. Phys. Lett. 112, 171905 (2018).


The long range perspective of these approaches and experiments is to further advance the understanding of structure-property correlations for hierarchically modulated structures and hybrid systems over a variety of different length-scales under highly non-equilibrium thermodynamic and kinetic conditions. The goal is to gain a descriptive and quantitative picture of phase formation, transformation, dynamics and property design under extreme conditions, such as ultra-fast heating and cooling on extremely short time scales with or without external mechanical, electrical or magnetic stimulus. Whereas some of these approaches are already followed for crystalline materials, research on disordered and interface dominated materials along these lines touches almost unknown grounds, since the structural diversity represented by disorder in a material represents a holy grail of materials science and promises to overcome the compositional and structural constraints of crystalline materials. The ability to predict and design disorder in architected materials with unique functionality via property-directed material design provides vast opportunities for new structural and functional materials including high-strength-lightweight systems, biomedical implants or micromechanical components with unique performance characteristics. But not only the basic fundamental mechanisms of structure formation and property development are of interest, but also the question how the findings can be transferred into parts, devices and systems for MEMS/NEMS, sensor and actuator applications, flexible microelectronics, as well as into materials for energy applications and energy harvesting. Also biocompatible (biodegradable) bulk materials, porous structures, coatings and surfaces are in the focus of interest, e.g. for tailored orthopedic implants or for

advanced personalized medical devices.

For this purpose state-of-the-art techniques from the fields of materials physics, structure analysis, *in situ* structure investigations under different applied fields (e.g. mechanical, electrical, magnetic), and also structure-biological mimetic and 3d printing techniques are used to generate architected materials built from disordered building blocks. Modelling and simulation supplement and strengthen the experimental efforts. Multi-scale modelling techniques based on hierarchies of overlapping scales including quantum mechanics based structure modelling, atomistic modelling and numerical methods can be involved. A variety of simulation and modelling of length and time scales is utilized, and complemented by Bayesian Interference (BI) and machine learning algorithms to better characterize the local property statistics not assessable with direct measurements. The outcome of this approach allows for both a quantitative parameterization of local properties and protocols by which they are, in general, to be measured. This is a vital input for property-directed material design of disordered systems, and promises to open new avenues for nanoscale structure formation in architected materials with unique functionality through generating an atomic structural – functional understanding of the properties, performance and correlation of hierarchical thin film structures and membranes, tailored interface structures, nano- and multiscale hybrid systems and tailored “lattice materials”.

# Artificial Intelligence & Robotic Solutions for Complex Applications

## by Andrew Goldenberg, Member EUAS

Short Biography

*Dr. Goldenberg is the founder of Engineering Services Inc. (ESI) - www.esit.com, established in 1982. ESI is a high-technology company involved in the development of robotics-based automation and technology. Under his leadership the company has achieved significant growth and a global leading role in a wide range of industrial sectors. From 2000 - 2001 Dr. Goldenberg was also the President of Virtek Engineering Science Inc. (VESI), a high-technology company formed after the acquisition of part of ESI by Virtek Vision International Ltd., a publicly listed company. Dr. Goldenberg is also President of ANVIV Mechatronics Inc. (AMI), which he founded in 2006. ANVIV is a high-technology company involved in the development of mechatronics products.*

*In May 2015 ESI has been acquired by a Chinese consortium located in Shenzhen, P.R. China. He has been the President of ESI after the acquisition until the Chinese consortium became a public company listed in Hong Kong. Dr. Goldenberg has been the Chief Technology Officer of the public company until May 12, 2019. Dr. Goldenberg left the public company in May 2019.*

*Dr. Goldenberg is also the founder of the field of Robotics at University of Toronto where he has been since 1982 as a Professor of Mechanical and Industrial Engineering, cross appointed in the Institute of Biomaterials & Biomedical Engineering, and previously cross-appointed in the Electrical and Computer Engineering. He is currently a Professor Emeritus. Dr. Goldenberg is also an Adjunct Professor at Ryerson University, Guest Professor at Nanjing University of Science and Technology, P.R. China and Guest Professor at the Institute of Biomedical Engineering, Chinese Academy of Science, Tianjin, P. R. China. From 1975-1981 Dr. Goldenberg has been an employee of SPAR Aerospace Ltd., of Toronto, working on the development of the first Space Shuttle Remote Manipulator System (Canadarm).*

*Dr. Goldenberg has supervised to-date the largest number of graduate students in the Faculty of Applied Science and Engineering (46 PhD and 64 MASc). He has an exceptional publication record with over 7500 citations (128 archival journal papers, 294 papers in major conferences, 15 book chapters and 85 patents granted and applied).*

*As of May 2019, he has returned to the University on part-time basis to work on graduate research in the use of Artificial Intelligence in Advanced Robotics, focusing on Personal Service Robots.*
*Dr. Goldenberg is a Life Fellow of the Institute of Electrical and Electronics Engineers, Inc. (IEEE), a Fellow of the American Society of Mechanical Engineers (ASME), a Fellow of the Engineering Institute of Canada (EIC), a Fellow of the Canadian Academy of Engineering (CAE), a Fellow of The American Association for the Advancement of Science (AAAS), a Member of the Professional Engineers of Ontario (PEng), and a Designated Consulting Engineer in Ontario. He is the recipient of the 2010 PEO Engineering Medal for Entrepreneurship, the 2013 EIC Sir John Kennedy Medal for Outstanding Merit in the Engineering Profession and the 2016 IEEE A.G.L. McNaughton Gold Medal for Exemplary Contributions to the Engineering Profession.*

*Dr. Goldenberg is a former editor of the archival international journal IEEE Transactions on Robotics and Automation, and a member of the editorial boards of Robotica, Robotics in Japan,*

*Journal of Robotics, Robotics Journal, Scientific World Journal, Industrial Engineering and Management Journal, SOJ Robotics and Automation and International Journal of Automation and Computing.*

*Dr. Goldenberg obtained the PhD degree in 1976 at the University of Toronto, and the M.A.Sc and B.Sc. degrees at the Technion, Israel Institute of Technology, in 1969 and 1972, respectively. Dr. Goldenberg was born in Bucharest, Romania.*

## Description of Current Research

In the recent years Artificial intelligence (AI) has been frequently mentioned in conjunction with robotic solutions for complex applications, leading to considerations of Machine Learning capabilities in the robotics domain. While AI is not yet close enough to reaching its full potential, as it continues to advance, the field of robotics will advance alongside with it. In the context of robotic systems, AI embedded in the robots would allow them to autonomously perform complex tasks that cannot be done based on the state-of-the-art knowhow.

My laboratory and company's robotics business include development projects in which the AI plays a key role. The business development focuses on applications where the key feature is the execution of autonomous tasks. The emerging 'Intelligent Robots' will eventually co-exist with humans in such a way that there will be benefits to humans from their interaction and association with Autonomous Robots.

Our Intelligent Robots applications are in the following domains: Intelligent Home, Robot as a Service (RaaS), Health Care, Personal Robots, Security Robots.

The main thrust of the research is to address two distinct issues in the AI-embedded robots. Well-established AI methods typically require significant a priori knowledge of the task and environment. Also, uncertainties are modelled as a probability field, and the convergence of the learning processes is dependent on optimization criteria. These approaches have the following shortcomings:

- extensive a priori training;
- use of probability to quantify uncertainties
- use of optimization to converge the learning process

The research aims to provide significant relief from these limitations by introducing new AI methodologies: (i) Repetition Practising (RP); (ii) Advanced Control Embedded with Dynamic Motion Primitives (ACDMP); and (iii) Model-free control using contact task coordinates (MFHC). Established AI methodologies

will provide the key tools required to achieve their implementation.

With the new approaches embedded into the control of a robot systems there are two improvements:

1. Extensive training typically required by traditional AI approaches can be dramatically reduced. From a practical point of view, the difference is a dramatic improvement in the implementation. Using traditional methods, a detailed digital model of the robot, target and environment needs to be generated, parameterized and then learned by the embedded AI controller. This is a time and effort- intensive exercise with the end results being valid only if the digital model is a valid approximation of the real world. Any substantive change to the real world implies that a new digital model needs to be created and the learning be repeated.

With the new approach of repetition practising (RP), the actual learning by the robot can be performed in the real environment in a few repeated iterations. The implications are significant: (a) if the environment changes, the learning steps can be repeated with the actual robot; and (b) if the task changes, the new task can be learned directly in the real world. This is a paradigm shift in the application of AI to robotic systems.

2. Use of probability to quantify uncertainties and optimization to converge the learning process required by traditional AI approaches can be diminished. From a practical point of view, the difference is a dramatic improvement in the implementation. Using traditional methods, management of uncertainties requires quantification of the uncertainties done using probabilities of occurrence. Furthermore, the convergence of the learning process is dependent on optimization criteria that are difficult to generate. Instead, it is proposed to embed well established control methods in the trajectory generation based on imitation learning using dynamic motion primitives. The advanced control methods would steer the trajectories towards the targeted goal in the presence of location or shape uncertainties. This method of convergence could still be enhanced using Reinforcement Learning to obtain the optimal solution.

With the new approach of fusing advanced control methods with the dynamic motion primitives (ACDMP) the robot control is significantly improved as follows: (i) if the environment changes, the ACDMP can be repeated with the actual robot in real time; (ii) if the task changes, the ACDMP can control the new task directly without learning. This is a paradigm shift in the application of AI to robotic systems

# Aerosol Sciences and Nanoparticle Technology to Biophysics

## by Wolfgang Kreyling, Member EUAS

Short Biography

*Wolfgang G. Kreyling is a biophysicist recently retired from the Helmholtz Center Munich – German Research Center for Environmental Health (HMGU) where he coordinated all aerosol and engineered nanoparticle related research across five HMGU-institutes spanning research and development ranging from material sciences to toxicology and epidemiology. He additionally chaired the research and development program of the HMGU's Institute of Lung Biology and Disease on dosimetry of ultrafine aerosol particles and engineered nanoparticles in the respiratory tract and secondary target organs like the cardiovascular and the central nervous system. He currently serves as an external scientific advisor of the HMGU Institute of Epidemiology 2.*

*His research interests range from aerosol sciences and nanoparticle technology to biophysics of the lungs reaching from the particle characterization to dosimetry and nanoparticle lung interactions on the level of the entire organism, cells like alveolar macrophages, and molecular compounds. In 1985-1985 Dr. Kreyling spent a sabbatical year in the Respiratory Biology Program at the Harvard School of Public Health, and that collaboration continues to this day. From 1999 until his retirement Dr. Kreyling also coordinated toxicological and epidemiological collaborations between the U.S. Environmental Protection Agency, National Health and Environmental Effects Research Laboratory, and HMGU on ambient air pollution research. In recent years he has been very much engaged with the International Society for Aerosols in Medicine, serving as its President from 2003-2005. He also served as a member of several expert panels of International, European and German committees. He is currently an associated editor of Particle & Fibre Toxicology as well as an editorial board member of several international particle-related journals. He has published more than 250 peer-reviewed articles and book chapters and reports of international panels. Dr. Kreyling was recently named a Highly Cited Researcher (2014, 2015 and 2016) by Thomson Reuters and was announced as one of the world's leading scientific minds in toxicology.*

## Recent Research

Kreyling WG, Holzwarth U, Schleh C, Hirn S, Wenk A, Schäffler M, Haberl N, Semmler-Behnke M, Gibson N: **Quantitative biokinetics over a 28 day period of freshly generated, pristine, 20 nm titanium dioxide nanoparticle aerosols in healthy adult rats after a single two-hour inhalation exposure.** Particle and Fibre Toxicology 2019, 16:29, (DOI: 10.1186/s12989-019-0303-7).

### Abstract

**Background:** Industrially produced quantities of $TiO_2$ nanoparticles are steadily rising, leading to an increasing risk of inhalation exposure for both professionals

and consumers. Particle inhalation can result in inflammatory and allergic responses, and there are concerns about other negative health effects from either acute or chronic low-dose exposure.

**Results:** To study the fate of inhaled $TiO_2$-NP, adult rats were exposed to 2-hour intra-tracheal inhalations of $^{48}$V-radiolabeled, 20nm $TiO_2$-NP aerosols (deposited NP-mass 1.4±0.5 µg). At five time points (1h, 4h, 24h, 7d, 28d) post-exposure, a complete balance of the [$^{48}$V]$TiO_2$-NP fate was obtained by quantifying the [$^{48}$V]$TiO_2$-NP in selected organs, tissues, carcass, lavage and body fluids, including excretions.

After fast mucociliary airway clearance (fractional range 0.16-0.31), long-term macrophage-mediated clearance (LT-MC) from the alveolar region is twice as high after 28d (integral fraction 0.31±0.04) as translocation across the air-blood-barrier (integral fraction 0.15±0.01). There was no detectable lymph-node clearance. A high NP fraction remains in the alveoli (0.44±0.05 after 28d), half of these on the alveolar epithelium and half in interstitial spaces. There is clearance from both retention sites at fractional rates (0.02-0.03 $d^{-1}$) by LT-MC. Prior to LT-MC, [$^{48}$V]$TiO_2$-NP are re-entrained to the epithelium as reported earlier for 20nm inhaled gold-NP (AuNP) and iridium-NP (IrNP).

**Conclusion:** Comparing the 28-day biokinetics patterns of three different inhaled NP materials $TiO_2$-NP, AuNP and IrNP, the long-term kinetics of interstitial relocation and subsequent re-entrainment onto the lung-epithelium is similar for AuNP and Ir-NP but slower than for $TiO_2$-NP. Additionally, after 28 days the integral translocated fractions of $TiO_2$-NP and IrNP across the air-blood-barrier (ABB) are similar and become 0.15 while the translocated AuNP fraction is only 0.04. Translocated $TiO_2$-NP and IrNP are predominantly excreted in urine (~0.1) while the urinary AuNP excretion amounts to a fraction of only 0.01. Urinary AuNP excretion is below 0.0001 during the first week but rises tenfold thereafter suggesting delayed disagglomeration. Of note, all three NP dissolve minimally, since no ionic radio-label release was detectable. These biokinetics data of inhaled, same-sized NP suggest significant time-dependent differences of the ABB translocation and subsequent fate in the organism.

Holzwarth U, Cossío U, Llop J, Kreyling WG: **Unpredictable Nanoparticle Retention in Commonly Used Plastic Syringes Introduces Dosage Uncertainties That May Compromise the Accuracy of Nanomedicine and Nanotoxicology Studies.** *Front Pharmacol :* 2019, **10:**1-12, (DOI: 10.3389/fphar.2019.01293).

**Abstract:**

In recent animal experiments with suspensions of radiolabelled $TiO_2$ nanoparticles large and highly variable radioactivity fractions were retained in disposable plastic syringes. After unloading between 10% and up to 70% of the loaded dose were still present in the syringes. As a consequence the effectively delivered nanoparticle

dose to the animals was frequently much smaller than the nominal dose of the nanoparticles loaded into the syringe. The high variability of this nanoparticle retention challenges the application of a precise, predefined dose and creates a major error source when normalizing organ and tissue contents to the dose loaded into the syringe which is usually set as the applied dose.

A control study was performed employing six commonly used syringe types with seven types of radiolabelled oxide and metallic nanoparticles. For this purpose the syringes were loaded with a given volume of nanoparticle suspension, the radioactivity was measured, the syringe was unloaded and the activity measurement was repeated with the empty syringe. The highest retention values were found when using $TiO_2$ nanoparticle suspensions with Tuberkulin type syringes. In the worst case between 6.6% and 79.1% of the nanoparticles were retained in the syringe. When using the same nanoparticle suspension with an Insulin-type syringe the retention was reduced to 1.4% to 20.6%. For amorphous silica nanoparticles the maximum observed retention was 8% and for Au nanoparticles it was 5.1%.

Further data gathered from *in vivo* animal imaging studies show that nanoparticle retention in syringes also affects experiments with nanoparticles such exosomes, polymersomes and protein-base nanoparticles investigated for possible applications in nanomedicine. Since this retention is highly variable the effectively applied dose cannot be determined by applying a simple syringe retention factor.

The present work shall illustrate the problem and proposes as mitigation strategy adequate checks with different syringe types in order to find out whether a given combination of syringe type and nanoparticle suspension is affected by nanoparticle retention and, if necessary, to select a different syringe type that minimizes retention.

# Application of Neutron Radiography to Study Water Movement in Porous Materials

**by Folker H. Wittmann, Member EUAS**

Short Biography

*1936. 04. 20: born in Karlsruhe, Germany, son of Alfred and Angela Wittmann*
*1942-1946 Elementary school in Berghausen near Karlsruhe*
*1947-1955 High school, Markgrafen Gymnasium Karlsruhe-Durlach*
*1955-1958 Studied Physics and Mathematics at University Karlsruhe (KIT), Vordiplom*
*1958-1961 Studied Physics at Munich University (MU), Diplom*
*1961-1965 Further studies for PhD (Dr. rer. nat) at Munich University of Technology (TUM)*
*1965-1969 Research Fellow at Building Materials Testing Laboratory and Institute for Concrete Structures at Munich University of Technology (TUM)*
*1969 Habilitation in Building Materials Science, Civil Engineering Department of Munich University of Technology (TUM)*
*1969-1976 Lecturer (Privatdozent) and Head of the Laboratory for Building Materials Science, Munich University of Technology (TUM)*
*1976-1980 Professor and Head of the Laboratory for Building Materials Science, Delft University of Technology (TUD), The Netherlands*
*1980-1988 Professor and Head of the Laboratory for Building Materials Science, Swiss Federal Institute of Technology, Lausanne (EPFL), Switzerland*
*1988-2001 Professor and Head of the Laboratory for Building Materials, Swiss Federal Institute of Technology (ETHZ)*
*2002-2020 Head of a Research Group at Qingdao University of Technology (QUT), Qingdao, China*
*1973 Winner of the RILEM Medal, Réunion Internationale des Laboratoires d'Essais et de Recherches sur les Matériaux et les Constructions.*
*1985 Advisory Professor for Tongji University, Shanghai, China*
*1991 Member of the Academy of Technological Sciences, Moscow, Russia*
*1995 Honorary Member of Wissenschaftlich-Technische Arbeitsgemeinschaft für Bauwerkserhaltung und Denkmalpflege, (WTA)*
*2010 The International Science and Cooperation Award of the People`s Republic of China*
*2018 Member of the EU Academy of Sciences*
*2018 Tenured Honorary Professor of China Building Materials Academy (CBMA), Beijing, China*

## INTRODUCTION

Concrete is a rather brittle material. This means that concrete may crack under modest thermal or hygral gradients and under applied load. Cracks must be considered to be easy pathways for penetration of water and aqueous salt solutions into a structural element. Recently it was found that ductility of cement-based materials can be increased enormously by adding fibers with a high elastic modulus and high tensile strength to a fine grained mortar [1-3]. Initially this new material was called Engineered Cementitious Composites (ECC) but soon the more meaningful name Strain Hardening Cementitious Composites (SHCC) was generally accepted [2]. The ultimate strain of SHCC under tension can reach up to 5%, which is more than 300 times the ultimate strain of conventional cement-based materials. If this material is applied in a protected environment,

without exposure to water or to salt solutions the full strain capacity can be used, as for instance for dampers for high rise buildings in seismic areas. However, as the extreme ductility of SHCC is reached by multi-crack formation, in cases where the material is exposed to natural environment, as for instance in contact with seawater or with de-icing salt solutions, durability and service life become a crucial problem. Under these conditions the high ductility reached by multi-crack formation must be considered to be a serious risk for durability in general and for service life in particular.

Penetration of water and salt solutions into the open pore space of concrete and into cracks can be reduced if not totally prevented by water repellent surface treatment [4-7]. Martinola et al. [4] and Sahmaran et al. [5] have studied the influence of addition of water repellent agents to SHCC on capillary water absorption. There are two different methods to avoid or reduce at least capillary water absorption of cement-based materials: (a) surface impregnation with a water repellent agent and (b) addition of a water repellent agent to the fresh mix. In this contribution results of studies of the influence of the imposed tensile strain on water repellent SHCC will be described in detail. In the past we could show that neutron imaging is a powerful method to visualize and to study quantitatively water movement into porous materials and into cracked concrete in particular. In this contribution the influence of surface impregnation and of integral water repellent SHCC on capillary absorption and of water movement into fine cracks in particular was investigated. The influence of imposed strain on capillary water absorption was studied in particular.

## EXPERIMENTAL

The composition of SHCC prepared for this project was as follows: 550 kg/m$^3$ ordinary Portland cement Type 42.5, 650 kg/m$^3$ local fly ash, 550 kg/m$^3$ fine sand with a maximum grain size of 0.3 mm, and 395 kg/m$^3$ water. 26 kg/m$^3$ of PVA fibers with a diameter of 40 µm, produced by Kuraray Company, Japan, were added to the fresh mix. A second batch was prepared to which 2.0 % (related to the mass of binder) of an alkyl silane emulsion (Protectosil MH50, produced by Evonik, Germany) were added to the fresh mix in order to obtain integral water repellent SHCC.

After compaction in steel forms, all specimens were allowed to harden in the concrete laboratory under wet burlap for 24 hours. Then the steel form was removed and the specimens were stored for 21 days in a moist curing room (20 °C, 95% RH). In this project, dumbbell shaped specimens with a thickness of 30 mm and an overall length of 330 mm were cast in steel forms. The width at both ends is 90 mm and the center part with a length of 120 mm has a width of 60 mm. In order to characterize mechanical properties of the SHCC under investigation, stress-strain diagrams have been determined. Typical results are shown in Fig. 1. The average first cracking stress of this type of SHCC was approximately 2.1 MPa and the average ultimate tensile strain was approximately 3.8 %. The center part of the specimens, which was subsequently subjected to a uniform tensile stress, had the following size: 120×60×30mm. Finally, in order to determine capillary water absorption by means of neutron digital imaging, the center part has been cut out of the specimen after a predetermined tensile strain had been applied.

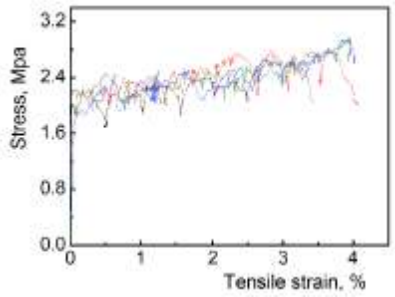


**Figure 1**: Typical stress-strain diagrams of the SHCC under investigation.

After curing for 21 days a tensile strain of 0.5 % and 1.5 % was applied for a duration of 15 minutes to both types of specimens. After unloading, some of the stressed samples were surface impregnated with 400 g/m$^2$ of silane gel.

In the next step all three types of specimens, the control, the integral water repellent, and the surface impregnated SHCC specimens were exposed to a neutron beam at Paul Scherrer Institute (PSI), Switzerland. A first image was taken from the dry specimens. Then one surface of the specimens (120 x 30 mm) was put in contact with tap water. While in contact with water, neutron images were taken in regular intervals to follow the process of water penetration into the pore space and the cracks of SHCC. More details on neutron technology can be found in recent publications [9, 10].

## RESULTS AND DISCUSSION

Neutron images were taken first on unloaded SHCC specimens. They served as reference. Images taken after 60 minutes of capillary absorption and the corresponding moisture distributions in a SHCC sample are shown in the left part of Fig. 2. For comparison a typical result as obtained on an ordinary concrete sample (W/C = 0.6) is shown in the right part of Fig. 2. It can be seen that the SHCC specimen which has not been exposed to tensile strain absorbed very little water in contact with water for 60 minutes compared to ordinary concrete. This indicates that undamaged SHCC absorbs comparatively little water.

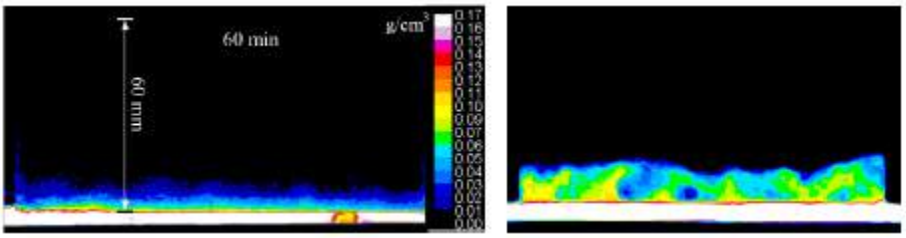


**Figure 2**: Neutron images of water penetration into un-cracked SHCC (left) and into ordinary concrete (W/C=0.6) after 60 minutes of contact of the lower surface with water.

The process of water penetration into neat SHCC exposed to different levels of tensile strain were visualized by neutron imaging. Selected images taken after 5, 15 and 90 minutes of capillary absorption are shown in Fig. 3. It can be seen from these results that after exposure to 0.5 % tensile strain, few cracks are created in the type of SHCC prepared for this project. Wider cracks, become water filled up to the height of the specimens within 15 minutes. After this period finer cracks become visible. The moisture distribution in SHCC in contact with water was quantitatively determined after 15 and 90 minutes.

Results obtained in the two rectangular areas in Fig. 3 are again shown in Fig. 4. Water profiles obtained after 15 and 90 minutes of capillary absorption on specimens exposed to a tensile strain of either 0.5 % or 1.5 % are shown. Obviously, the lower part absorbed more water than the center of the specimen. The wide cracks, which reach the upper surface, soon contain significantly more water than the fine cracks. The profiles show that in the sample subjected to 1.5 % tensile stress, more and wider cracks were formed. As a consequence, they absorb significantly more water. From these results we may conclude that SHCC exposed to 0.5 % and 1.5 % of strain cannot be considered to provide long term protection in aggressive environment.

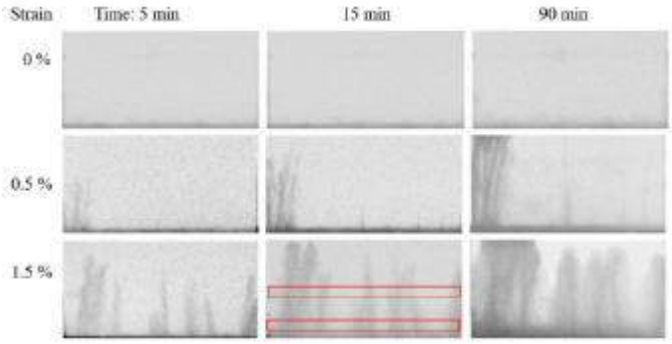


**Figure 3:** Neutron images of water penetration into neat SHCC before and after imposed tensile strain of 0.5 % and 1.5 %.

These results underline the fact that SHCC has a high strain capacity. If the mechanical properties are of main interest in a given application, then one can take full advantage of the strain capacity. If durability is an issue, however, the ultimate strain that may be allowed is rather limited.

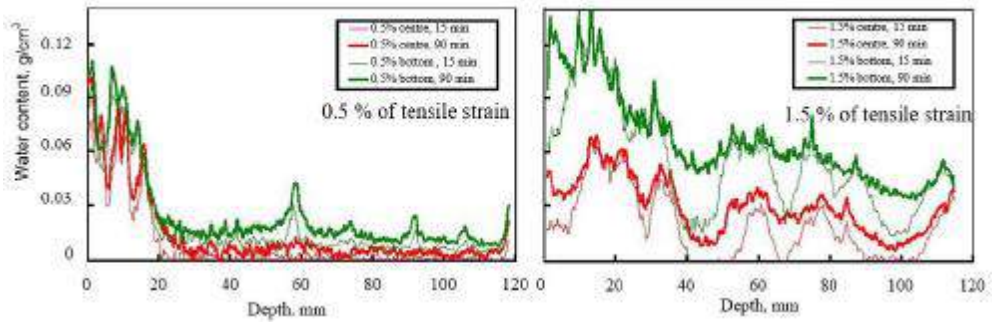


**Figure 4**: Horizontal quantitative water profiles in the center and at the bottom of cracked SHCC, as indicated with rectangular areas in Fig. 3 after imposed tensile strain of 0.5% (left) and 1.5 % (right).

By addition of silane emulsion to the fresh mix of SHCC integral water repellent SHCC was produced. The water repellent cementitious matrix should prevent or at least reduce water absorption. Water penetration into the cracks formed under the influence of tensile strain should also be avoided or at least reduced. Typical results are shown in Fig. 5. Specimens which were not exposed to an applied strain practically do not absorb any water after 90 minutes of contact with water. Even after application of 0.5 % strain, a small amount of water can be observed in the cracks only. However, when a strain of 1.5 % was imposed, wider cracks begin to absorb water and water penetrates up to the upper surface

of the specimens.

The moisture profiles for the integral water repellent SHCC after application of 0.5 % and 1.5 % strain are shown in Fig. 6. Compared with the results shown in Fig. 4, far less water enters the crack-free zones and fewer cracks absorb water. However, water enters the cracks and migrates into the matrix. This means that integral water repellent treatment is effective in protecting SHCC from penetration of water or aqueous salt solutions as long as there are no cracks. But once micro-cracks are formed under a certain level of imposed tensile strain water can still penetrate into the matrix of the SHCC. This underlines again that SHCC is beneficial only under mild mechanical strain and under imposed moderate strain it is not a reliable protection in aggressive environment.

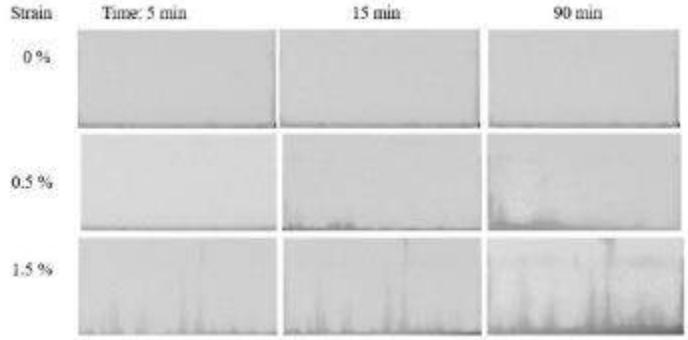


**Figure 5**: Neutron images of water penetration into integral water repellent SHCC before and after imposed tensile strain of 0.5 % and 1.5 %

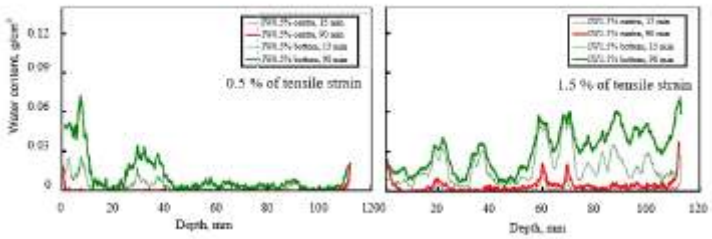


**Figure 6**: Horizontal quantitative water profiles in the center and at the bottom of integral water repellent SHCC after imposed tensile strain of 0.5 % (left) and 1.5 % (right).

**Selected Relevant Literature:**

1.) P. Zhang, F. H. Wittmann, T. Zhao and E. Lehmann, Neutron Imaging of water penetration into cracked steel reinforced concrete, Physica B 405, 2010, 1866-1871
2.) P. Zhang, F. H. Wittmann, Zhao T. J. et al. Observation of water penetration into ater repellent and cracked cement-based materials by means of neutron radiography, Int. J. Restor. Build. Monum., 15(2) 2009, 91-100
3.) P. Zhang, F. H. Wittmann, M. Haist, H. S. Müller, P. Vontobel and T. J. Zhao, Water Penetration into Micro-cracks in reinforced concrete, Rest. Buil. Monum. 20, 2014, 85-94
4.) F. H. Wittmann, P. Zhang, E. Lehmann, and T.Zhao, Visualisation of frost damage in concrete by means of neutron radiography, in Wittmann F. H. and Mercier O., Basic research on Concrete and Applications, Aedificatio Publishers, 2011, 155-174
5.) P. Zhang, F. H. Wittmann, P. Lura, H. S. Müller, S. Han, Applications of Neutron Imaging to Study Aspects of Durability of Cement-based Materials: an Overview, Cement and Concrete Research, 108, 2018, 152-166

# Spray-on Piezoelectric Transducer Technology

## by Bernhard R. Tittmann, Member EUAS

Short Biography

*Schell Professor of Engineering, Emeritus*
*Director of Engineering Nanostructure Characterization Center*
*The Pennsylvania State University*

***Academic Training***

*B.S. (Physics and Mathematics), George Washington University, Washington, DC, 1957*
*Ph.D. (Solid State Physics), University of California at Los Angeles, CA, 1965*

***Teaching Experience**:*

*Professor, The Pennsylvania State University, University Park, PA 16802, 1989-present;*
*Visiting Professor, Fall 2017, University of California, Santa Barbara, CA*
*Visiting Professor, Spring 1995-1997. Johannes Kepler University, Linz, Austria.*
*Visiting Professor, University of Paris III, Physics Department, 1977, 1979, 1982.*
*Assistant Professor (in residence), 1965-1966. Physics Department, University of California at Los Angeles, CA.*

***Industrial Experience***

*Manager, Materials Characterization. Science Center, Rockwell Intern., 1979 - 1989.*
*Member Staff, Materials Mechanics Group. Science Center, Rockwell, 1966-1977.*
*Howard Hughes Fellow – Microwave Antenna Dept.; Hughes Research Lab., Culver City, CA, 1957-1962.*

***Professional Societies and Activities***

*American Ceramic Society (ACS), Member 1995 – present*
*American Society for Metals (ASM) International, Member 1993, Fellow 2006 – present*
*American Society of Nondestructive Testing (ASNT), Member 1980 – present*
*Materials Research Society (MRS), Member, 1995 – present*
*American Society of Mechanical Engineers (ASME), Member, 2001 – present*
*Acoustical Society of America (ASA), Fellow, 2001 – present*
*Technical Program Committee - Standing Member, 1999 to present*
*Institute of Electrical and Electronics Engineering (IEEE), Fellow, 1990 – present*
*Distinguished IEEE – UFFC Lecturer, June 1998 – December 1999*
*Vice-Chair of Awards Committee, IEEE – UFFC, 2003-present*
*International Society for Optical Engineering (SPIE), Senior Member*

***Awards/Honors***

*Marquis Who's Who Albert Nelson Marquis Lifetime Achievement Award 2018*
*Top 100 Registry Professors of the Year, 2018*
*EU Academy of Sciences, January 2018*
*Schell Professor, Emeritus July, 2017.*
*Endowed Chair at Penn State College of Engineering Schell Professor of Engineering 1989 (renewed 5 times) to June, 2017.*
*IEEE-UFFC Distinguished Service Award 2017*
*IEEE-UFFC Invited Speaker at 2017 Int. Ultrasonics Symposium, Washington, D.C.*
*Named Consulting Editor of Archives of Acoustics, Polish Academy of Sciences, Warsaw, 2003*
*Penn State Engineering Society Outstanding Research Award, 1998*
*Senior Fulbright Fellowship, Spring and Summer 1999*
*Rockwell Award for Highest IR&D Score Rockwell Science Center (1988)*
*NASA Principal Investigator Award for "Elastic and Anelastic Properties of Lunar Rock (1979)."*
*Howard Hughes Fellow (1957-1962).*

*Phi Beta Kappa (1957).*
*Graduation Cum Laude (1957).*
*G. Washington Tuition Scholarship (1953-1957).*
***Accomplishment***
*Graduated 11 PhD students and 25 MS students.*
*Citations 4028; h-index 32*
*Nearly 500 publications including refereed journal publications and refereed Proceedings.*
*8 Patents*

## Introduction

Damage detection in the power industry is always vying for optimized and cheaper techniques. Most components in the energy sector utilize metallic structure, whether it is for power generation, storage, transportation, or waste management. Many components operate at a high temperature adding further challenges for their health monitoring. Given that commercial transducers rated for elevated temperatures are limited and expensive, the use of spray-on film transducers for such purposes has been researched while keeping the fabrication simple enough for anyone to create them.

## Methodology

Bismuth titanate ($Bi_4Ti_3O_{12}$) is an excellent piezoelectric which has a $T_c$ of 670 °C and a safe operating level until about 500 °C, considerably higher than PZT. Unlike the preceding sol–gel method [18–26], this fabrication process involves a lithium-silicate-based inorganic binder and water to mix with the $Bi_4Ti_3O_{12}$ powder.

With the initial bulk-wave characterization of the film, it was noted that despite the lower piezoelectric coefficient compared to PZT, the film transducers were able to function at higher temperatures. Another major advantage is the straightforward fabrication procedure and the ability for these films to cure at room temperature. Another method to produce these films consisted of using organic compounds instead of the high-temperature inorganic binder. The organic films were also excellent in heat resistance despite having a slightly complicated fabrication procedure compared to the inorganic films. High-temperature lithium niobate ($LiNbO_3$) spray-on films were also fabricated under the same inorganic film fabrication procedure.

**Figure 1.** Bismuth titanate, lithium niobate/barium titanate, and organic bismuth titanate film transducers (**left** to **right**). Good adhesion was observed for extended periods of time. One film transducer is still working normally after several years of use. [1]

## Results and Discussion

Figure 2 shows A-scan pulse-echo measurements of $Bi_4Ti_3O_{12}$ (left), $LiNbO_3$ (center), and organic $Bi_4Ti_3O_{12}$ (right) thick-film transducers deposited on a steel cylinder (7 mm) at 40 dB gain, film thickness ~200 micron, and frequency ~1.5 MHz [1].

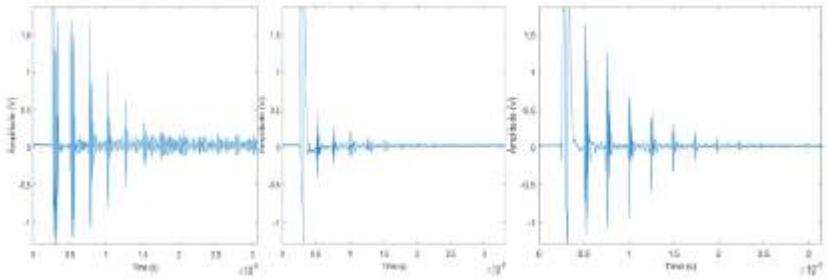

**Figure 2.** A-scan pulse-echo measurements of $Bi_4Ti_3O_{12}$ (**left**), $LiNbO_3$ (**center**), and organic $Bi_4Ti_3O_{12}$ (**right**) thick-film transducers deposited on steel cylinder (7 mm) at 40 dB gain, film thickness ~200 micron, and frequency ~1.5 MHz [1].

The Curie–Weiss temperatures of $Bi_4Ti_3O_{12}$ and $LiNbO_3$ make them ideal candidates for high-temperature testing. These films were inserted in the tube furnace and peak-to-peak voltage measurements for the first and second reflection from an edge were recorded. The furnace was set to increase the temperature of the films at a rate of about 6 °C/min. The $Bi_4Ti_3O_{12}$ films were tested up to a temperature of 650 °C, whereas the $LiNbO_3$ films were tested to a temperature of 900 °C. The first and second echoes were recorded in terms of the signal amplitude and plotted in relation with the temperature ramp seen here in Figures 3. Fig 4 shows the results for $LiNbO_3$.

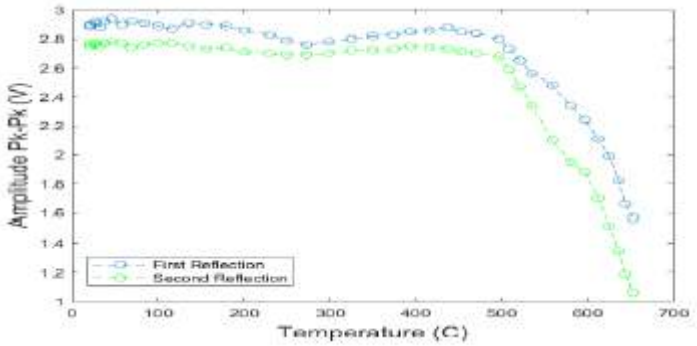


**Figure 3.** Signal amplitude (peak-to-peak) for the first two reflections as a function of temperature for bismuth titanate thick-film, spray-on transducer [1].

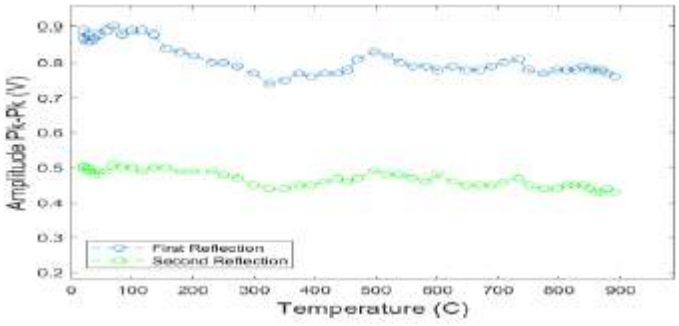


**Figure 4.** Signal amplitude (peak-to-peak) for the first two reflection as a function of the temperature for lithium niobate thick-film, spray-on transducer [1].

To demonstrate their ability to perform as a guided-wave sensor, the primary Lamb wave modes (A0, S0, A1, S1) were generated using a comb transducer arrangement. Furthermore, 6061 aluminum plates of several different thicknesses ranging from 2 to 4 mm were chosen as the waveguides. Sets of comb transducers were then applied onto the plate a certain distance apart in a through-transmission setup as shown in Figures 5a and 5b.

The number of actuating and receiving elements were altered to give rise to various configurations for better transducer characterization. Calculations solving the thin-plate Lamb wave transcendental equations were performed for the comb elements to be spaced by the same length as the wavelength of the preferential excited mode. See Figure 6 for graphs of the corresponding dispersion curves. A tone-burst of 15 cycles was introduced in the actuator set of the transducers and the A-scan was plotted. According to the excitation parameters and the comb spacing, the S1 mode should be the first to be received as shown in Figure 18. The readings were then recorded through various receiving elements and calculation were performed to compare the experimental group velocity for S1 mode with its theoretical value at that specific frequency.

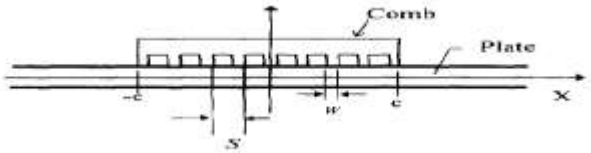


**Figure 5a.** S is the element width, W is the element gap, W + S is the wavelength of the traveling wave.[1].

**Figure 5b.** Schematic of the experiment setup for generation of Lamb waves in a 3.2 mm thick 6061 aluminum plate [1].

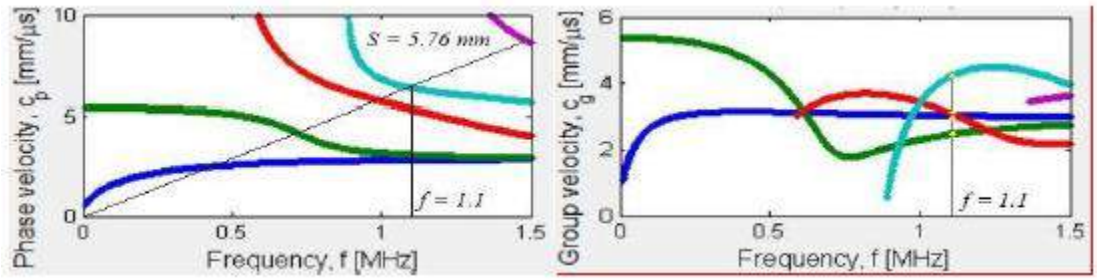


**Figure 6.** Dispersion curves for a 3.2 mm thick aluminum 6061 plate showing the activation line on the phase velocity and corresponding group velocities at that frequency.

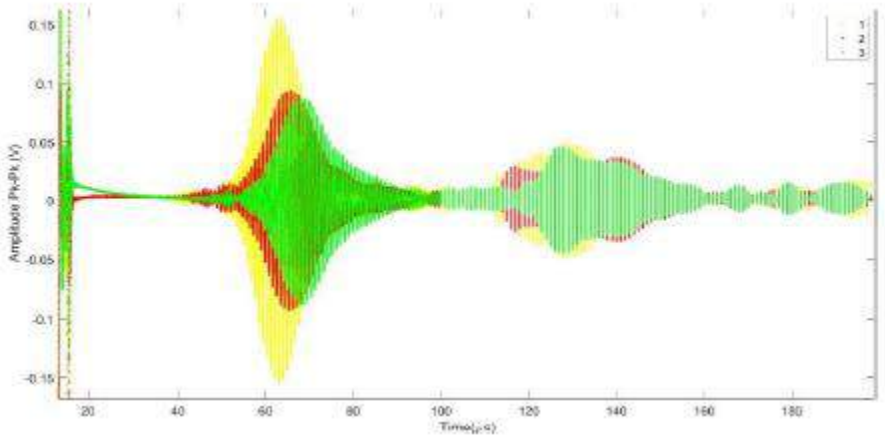


**Figure 7.** A-scan for one of the tested plates showing the superimposed guided-wave modes from three different elements.[7]

## Conclusion

The inorganic films are easy to produce and extremely inexpensive, as the films use very small quantities. A batch of 5 g powder with another 5 g of the solvents is enough to coat at least two of the stainless cubes used for the pulse-echo measurements. For spraying films on bigger areas, the slurry quantity would also have to be increased, but compared to the cost of commercial sensors these transducers are affordable. The respective SNR of 20.72, 14.93, and 19.93 dB for the BIT, LiN, and organic BiT films is comparable to commercial transducers. According to the study done by Kobayashi, the films on the planar surfaces yielded an SNR of 16 dB and a center frequency of 3.6 MHz, where the BIT was doped with PZT. Here, without a strong piezoelectric material such as PZT, the signal strength is quite strong. The center frequencies for the BIT, LiN, and organic BiT films were 1.4, 1.22, and 1.42 MHz, respectively. With the premise of a working transducer, the films were then subjected to temperature testing. From the capacitance, other parameters to characterize the films could be calculated such as the dielectric constant, dielectric loss, amount of charge in the film, and even piezoelectric constant after some analysis.

## References

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# Mechanical and Physiological Role of Bone Microdamage/Bone Quality

## by David B. Burr, Member EUAS

Short Biography

*David B. Burr*
*Distinguished Professor of Anatomy and Cell Biology, and Biomedical Engineering*
*Indiana University School of Medicine, and Indiana University-Purdue University Indianapolis (IUPUI)*

***Positions Held***

*2001-2002* *President, Association of Anatomy, Cell Biology and Neurobiology Chairpersons*
*2007-2009* *President, American Association of Anatomists*
*2008-2009* *President, Orthopaedic Research Society*
*2009-2013* *Delegate, General Assembly, International Federation of Associations of Anatomists*
*2013-present* *Editor, Bone*
*2011* *Guest Editor (with R. Graham G. Russell) for Special Issue of BONE on Bisphosphonates*
*2012-2018* *Associate Vice Chancellor for Research, IUPUI*
*2014-2021* *Editor-in-Chief, Current Osteoporosis Reports*
*2014-2018* *Board of Directors, Federation of Associated Societies of Experimental Biology (FASEB)*
*2015-2018* *Chair, Scientific Advisory Board, Fibrous Dysplasia Foundation*

***Honors***

*1997* *Honorary Chairman, 27th International Sun Valley Hard Tissue Workshop*
*2002* *First Louis V. Avioli Best Article Award, Calcified Tissue International and Springer-Verlag*
*(co-recipient with Jiliang Li and Tasuku Mashiba)*
*2008* *Borelli Award, American Society of Biomechanics*
*2009* *Fellow, American Association of Anatomists*
*2010* *Chief Scientist Pro-Tempore, Hospital for Special Surgery*
*2010* *Gideon A. Rodan Award for Excellence in Mentorship, American Society for Bone and Mineral Research (ASBMR)*
*2013* *Named Distinguished Professor of Indiana University*
*2015* *Henry Gray Scientific Award, American Association of Anatomists*
*2018* *Fellow, Orthopaedic Research Society*
*2018* *Albert Nelson Marquis Lifetime Achievement Award, Marquis Who's Who*

*I am an Indiana University Distinguished Professor Emeritus in the Department of Anatomy, Cell Biology, and Physiology, and Professor of Biomedical Engineering at IUPUI. I have 40 years of experience in studies involving histological and histomorphometric endpoints in both bone and cartilage. My primary area of research emphasis is to evaluate the effects of pharmacologic agents used to treat osteoporosis on bone matrix quality, specifically, the accumulation and repair of microdamage, changes in mineralization and alterations to the collagenous matrix. We have been investigating matrix effects of bisphosphonates and other anti-remodeling agents for many years using canine models. Since the early 1980's, I have studied the cross-talk between subchondral bone and cartilage deterioration, and still am frequently asked to talk about this in national and international venues. In the past several years, we have begun to investigate changes in matrix in Type 2 diabetes using similar approaches in the ZDSD and ZDF rat models of diabetes. My laboratory is equipped to characterize histological, immunohistochemical and dynamic histomorphometric features of different tissues, and to utilize bone density (BMD) and imaging*

*techniques (µCT, pQCT) to analyze tissues in animal models. This has allowed me to bring both biological and mechanical concepts to the study of biological form, function and physiological processes at various length scales.*

## A. Mechanical and Physiological Role of Bone Microdamage/Bone Quality

It is now generally accepted that microdamage in bone is a naturally occurring event, important for skeletal health. When we began to study skeletal microdamage in 1983, its existence was not accepted as a physiological feature of bone. Although Harold Frost had first proposed its existence in 1960, "cracks in bone" were considered to be an artifact of preparation. We were the first to demonstrate conclusively that microcracks in bone are not artifactual but are a common physiologic occurrence consequent to normal human activity and bone loading [2]. Once we had validated the technique for exposing them, the phenomenon of microdamage was observed in multiple labs using different techniques, and their occurrence is now accepted by nearly everyone, including government regulatory agencies such as the FDA.

Most investigators tended to think of microdamage as only a mechanical event. However, we were able to show in two papers starting in 1985 that microdamage is "targeted" for repair by the bone remodeling system [1] and that microcracks were signaling for their own repair [3]. We now know that this occurs when microdamage disrupts osteocytic canalicular processes. This causes apoptosis of osteocytes close to the damage, and these osteocytes upregulate the production of RANKL. If apoptosis is prevented, repair of the damage does not occur. Thus, osteocytes in areas of microdamage recruit osteoclasts to specific areas to remove damage; because the osteoclasts are coupled to osteoblasts, new bone is formed once the old bone is removed, and the damaged region is repaired. This process is fundamental to maintain bone's strength and to prevent fracture [4]. We recently reviewed the role that bone microstructure plays in creating stress concentrations that can lead to the initiation and arrest of bone microcracks [5].

(1) Bone remodeling in response to in vivo fatigue microdamage. D.B. Burr, R. B. Martin, M.B. Schaffler, E.L. Radin, J. Biomech. 1985; 18:189-200.
(2) Validity of the bulk staining technique to separate artifactual from in vivo bone microdamage. D.B. Burr and T. Stafford. Clin. Orthop.1990; 260:305-308.
(3) Increased intracortical remodeling following fatigue damage. S. Mori and D.B. Burr, Bone 1993; 14:103-109.
(4) Bone microdamage and skeletal fragility in osteoporotic and stress fractures. D.B. Burr, M.R. Forwood, D.P. Fyhrie, R. B. Martin, M.B. Schaffler, and C.H. Turner. J. Bone Miner. Res. 1997; 12:6-15.
(5) Stress concentrations and bone microdamage: John Currey's contributions to understanding the initiation and arrest of cracks in bone. D. B. Burr. Bone 2019; 127: 517-525.

## Bone Fatigue and Stress Fractures

Because of my interest in the mechanical adaptation of bone, I began to study the origin and pathogenesis of stress fractures. One notable early set of experiments involved applying strain gages to my tibia to measure bone strains that occurred during vigorous activities [1]. At that time, strain gages had been applied to human bone only one time before. Therefore, these data became well-known and led to a number of other studies with Israeli collaborators. These studies resulted in many refereed publications evaluating the role of impact and muscle fatigue on bone strain. I also developed a rabbit model of stress fracture by adapting the rabbit impact loading device that we used to study osteoarthrosis

to create tibial stress fractures in rabbits. In combination, this work led to the publication of several review type articles and a co-edited book on muscular fatigue and stress fractures [2,3]. This has become particularly pertinent recently with the observation that atypical femoral fractures are a type of insufficiency stress fracture. This observation, in combination with our other work showing that long-term bisphosphonate (BP) use could cause deterioration in the mechanical and material properties of bone, led us more recently to investigate the effect of BP administration on the fatigue life of bone [4]. This work shows that treatment with BPs, at least at high doses, is associated with a 3-fold reduction in fatigue life and demonstrates the proof-of-principle that BPs could be implicated in the pathogenesis of atypical femoral fractures.

(1) In vivo measurement of human tibial strains during vigorous activity. D.B. Burr, C. Milgrom, D. Fyhrie, M. Forwood, M. Nyska, A. Finestone, S. Hoshaw, E. Saiag and A. Simkin. Bone 1995; 18:405-410.
(2) Musculoskeletal Fatigue and Stress Fractures. D.B. Burr and C. Milgrom (eds). Boca Raton: CRC Press; 2001.
(3) Bone stress injuries. S.T. Warden, D.B. Burr. Primer on the Metabolic Bone Diseases and Disorders of Mineral Metabolism. 9th Ed., ASBMR; 2018.
(4) The resistance of cortical bone tissue to failure under cyclic loading is reduced with alendronate. D. Bajaj, J.R. Geissler, M.R. Allen, D.B. Burr, J.C. Fritton. Bone 2014; 64:57-64.

**Mechanical Properties/Adaptation of Bone**

An early interest in the skeletal adaptation of nonhuman primates related to locomotion led to an interest in dynamic bone remodeling and adaptation. Early studies using a canine model employing an ulnar osteotomy to overload the radius showed that increased bone mass in response to elevated strain resulted from increased activation of modeling on periosteal and endocortical surfaces [1]. Extreme overload led to a woven bone response that was not associated with damage to the bone. There was no evidence that elevated strain changed the individual vigor of osteoclasts or osteoblasts or altered the remodeling period. Subsequently, we studied the effects of cyclic loading on bone fatigue. This work showed that fatigue of compact bone was a realistic expectation of the normal loading environment, but that fatigue of bone did not progress to failure in a physiologically reasonable number of loading cycles when tested at physiological strains and strain rates [2]. This led to the hypothesis that an intermediate remodeling reaction might be required to cause stress fractures. These data suggested it was important to develop approaches that could maximize bone response to normal loading events. With Charles Turner and Alex Robling, we were the first to demonstrate that providing a rest period between loading bouts increased the osteogenic effectiveness of loading [3]. Additional experiments showed that the refractory period for osteoblasts was about 8-12 hours. Because of my long-term interest in mechanical properties of bone, I collaborated on a book to explore the broad areas of skeletal mechanics and adaptation [4].

(1) The effects of altered strain environments on bone tissue kinetics. D.B. Burr, M.B. Schaffler, K.H. Yang, D.D. Wu, M. Lukoschek, N. Sivaneri, D. Kandzari, J.D. Blaha and E.L. Radin. Bone 1989; 10:215-221.
(2) Long term fatigue behavior of compact bone at physiological strains. M.B. Schaffler, E.L. Radin and D.B. Burr. Bone 1990; 11:321-326.
(3) Partitioning a daily mechanical stimulus into discrete loading bouts improves the osteogenic response to loading. A.G. Robling, D.B. Burr, and C.H. Turner. J. Bone Miner. Res. 2000; 15:1596-1602.
(4) Skeletal Tissue Mechanics. R.B. Martin, D.B. Burr, and N. Sharkey. New York: Springer-Verlag; 1998. (2nd edition published in 2015 with Dr. David Fyhrie as an additional co-author).

**Treatments for Osteoporosis/Bone Matrix Quality**

My lab has been engaged for the past 20 years in studies to examine the effect of suppressed bone remodeling on bone quality. Although bisphosphonates (BPs) are effective at preventing bone loss and do reduce the risk of fracture in most people, it seemed to us that inhibition of damage repair could represent a significant risk factor for women on long-term BP therapies. Using a pre-clinical animal model, we demonstrated in a series of papers starting in 2000 that treatment with BPs could reduce the amount of energy required for bone to fracture (ie reduce the mechanical "toughness" of bone) [1]. We have published numerous papers on this topic, and other labs have found similar results. Although suppressing bone turnover increases bone mineral density and makes the whole bone stronger, the bone matrix itself is more brittle and can absorb less energy per unit of mass before it breaks.

In 2006, an increased incidence of femoral shaft fractures was detected, especially in women taking BPs for long periods of time. Femoral shaft fractures are not that common, and these had "atypical" characteristics different from other femoral fractures. This was consistent with our observations that BP treatment makes bone more brittle and reduces the energy required for fracture. In 2009 I was asked to Co-Chair an International Task Force for the ASBMR to define atypical femoral fractures and provide recommendations for BP treatments. Two Task Force Reports [2] altered clinical practice related to the administration of BPs to patients. Whereas in the past, these were used to prevent bone loss in younger women (in their 50's), most physicians now will not prescribe them without a clear diagnosis of osteoporosis.

We have begun to explore the idea that it is possible to improve bone material properties and reduce fracture risk without interfering with normal cellular activity. This is part of the basis for the fracture efficacy of raloxifene [3]. This work could lead to the development of a new class of drugs to treat bone fragility.

We have continued our work more recently to investigate other changes related to bone matrix changes that may affect bone fragility in aging and in osteoporosis. We have explored the regulation of mineralization in animal models as a means to further understand bone matrix quality changes in osteoporosis [4]. This work shows that, in addition to the well-established effects on turnover rates and bone mass, estrogen depletion alters the regulation of mineralization by GAGs and pyridinoline. We have also begun to explore some of the molecular mechanisms for bone matrix changes [5,6]. We recently published an article reviewing the numerous changes to bone quality that occur during the aging process [7].

(1) Suppressed bone turnover by bisphosphonates increases microdamage accumulation and reduces some biomechanical properties of dog rib. T. Mashiba, T. Hirano, C.H. Turner, M.R. Forwood, C.C. Johnston, and D.B. Burr, J. Bone Miner. Res. 2000; 15:613-620

(2) Atypical subtrochanteric and diaphyseal femoral fractures: Report of a task force of the American Society for Bone and Mineral Research. E. Shane, D. Burr (co-chairs) et al. (25 other co-authors). J Bone Miner Res 2010; 25:1-28. [Accepted for inclusion to the National Guideline Clearinghouse (NGC)]. Second Report of the AFF Task Force, J Bone Miner Res 2014; 29:1-24.

(3) Bone cell-independent benefits of raloxifene on the skeleton: A novel mechanism for improving bone material properties. M.A. Gallant, D.M. Brown, M. Hammond, J.M. Wallace, J. Du, A. C. Deymier-Black, J.D. Almer, S.R. Stock, M.R. Allen, D.B. Burr. Bone 2014; 61:191-200.

(4) Estrogen depletion alters mineralization regulation mechanisms in an ovariectomized monkey animal model. E.P. Paschalis, S. Gamsjaeger, K. Condon, K. Klaushofer, D. Butr, Bone 2019; 120:279-284.

(5) Nrf2 regulates mass accrual and the antioxidant endogenous response in bone differently depending on the sex and age. G. G. Pellegrini, M. Cregor, K. McAndrews, C. C. Morales, L.D. McCabe, G.P. McCabe, M. Peacock, D. Burr, C. Weaver, T. Bellido. PLoS One 2017; 0171161.

(6) Loss of Nmp4 optimizes osteogenic metabolism and secretion to enhance bone quality. Y. Shao et al. Am. J. Physiol. Endocrinol. Metab. 2019; 316:E749-E772.
(7) Changes in bone matrix properties with aging. D. B. Burr. Bone 2019; 120-85-93.

**Osteoarthritis**

I began to work in the field of osteoarthrosis (OA) when I joined Dr. Eric Radin at West Virginia University in 1980. At that time, the hypothesis was that the progression of OA was driven by sclerotic subchondral bone that prevented the bone from absorbing stresses that would otherwise be distributed to the cartilage. We primarily employed two different models to study OA: the rabbit impact loading model [1,2], and a sheep model in which the subchondral bone was artificially stiffened. I am frequently asked to speak on this topic and was recently asked by *Nature Reviews* to consider the current status of our understanding of subchondral bone remodeling and bone density on the initiation and progression of osteoarthritis [3]. More recently, we have collaborated with the laboratory of Ellen Gravallese to study the role of bone erosions in the inflammatory arthritides [4]. A review of studies showing how agents designed to reduce skeletal remodeling and be used to treat or prevent osteoarthritis. The work reviewed in this paper suggests that subchondral bone is an important part of the etiology for OA.

(1) Effects of mechanical loading on the tissues of the rabbit knee. E.L. Radin, R.B. Martin, D.B. Burr, B. Caterson, R.D. Boyd, and C. Goodwin. J. Orthop. Res. 1984; 2:221-234.
(2) Mechanical determinants of osteoarthrosis. E.L. Radin, D.B. Burr, B. Caterson, D. Fyhrie, T.D. Brown and R.D. Boyd. Sem. Arth. Rheum. 1991; 21 (suppl. 2):12-21.
(3) Bone remodeling and osteoarthritis. D.B. Burr, M.A. Gallant. Nature Reviews Rheumatology 2012; 8:665-673.
(4) Resolution of inflammation induces osteoblast function and regulates the Wnt signaling pathway. M.M. Matzelle, M.A. Gallant, K.W. Condon, N.C. Walsh, C.A. Manning, G.S. Stein, J.B. Lian, D.B. Burr, E M Gravallese. Arth Rheumat, 2012; 64:1540-1550.
(5) Using agents that suppress bone remodeling to treat or prevent joint disease: Quo Vadis? D.B. Burr. Actual Osteol, 2016; 12:197-214.

**Type II Diabetes**

Because of our finding that raloxifene can improve bone toughness, we decided to apply this treatment to Type II diabetes, a condition in which fracture risk is increased, even though bone mass is normal or even elevated. With diabetes, the high glucose causes glycation of bone collagen, making the bone more brittle and more prone to fracture. We used a rat model in which diabetes is induced by a high fat diet [1]. Femoral toughness was improved in rats treated with raloxifene compared to both diabetic and non-diabetic vehicle-treated rats. Surprisingly, raloxifene treated rats had a lower incidence of diabetes compared with vehicle-treated rats. Treatment prevented the onset of diabetes in all female rats, and in about half of the male rats. Moreover, in those male rats that did become diabetic, the onset of diabetes was 3-4 later than in vehicle-treated rats. This suggests that raloxifene may be helpful in diabetes, both in delaying onset, and in rescuing bone mechanical properties. We recently determined the mechanism by which raloxifene interacts with bone organic matrix to improve its material properties and reduce brittleness [2].

(1) Raloxifene prevents skeletal fragility in adult female Zucker Diabetic Sprague-Dawley rats. K.M. Hill Gallant, M.A. Gallant, D.M. Brown, A.Y. Sato, J. N. Williams, D. B. Burr. PLoS One 2014; 9:e108262.
(2) Structural features underlying raloxifene's biophysical interaction with bone matrix. N. Bivi, H. Hu, B. Chavali, M.J. Chalmers, C.T. Reutter, G.L. Durst, A. Riley, M. Sato, M.R. Allen, D. B. Burr, J.A. Dodge. Bioorganic and Med Chem 2016; 24:759-767.

# Recent Contributions of Thermodynamics & Kinetics of Nanomaterials

**by Qing Jiang, Member EUAS**

Short Biography

*Qing Jiang is Professor of the School of Materials Science and Engineering, Jilin University, and Director of the Key Laboratory of Automobile Materials, Ministry of Education, China. He received his BSc and MSc in Materials Science from Jilin University of Technology (combined into Jilin University in 2000) in 1982 and 1984, respectively, and PhD in Chemistry from University of Stuttgart, Germany in 1990. After working at Technical University of Berlin as a postdoc for two years, Dr. Jiang joined Jilin University of Technology as a professor in 1992. In 2000, he was granted The National Science Fund for Distinguished Young Scholar by National Natural Science Foundation of China. In 2001, Dr. Jiang was awarded as the Chueng Kong Scholar Professor from Ministry of Education, China. During the time from 1996 to 2012, Dr. Jiang worked as vice dean/excusive vice dean of school of Materials Science and Engineering, Jilin University. As visiting professors, Dr. Jiang worked in University of California (Irvine), USA (1997), Forschungszentrum Karlsruhe, Germany (1999), and Tohoku University, Japan (2013).*

*Now Dr. Jiang is a Fellow of The Institute of Physics (U.K.), an Academician of the Asia Pacific Academy of Materials and a Member of the EU Academy of Sciences. He also serves several international journals as the members of the editorial board or advisory boards. He earned the first class prize of science and technology of Jilin province, China, for two times.*

*Dr. Jiang has published more than 500 papers in peer-reviewed journals, including Nature series, Cell series, Adv. Mater., Phys. Rev. Lett., Angew. Chem. Int. Ed., Environ. Energy Sci., et al, which have been cited more than 15,000 times with h-index of 64 (Web of Science). Contributions have also been recorded in 1 monograph, 16 monographic reports and over 50 keynote or invited talks at international conferences. In addition, Dr. Jiang has supervised/co-supervised more than 60 PhD students.*

*Dr. Jiang was elected as a Member of the EU Academy of Sciences in 2018, and an Academician of the Asia Pacific Academy of Materials in 2015. He is a Fellow of The Institute of Physics (U.K.), and several editor board members of academic journals.*

## Research

Y. Q. Li, H. Shi, S. B. Wang, Y. T. Zhou, Z. Wen, X. Y. Lang, Q. Jiang, "Dual-phase nanostructuring of layered metal oxides for high-performance aqueous rechargeable potassi-um ion microbatteries", Nat. Commun. 10 (2019) 4232

### Abstract

Aqueous rechargeable microbatteries are promising on-chip micropower sources for a wide variety of miniaturized electronics. However, their development is plagued by state-of-the-art electrode materials due to low capacity and poor rate capability. Here we show that layered potassium vanadium oxides, KxV2O5·nH2O, have an amorphous/crystalline dual-phase nanostructure to show genuine potential as high-performance anode materials of aqueous rechargeable potassium-ion microbatteries. The dual-phase nanostructured KxV2O5·nH2O keeps large interlayer spacing while removing secondary-bound interlayer water to create sufficient channels and accommodation sites for hydrated potassium cations. This unique nanostructure facilitates accessibility/transport of guest hydrated potassium cations to significantly improve practical capacity and rate performance of the constituent KxV2O5·nH2O. The potassium-ion microbatteries with KxV2O5·nH2O anode and KxMnO2·nH2O cathode constructed on interdigital-patterned nanoporous metal current microcollectors exhibit ultrahigh energy density of 103mWh cm−3 at electrical power comparable to carbon-based microsupercapacitors.

W. T. Jing, Y. Zhang, Y. Gu, Y. F. Zhu, C.C. Yang, Q. Jiang, "N-doped carbon nanonecklaces with encapsulated Sb as a sodium-ion battery anode", Matter 1 (2019) 720-733

**Summary**

The sodium-ion battery has shown great potential to replace the lithium-ion battery, especially for large-scale energy-storage systems. In this work, a hybrid material of ultra-small Sb nanoparticles encapsulated in unique N-doped carbon nanonecklace (Sb/N-CNN) has been synthesized for the first time via electrospinning and in situ substitution. As an anode material in sodium-ion batteries, the as-fabricated Sb/N-CNN exhibits superior rate property (314 mAh g1 at 20 A g1) and cycling stability (401 mAh g1 after 6,000 cycles at 1 A g1), outperforming other Sb-based materials. Such excellent performances originate from the ingenious necklace-like structure of Sb/N-CNN, which supplies efficient electrolyte diffusion paths and more active sites for Na+ insertion/extraction, disperses the stress caused by the large volume change of Sb nanoparticles during the cycling process, and also reduces the electrode resistance. This study provides a facile strategy for construction of a well-designed structure for advanced energy-storage technologies.

Y. H. Zhu, Q. Zhang, X. Yang, E. Y. Zhao, T. Sun, X. B. Zhang, S. Wang, X. Q. Yu, J. M. Yan, Q. Jiang, "Reconstructed orthorhombic V2O5 polyhedra for fast ion diffusion in K-Ion batteries", Chem 5(2019)168-179

**Summary**

Potassium-ion batteries (KIBs) are a promising alternative to lithium-ion batteries because of the abundance, low cost, and redox potential of K; however, the significantly larger radius of K+ inevitably destabilizes the crystal structure of the cathode material, impeding the diffusion of K+. Here, to lower the insertion energetics and diffusion barriers of K+, we synthesizedd-K0.51V2O5 nanobelts (KVOs) with a large interlayered structure and optimized growth orientation by reconstructing the V–O polyhedra of orthorhombic V2O5; these exhibited a high average voltage (3.2 V), high capacity (131 mAh g1), and superior rate capability even at 10 A g1. By coupling the electrochemical experiments with

theoretical calculations, we found that the excellent K-ion storage performance of KVO is attributed to its large interlayered structure and unique 1D morphology. Additionally, we assembled a full KIB composed of KVO and graphite with high energy and power densities, proving its feasibility as a promising new battery.

S. J. Li, Y. T. Zhou, X. Kang, D. X. Liu, L. Gu, Q. H. Zhang, J. M. Yan, Q. Jiang, "A simple and effective principle for a rational design of heterogeneous catalysts for dehydrogenation of formic acid", Adv. Mater. 31(2019)1806781

**Abstract**

Efficient and selective dehydrogenation of formic acid is a key challenge for a fuel-cell-based hydrogen economy. Though the development of heterogeneous catalysts has received much progress, their catalytic activity remains insufficient. Moreover, the design principle of such catalysts are still unclear. Here, experimental and theoretical studies on a series of mono-/bi-metallic nanoparticles supported on a NH2-N-rGO substrate are combined for formic acid dehydrogenation where the surface energy of a metal is taken as a relevant indicator for the adsorption ability of the catalyst for guiding catalyst design. The AuPd/NH2-N-rGO catalyst shows record catalytic activity by reducing the energy barrier of rate controlling steps of formate adsorption and hydrogen desorption. The obtained excellent results both in experiments and simulations could be extended to other important systems, providing a general guideline to design more efficient catalysts.

K. H. Liu, J. Z. Wang, M. M. Shi, J. M. Yan, Q. Jiang, “Simultaneous achieving of high faradaic efficiency and CO partial current density for CO2 reduction via robust, noble-metal-free Zn nanosheets with favorable adsorption energy”, Adv. Energy Mater. 9(2019)1900276

**Abstract**

Electrocatalytic CO2 reduction to fuels is considered a promising strategy for the sustainable carbon cycle. However, the improvement of the catalytic performance of CO2 electrocatalysts still poses many challenges, especially achieving the large partial current density of product and high faradaic efficiency simultaneously, which are essential for future applications of the electrochemical CO2 reduction reaction. In response, herein, an in situ porous Zn catalyst is prepared and exhibits high faradaic efficiency and large CO partial current density at the same time, benefiting from the porous architecture with increased exposure and accessibility of active sites. Furthermore, density functional theory calculations demonstrate that the high faradaic efficiency is attributed to the favorable adsorption energy of the key intermediate, which promotes CO2 electroreduction to CO.

# Atomic Layer Deposition of Emerging 2D Semiconductors, HfS2 and ZrS2, for Optoelectronics

## by Markku Leskelä, Member EUAS

Short Biography

***Markku Leskelä*** *(born 1950), ORCID 0000-0001-5830-2800*
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*https://tuhat.helsinki.fi/portal/en/persons/markku-leskela(78010015-5f49-49b7-b712-54b1b327ac7b).html*

***Education and degrees completed***

*D. Techn. 1980, MSc 1974, Helsinki University of Technology*

***Current position***

*Professor emeritus, University of Helsinki*

***Previous work experience***

*PhD student Helsinki University of Technology (1973-1979); Associate professor University of Oulu (1979-1981; 1982-1986); Professor Helsinki University of Technology (1981-1982); Professor University of Turku (1986-1990); Professor University of Helsinki, 1990 – 2018; Academy professor 2004-2009*

***Research interests***

*Research activities include thin films and nanostructured materials made by various chemical methods (Atomic Layer Deposition, electrodeposition and Successive Ionic Layer Adsorption and Reaction) for applications in micro- and optoelectronics. The studies include all stages in film growth from precursor synthesis to applications. The other research topic is catalysis where the focus is in activation of small molecules by metal complexes in homogeneous systems. Co-author of 713 peer reviewed papers, 66 reviews and holder of 53 patents. Number of citations 26 600; h-index 74 (Web of Science)*

***Personal research funding***

*Number of research grants during whole carrier is about 80. Most important recent fundings:*
*Interfacial engineering of semiconductors for highly selective light-driven chemical transformations (Academy of Finland 2020-2023) 315 000€; European Research Training Network of Functional Hybrid Coatings by Molecular Layer Deposition (EU, 2017-2021) 538 000€; Finnish Centre of Excellence in Atomic Layer Deposition (Academy of Finland, University of Helsinki, 2015-2019) 2 920 000 €; Building-up Centre of Excellence for advanced materials, (EU Teaming project, 2015-16) 130 000 €; Development of ALD processes for microelectronic applications (ASM Microchemistry, 2014-2018) 1 300 000 €*

***Awards and honours***

*Member of Finnish Academy of Science and Letters 1991- ; Finnish Academy of Technical Sciences 1996-; Finnish Society of Sciences and Letters 2005-; SVR I 2005; Magnus Ehrnrooth Foundation Award 2002; ISI Highly cited scientist 2004-; A.I Virtanen award 2011; American Vacuum Society ALD award 2012; Award of Finnish Academy of Sciences and Letters 2014; Honorary member of Finnish Chemical Society 2014; Honorary doctor, University of Tartu 2016; Member of EU Academy of Sciences 2018*

***Other scientific or academic merits***

*Member of board of governors in University of Helsinki, 2010-2017; opponent for 35 PhD theses, pre-examiner for 37 PhD theses, referee for 30 professor positions, evaluator for research proposals in 14 countries, ca. 100 invited talks in international conferences, numerous positions in trust in Finnish and international scientific societies, editorial board member of 6 journals (1989-2019), board member of seven foundations (1992-2019).*

**Atomic Layer Deposition of Emerging 2D Semiconductors, HfS2 and ZrS2, for Optoelectronics**

Miika Mattinen, Georgi Popov, Marko Vehkamäki, Peter J. King, Kenichiro Mizohata, Pasi Jalkanen, Jyrki Räisänen, Markku Leskelä, and Mikko Ritala

**Chemistry of Materials 2019, 31, 5713−5724**
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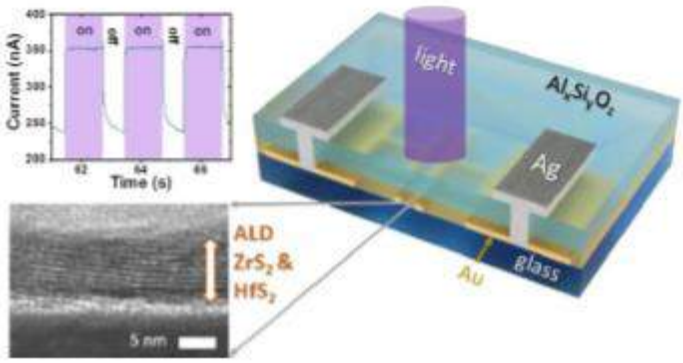
Semiconducting two-dimensional (2D) materials are studied intensively because of their promising performance in diverse applications from electronics to energy storage and catalysis. Recently, $HfS_2$ and $ZrS_2$ have emerged as potential rivals for the commonly studied 2D semiconductors such as $MoS_2$ and $WSe_2$, but their use is hindered by the difficulty of producing continuous films. Herein, we report the first atomic layer deposition (ALD) processes for $HfS_2$ and $ZrS_2$ using $HfCl_4$ and $ZrCl_4$ with $H_2S$ as the precursors. We demonstrate the deposition of uniform and continuous films on a range of substrates with accurately controlled thicknesses ranging from a few monolayers to tens of nanometers. The use of semiconductor industry-compatible precursors and temperatures (approximately 400 °C) enables facile upscaling of the process. The deposited $HfS_2$ and $ZrS_2$ films are crystalline, smooth, and stoichiometric with oxygen as the main impurity. As an important step toward applications of $HfS_2$ and $ZrS_2$, we show that their sensitivity toward oxidation can be overcome by minimizing the impurities in the reactor and by depositing a protective $Al_xSi_yO_z$ layer on the top without a vacuum break. Finally, we demonstrate $HfS_2$ and $ZrS_2$ photodetectors exhibiting good performance and stable operation in ambient conditions. Photoresponsivity comparable to thin films or even single flakes of $HfS_2$ or $ZrS_2$ deposited at much higher temperatures is achieved, although the response speed seems to be limited by photogating, as is common for 2D photodetectors. We expect the first ALD processes for $HfS_2$ and $ZrS_2$ to enable further exploration of these materials for various semiconductor applications.




**Crystalline tungsten sulfide thin films by atomic layer deposition and mild annealing**

Miika Mattinen, Timo Hatanpää, Peter J. King, Kristoffer Meinander, Kenichiro Mizohata, Pasi Jalkanen, Jyrki Räisänen, Mikko Ritala, and Markku Leskelä

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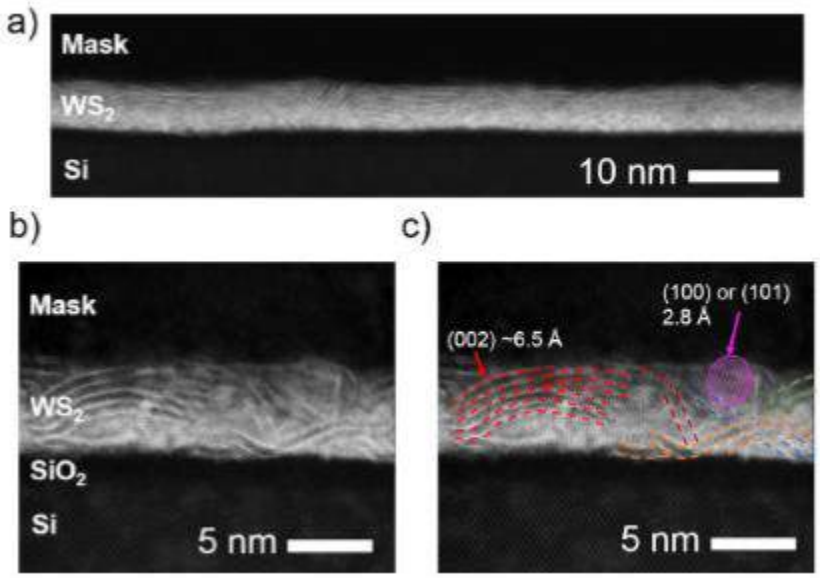
Tungsten disulfide ($WS_2$) is a semiconducting 2D material, which is gaining increasing attention in the wake of graphene and $MoS_2$ owing to its exciting properties and promising performance in a multitude of applications. Herein, the authors deposited $WS_x$ thin films by atomic layer deposition using $W_2(NMe_2)_6$ and $H_2S$ as precursors. The films deposited at 150 °C were amorphous and sulfur deficient. The amorphous films crystallized as $WS_2$ by mild post deposition annealing in $H_2S/N_2$ atmosphere at 400 °C. Detailed structural characterization using Raman spectroscopy, x-ray diffraction, and transmission electron microscopy revealed that the annealed films consisted of small (<10 nm) disordered grains. The approach proposed by the authors enables deposition of continuous and smooth $WS_2$ films down to a thickness of a few monolayers while retaining a low thermal budget compatible with potential applications in electronics as well as energy production and storage, for example.



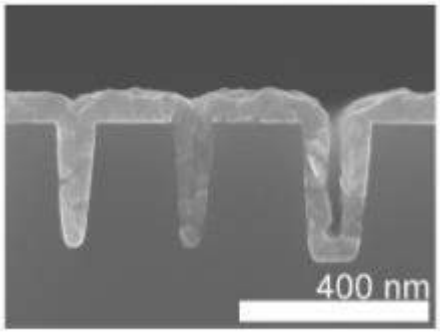

**Atomic Layer Deposition of Intermetallic $Co_3Sn_2$ and $Ni_3Sn_2$ Thin Films**

Katja Väyrynen, Timo Hatanpää, Miika Mattinen, Kenichiro Mizohata, Kristoffer Meinander, Jyrki Räisänen, Joosep Link, Raivo Stern, Mikko Ritala, and Markku Leskelä

**Advanced Materials Interfaces 2019, 6, 1801291 (1-7)**
DOI: 10.1002/admi.201801291

Intermetallics form a versatile group of materials that possess unique properties ranging from superconductivity to giant magnetoresistance. The intermetallic Co–Sn and Ni–Sn compounds are promising materials for magnetic applications as well as for anodes in lithium- and sodium-ion batteries. Herein, a method is presented for the preparation of $Co_3Sn_2$ and $Ni_3Sn_2$ thin films using diamine adducts of cobalt(II) and nickel(II) chlorides, $CoCl_2$(TMEDA) and NiCl2(TMPDA) (TMEDA = *N,N,N',N''*-tetramethylethylenediamine, TMPDA = *N,N,N',N''*-tetramethyl-1,3- propanediamine)

combined with tributyltin hydride. The films are grown by atomic layer deposition (ALD), a technique that enables conformal film deposition with sub-nanometer thickness control. The $Co_3Sn_2$ process fulfills the typical ALD qualifications, such as self-limiting growth, excellent film uniformity, and conformal coverage of a trench structure. X-ray diffraction (XRD) shows reflections characteristic to the hexagonal $Co_3Sn_2$ phase, which confirms that the films are, indeed, intermetallic instead of being mere alloys of Co and Sn. The films are extremely pure with impurity levels each below 1.0 at.%. $Ni_3Sn_2$ films similarly exhibit the expected XRD reflections for the intermetallic phase and are of high purity. The $Co_3Sn_2$ film show magnetic hysteresis with high coercivity values exceeding 500 Oe, indicating great potential in terms of applicability of the films.

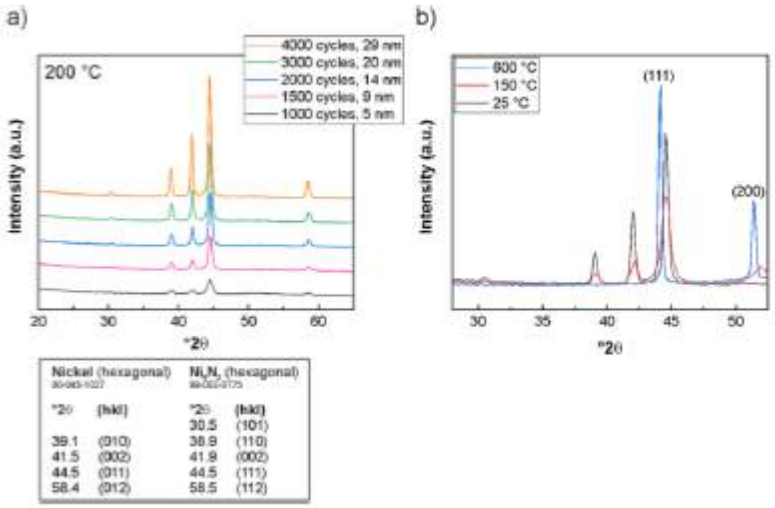



**Atomic Layer Deposition of Nickel Nitride Thin Films using $NiCl_2$(TMPDA) and Tert-butylhydrazine as Precursors**

Katja Väyrynen, Timo Hatanpää, Miika Mattinen, Mikko J. Heikkilä, Kenichiro Mizohata, Jyrki Räisänen, Joosep Link, Raivo Stern, Mikko Ritala, and Markku Leskelä

**Physica Status Solidi A 2019, 1900058** (1-9)
DOI: 10.1002/pssa.201900058

This article describes the atomic layer deposition (ALD) of nickel nitride and nickel thin films using a diamine adduct of Ni(II) chloride, $NiCl_2$(TMPDA) (TMPDA=*N*,*N*,*N*',*N*",-tetramethyl-1,3-propanediamine), as the metal precursor. Owing to the high reducing power of tert-butylhydrazine (TBH), the films are grown at low temperatures of 190–250 $^oC$. This is one of the few low temperature ALD processes that can be used to grow Ni3N and Ni metal on both insulating and conductive substrates. The films are characterized in terms of crystallinity, morphology, composition, resistivity, and coercivity. Xray diffraction shows reflections compatible with either hexagonal Ni or Ni3N. Composition analyses suggest that the films are close to stoichiometric $Ni_3N$. Despite the nitride component, the films exhibit low resistivity values and at the lowest, a resistivity of 37 μΩ cm is achieved. The result is lower than what is typically observed for $Ni_xN$ films and not much higher than the best results concerning ALD Ni metal. The nitrogen content of the films is lowered down to 1.2 at% by postdeposition reduction at 150 $^oC$ in 10% forming gas. After the reduction, the nonmagnetic nitride films are converted to ferromagnetic Ni metal.

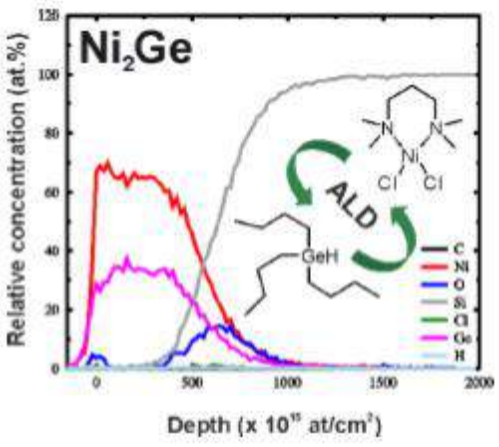



**Nickel Germanide Thin Films by Atomic Layer Deposition**

Katja Väyrynen, Anton Vihervaara, Timo Hatanpää, Miika Mattinen, Mikko J. Heikkilä, Kenichiro Mizohata, Jyrki Räisänen, Mikko Ritala, and Markku Leskelä

**Chemistry of Materials 2019, 31, 5314−5319**
DOI: 10.1021/acs.chemmater.9b01877

This work presents preparation of nickel germanide ($Ni_2Ge$) thin films by atomic layer deposition (ALD). The films were grown using $NiCl_2$(tmpda) (tmpda = N,N,N′,N″,-tetramethyl-1,3-propanediamine) and tributyl germanium hydride serving as a new, efficient reducing agent. This is the first time ALD $Ni_xGe_y$ films are prepared directly upon the combination of two precursors and without any annealing treatment. $Ni_xGey$ is an important contact material for enabling Ge-based transistors and thus circumventing the scaling issues related to current microelectronics. The $Ni_2Ge$ process was examined at low temperatures of 160−200 °C. Self-limiting, saturative growth with a high growth rate of 0.91 Å/cycle was observed at 180 °C. The films were thoroughly analyzed in terms of morphology, crystallinity, composition, and resistivity. The $Ni_2Ge$ films were pure, with the sum of contaminants being less than 1 at. %. Owing to their high purity, the films exhibited low resistivity, suggesting suitability for contact applications.

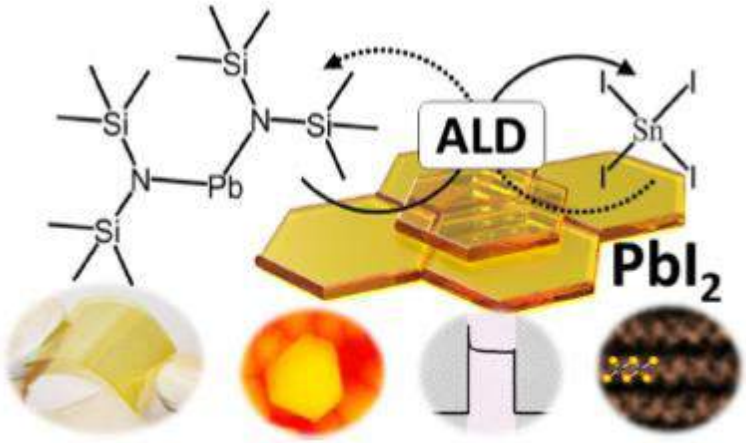


**Atomic Layer Deposition of PbI2 Thin Films**

Georgi Popov, Miika Mattinen, Timo Hatanpää, Marko Vehkamäki, Marianna Kemell, Kenichiro Mizohata, Jyrki Räisänen, Mikko Ritala, and Markku Leskelä

**Chemistry of Materials 2019, 31, 1101−1109**
DOI: 10.1021/acs.chemmater.8b04969

Atomic layer deposition (ALD) enables the deposition of numerous materials in thin film form, yet there are no ALD processes for metal iodides. Herein, we demonstrate an ALD process for $PbI_2$, a metal iodide with a two-dimensional (2D) structure that has applications in areas such as photodetection and photovoltaics. This process uses lead silylamide $Pb(btsa)_2$ and $SnI_4$ as precursors and works at temperatures below 90 °C, on a variety of starting surfaces and substrates such as polymers, metals, metal sulfides, and oxides. The starting surface defines the crystalline texture and morphology of the $PbI_2$ films. Rough substrates yield porous $PbI_2$ films with randomly oriented 2D layers, whereas smooth substrates yield dense films with 2D layers parallel to the substrate surface. Exposure to light increases conductivity of the ALD PbI2 films which enables their use in photodetectors. The films can be converted into a $CH_3NH_3PbI_3$ halide perovskite, an important solar cell absorber material. For various applications, ALD offers advantages such as ability to uniformly coat large areas and simple means to control film thickness. We anticipate that the chemistry exploited in the $PbI_2$ ALD process is also applicable for ALD of other metal halides.



# Contributions in Numerical Methods for Singularly Perturbed and Degenerate PDEs and PDE constrained Optimisation Problems in Classic and Financial Engineering

**by Song Wang, Member EUAS**

Short Biography

*Professor Song Wang, born in 1958 in Wuhan, China, received a B.Sc. degree in Applied Mathematics from Wuhan University of Hydraulic and Electric Engineering, Wuhan (now Wuhan University) in 1982 and a Ph.D. in Numerical Analysis from Trinity College Dublin in 1989, under the supervision of Professor John Miller. Upon his PhD graduation, he was employed by a Dublin-based hi-tech company Tritech Ltd as a senior software engineer and then the technical director. During the period of 1989 to 1992, he managed and was a main contributor to a number of research projects from the then EEC.*

*In late 1992, he migrated from Ireland to Australia to take up a research position at The University of New South Wales. He was then employed by Curtin University of Technology as a lecturer in 1995. From 1999 to 2014 he was an academic in the School of Mathematics & Statistics, The University of Western Australia (UWA), where he got promoted to senior lecturer, associate professor and professor. He also served as the Deputy Head of School at UWA in 2013. In 2014 he moved to Curtin University as a professor of computational mathematics and Head of Dept. of Maths & Stats. Currently he is a professor of Computational Mathematics at Curtin University.*

*In addition to his regular positions in Australia, has held visiting or adjunct professor positions at various overseas universities such as HK Polytechnic University, National Sun Yat-sen University, Sichuan Normal University, Tianjin University of Finance & Economics and Wuhan University. His also a distinguished visiting professor of Laboratory for General Applied Mathematics, Northeast Normal University China, and a director of the China-Australia Collaboration in Applied Optimization, a research centre jointly by Federation University, Curtin University, Shanghai University and Chongqing Normal University.*

*Professor Wang's research interests include scientific computation, numerical optimization and optimal control, optimum design and computational finance. He is a world-leading researcher in these areas and has published many research papers, mostly in well-established international journals. His research activities have been supported financially by government organisations and private sectors from Australia, China, Hong Kong and US. He has supervised numerous PhD students to completion and delivered plenary and keynote talks at many international conferences and workshops. Currently, he is on the editorial boards of several international journals. During 2019 his research activities were in computational mathematics, optimization and optimal control as detailed below.*

## Super-convergent fitted finite volume method for singularly perturbed convection-diffusion equations

A novel 'super-convergent' numerical method for a singularly perturbed convection-diffusion equation was developed by him and his collaborator. The method is based on a fitted finite volume spatial discretization and an implicit time stepping technique. Unlike conventional finite volume methods in which the dual mesh points are naively chosen to be the midpoints of the subintervals of the primal mesh, we construct the dual mesh judiciously using an error representation for the flux interpolation so that both the approximate flux and solution have the second-order accuracy at the mesh points without any increase in computational costs. Numerical results have been presented to demonstrate the super-convergence of the method.

## Penalty method for nonlinear complementarity problems (or Hamilton-Jacobi-Bellman equations)

Most of problem arising in financial engineering, particularly those from pricing financial options are Hamilton-Jacobi-Bellman (HJB) equations of the form:

$$\min\{L_1 v - f_1, L_2 v - f_2, \ldots, L_M v - f_M\} = 0$$

in a domain $\Omega$ and time interval $[0,T]$with terminal and boundary conditions, where $L_1$ is a 2nd-order differential operator, $L_2,\ldots,L_M$ are the 1st or 0th order operators, and $f_1,\ldots,f_M$ are given functions. This is equation is normally non-linear and non-smooth. In our early work, we developed a power penalty function approach to the differential linear and non-linear complementarity problems arising from pricing European and American options of various types. Such a problem is first reformulated as a variational inequality, and the resulting variational inequality is then approximated by a nonlinear parabolic partial differential equation with a power penalty term. It is shown that the solution to the penalized equation converges to that of the variational inequality problem with an arbitrary order. This arbitrary order convergence rate allows one to achieve the required accuracy of the solution to a problem with a small penalty parameter. A numerical scheme for solving penalized nonlinear partial differential equations is also proposed. Numerical results are given to illustrate the theoretical findings and to show the effectiveness.

Penalty methods for various types of linear and non-linear HJB equations of the above form in finite dimensions arising from the discretization of infinite-dimensional HJB equation of the above form have also developed and analysed. These includes both exterior and interior penalty methods. For each of the numerical methods developed, we have established a convergence theory. Numerical results show that our method provide very efficient and useful tools for solving HJB equations of practical significance.

## Novel numerical methods for control and fractional optimal control problems

We have developed a numerical algorithm for solving a class of optimal control problem with a dynamic system containing fractional differential equations of the following form.

$$min_{u\in U}\, F(u) = \int_0^T L\big(t, x(t), u(x)\big)dt \; + \; \mathrm{S(x(T))}$$
$$\text{subj. to} \quad D_t^{\alpha} x(t) = f\big(t, x(t), u(t)\big), \; t \in (0, T],$$
$$x(0) = x^0,$$
$$g\big(u(t)\big) \le 0, \; t \in (0, T).$$

We first propose a robust 2nd-order numerical integrating scheme for the fractional system, based a set of judiciously chosen quadrature points. We then apply a gradient-based search method, along with the numerical integration method to the optimal control problem. Formulas for calculating the gradients with respect to the unknowns defining the approximate control variables are derived. Numerical results are presented to demonstrate that the developed method is able to produces accurate numerical approximations to optimal problems with multiple state and control variables. The results also show that the method is robust with respect to the fractional orders of derivatives.

Numerical solution of other control problems, particularly consensus and event-triggered probabilistic control problems under uncertainty, have also been studies and various numerical methods have been proposed for solving the problems.

## Numerical solution of option evaluation problems

In this work we develop PDE-based mathematical models for valuing real options on investment project expansions when the underlying commodity price follows a geometric Brownian motion. The models developed are of a similar form as the Black-Scholes model for pricing conventional European call options, but, unlike the Black-Scholes' model, the payoff conditions are determined by a PDE system. A finite difference scheme is developed for solving the models and a convergence analysis is performed for the finite difference method. Numerical experiments have been performed using two examples in pricing project expansion options in the mining industry to demonstrate that our models are able to produce financially meaningful numerical results for the two non-trivial test problems.

## Representative significant publications during 2018-2019


1. S. Wang, An interior penalty method for a large-scale finite-dimensional nonlinear double obstacle problem, *Applied Mathematical Modelling*, **58** (2018) 217-228.
2. Y. Yin, Y. Liu, K.L. Teo, S. Wang, Event-triggered probabilistic robust control of linear systems with input constraints: by scenario optimization approach, *Int. J. Robust Nonlinear Control*, **28** (2018) 144—153.
3. Y. Shi, Y. Yin, S. Wang, Y. Liu and F. Liu, Distributed Leader-following Consensus of Nonlinear Multi-agent Systems with Nonlinear Input Dynamics, *Neurocomputing*, **286** (2018) 193-197.
4. S. Wang, K. Zhang, An interior penalty method for a finite-dimensional linear complementarity problem in financial engineering, *Optim. Lett.*, **12** (2018) 1161-1178.
5. S. Zhang, X. Wang, S. Wang, Modeling and computation of energy efficiency management with emission permits trading, *Journal of Industrial and Management Optimization*, **14** (2018) 1349-1365.
6. L. Zhu, Y. Yin, F. Liu and S. Wang, $H_\infty$ filtering for uncertain periodic Markov jump systems with periodic and partly unknown information, Circuits, Systems, and Signal Processing, 37 (2018) 4200-4214.
7. X.-B. Li, S. Wang, Characterizations of robust solution set of convex programs with uncertain data, *Optim. Lett*, **12** (2018) 1387-1402

8. N Li, S. Wang, Pricing options on investment project expansions under commodity price uncertainty, *Journal of Industrial and Management Optimization*, **15** (2019) 261-273.
9. W. Li, S. Wang, V. Rehbock, Numerical solution of fractional optimal control, *Journal of Optimization Theory and Applications*, **180**, No.2 (2019) 556—572.
10. Y. Liu, Y. Yin, K.L. Teo, S. Wang, F. Liu, Probabilistic control of Markov jump systems by scenario optimization approach, *Journal of Industrial and Management Optimization*, **15** (2019) 1447-1453.
11. L. Angermann, S. Wang, A super-convergent unsymmetric finite volume method for convection-diffusion equations, *Journal of Computational & Applied Mathematics*, **358** (2019) 179-189.
12. J. Zhao, S. Wang, A power penalty approach to a discretized obstacle problem with nonlinear constraints, *Optim. Lett.* **13** (2019) 1483-1504.
13. Y. Yin, Y. Shi, F. Liu, K.L. Teo, S. Wang, Second-order consensus for heterogeneous multi-agent systems with input constraints, *Neurocomputing*, **351** (2019) 43-50.
14. Y. Yin, Y. Liu, K.L. Teo, S. Wang, F. Liu, Event-triggered ε-level $H_\infty$ probabilistic control of uncertain systems, *Journal of Franklin Institute*, **356** (2019) 10564-10575.

# Sleep Scheduling in Energy Harvesting Wireless Body Area Networks

## by Amiya Nayak, Member EUAS

Short Biography

*a)* *NAME:*
*NAYAK, Amiya, Professor*
*Member of Faculty of Graduate & Postgraduate Studies*

*b)* *DEGREES:*
*Ph.D., Systems & Computer Engineering, Carleton University, Ottawa, Ontario, 1991*
*M.C.S., Computer Science, Carleton University, Ottawa, Ontario, 1986*
*B.Math., Computer Science and Combinatorics & Optimization, University of Waterloo, 1982*

*c)* *EMPLOYMENT HISTORY:*
*2006 - Professor, School of Information Technology & Engineering, University of Ottawa*
*2002-06 Associate Professor, School of Information Technology & Engineering, University of Ottawa*
*1994-04 Adjunct Research Professor, School of Computer Science, Carleton University*
*1996-02 Member of Scientific Staff, Nortel Networks, Ottawa*
*1985-96 Systems Designer, CMC Electronics, Ottawa*

*d)* *SCHOLARLY AND PROFESSIONAL ACTIVITIES (Since 2010):*
*2018 -* ***Associate Editor****, IEEE Internet of Things Journal.*
*2017* ***Guest Editor****, IEEE Transaction on Industrial Informatics, Special Issue on Cloud Computing in Smart Grid Operation and Management.*
*2016* ***General Co-Chair****, International Workshop on Security, Trust, Privacy and Analytics in conjunction with 30th IEEE International Conference on Advanced Information Networking and Applications (AINA-2016), Crans-Montana, Switzerland.*
*2016* ***Steering Committee Member****, 2nd International Workshop on Future Information Security, Privacy and Forensics for Complex systems (FISP-2016) in conjunction with 11th International Conference on Future Networks and Communications (FNC-2016), Montreal.*
*2016* ***Workshop Chair****, 13th International Conference on Mobile Systems and Pervasive Computing (MobiSPC'16), Montreal, Canada.*
*2016* ***Steering Committee Member****, 1st International Workshop on Information Security and Privacy for Mobile Cloud Computing, Web and Internet of Things (ISCW-2016) in conjunction with 2016 IEEE International Conference on Cloud and Autonomic Computing (ICCAC), Augsburg, Germany.*
*2015--* ***Editorial Board Member****, Journal of Sensor and Actuator Networks (JSAN), MDPI.*
*2015--* ***Advisory Board Member****, International Journal of Distributed Sensor Networks (IJDSN), SAGE Publishing.*
*2015* ***Publicity Chair****, Ad-Hoc, Mobile and Wireless Networks (ADHOC-NOW), Athens, Greece.*
*2014* ***Workshop Chair****, 11th International Conference on Mobile Systems and Pervasive Computing (MobiSPC'14), Niagara Falls, Canada.*
*2013* ***Technical Program Committee Chair****, 10th International Conference on Mobile and Ubiquitous Systems: Computing, Networking and Services, Tokyo, Japan.*
*2013* ***Guest Editor****, IEEE Journal on Selected Areas in Communications, Special Issue on Networking Challenges in Cloud Computing Systems and Applications.*
*2013* ***Technical Program Committee Chair****, IEEE WCNC Mobile Cloud Computing and Networking Workshop, Shanghai, China.*
*2012* ***Program Vice-Chair****, 15th IEEE Int. Conference on Computational Science and Engineering, Nicosia, Cyprus.*
*2012* ***Publicity Chair****, 4th FTRA Int. Conference on Computer Science and its Applications, Jeju Island, Korea.*
*2011* ***Workshop Chair****, 13th IEEE Int. Conference on High Performance Computing and Communications (HPCC), Banff, Canada.*

*2010* ***Program Vice-Chair****, 5th Int. Conference on Frontier of Computer Science & Technology (FCST), Changchun, China.*
*2010- 2013* ***Associate Editor,*** *IEEE Transactions on Parallel & Distributed Systems.*
*2008- 2015* ***Associate Editor****, EURASIP Journal on Wireless Communications & Networking, Hindawi Publishing Corporation.*

**Sleep Scheduling in Energy Harvesting Wireless Body Area Networks**
Published in: IEEE Communications Magazine (Volume: 57, Issue: 2, February 2019)

**Abstract**

WBANs offer a variety of medical applications and have received considerable attention in recent years. Due to the limited energy of sensors, prolonging network lifetime is of paramount importance for WBANs. Although duty-cycling techniques can conserve energy consumption and energy harvesting techniques can provide extra energy supply, the former leads to huge data delivery delay and the latter cannot supply energy infinitely and stably. Therefore, how to maximize network lifetime at low latency is still an open and challenging problem. In this article, we introduce a three-level sleep scheduling strategy for EH-WABNs. The first level is sensor node scheduling, which minimizes the number of sensors in an active sensor group. The second level is active sensor group discovery, which finds the maximum number of active sensor groups to enable alternate work in different frames to the greatest extent. The third level is active sensor group scheduling, which assigns an active sensor group in each frame. Importantly, this article provides a novel route to reduce energy consumption in EH-WBNAs, i.e. a combination of sensor sleep scheduling and energy harvesting, and we believe that this design can also be useful for other network scenarios.

**A Scheme to Design Community Detection Algorithms in Various Networks**

Published in: Future Internet 2019, 11(2), 41

**Abstract**

Network structures, consisting of nodes and edges, have applications in almost all subjects. A set of nodes is called a community if the nodes have strong interrelations. Industries (including cell phone carriers and online social media companies) need community structures to allocate network resources and provide proper and accurate services. However, most detection algorithms are derived independently, which is arduous and even unnecessary. Although recent research shows that a general detection method that serves all purposes does not exist, we believe that there is some general procedure of deriving detection algorithms. In this paper, we represent such a general scheme. We mainly focus on two types of networks: transmission networks and similarity networks. We reduce them to a unified graph model, based on which we propose a method to define and detect community structures. Finally, we also give a demonstration to show how our design scheme works.

**Fair and Social-Aware Message Forwarding Method in Opportunistic Social Networks**
Published in**:** IEEE Communications Letters (Volume: 23, Issue: 4, April 2019)

**Abstract**

In opportunistic social networks, most of the existing store-carry-forward routing mechanisms have severe problems with unfair traffic distribution among nodes and unfair delivery success ratio for individuals. To address these issues, we propose a novel protocol, called fair and social-aware message forwarding (FSMF), for opportunistic social networks. FSMF first introduces a Markov chain model of users' social ties to evaluate users' social relationship and then formulates the problems of unfair traffic distribution and unfair delivery success ratio. Moreover, FSMF limits the number of message copies and restricts the number of forwarding copies according to users' social ties in order to improve fairness. The simulation results show that our protocol has a lower standard deviation of traffic distribution and delivery success ratio.

**Energy-Efficient Sleep Scheduling in WBANs: From the Perspective of Minimum Dominating Set**

Published in**:** IEEE Internet of Things Journal (Volume: 6, Issue: 4, Aug. 2019)

**Abstract**

Wireless body area networks (WBANs) that offer various medical applications have received considerable attention in recent years. Due to limited energy of sensors, duty-cycling technique is employed to prolong the network lifetime. However, it results in long delivery delay and suffers from reliability issues. In this paper, we introduce an efficient and reliable sleep scheduling scheme from the perspective of constructing m-fold dominating set (DS), where m is the number of links from a node outside DS to those in DS. The key idea is to activate partial nodes at each frame to form a DS which can guarantee the network reliability such that the other nodes can fall asleep to save energy. Technically, we formulate the sleep scheduling in a WBAN as a problem of constructing minimum weighted m-fold DS, which is proven NP-hard. We first design an $H(m + \delta)$-approximation algorithm, namely global approximation algorithm, by globally picking the optimal node based on a polymatroid function, where $H(\cdot)$ is the Harmonic number and $\delta$ is the maximum node degree. Then, we propose a simplified $1 + \ln(m\delta)$-approximation algorithm, referred to as local approximation algorithm, to reduce computational complexity and execution rounds. We further conduct extensive simulations to confirm the superiority of our proposed algorithms.

**Lightweight remote user authentication protocol for multi-server 5G networks using self-certified public key cryptography**

Published in: Journal of Network and Computer Applications 131: 66-74 (2019)

**Abstract**

Due to small cell deployments and multiple servers in 5G networks, a fast and anonymous mutual authentication protocol needs to be developed for complex 5G networks. In this paper, we propose a lightweight and untraceable authentication protocol for multi-server-based 5G networks. To reduce computational complexity, we employ self-certified public key cryptography based on elliptic curve cryptography to authenticate the validation of users and servers. Without pairing operations, our scheme could improve performance

efficiency. Also, a formal security model is designed to prove that our protocol is secure against forgery attack due to the discrete logarithm and the computational Diffie-Hellman problem. Performance analysis further shows that our protocol has a lower communication and computational overhead. Also, our protocol could support anonymous mutual authentication.

**Discovery method for distributed denial-of-service attack behavior in SDNs using a feature-pattern graph model**

Published in: Frontiers of Information Technology & Electronic Engineering
September 2019, Volume 20, Issue 9, pp 1195–1208

**Abstract**

The security threats to software-defined networks (SDNs) have become a significant problem, generally because of the open framework of SDNs. Among all the threats, distributed denial-of-service (DDoS) attacks can have a devastating impact on the network. We propose a method to discover DDoS attack behaviors in SDNs using a feature-pattern graph model. The feature-pattern graph model presented employs network patterns as nodes and similarity as weighted links; it can demonstrate not only the traffic header information but also the relationships among all the network patterns. The similarity between nodes is modeled by metric learning and the Mahalanobis distance. The proposed method can discover DDoS attacks using a graph-based neighborhood classification method; it is capable of automatically finding unknown attacks and is scalable by inserting new nodes to the graph model via local or global updates. Experiments on two datasets prove the feasibility of the proposed method for attack behavior discovery and graph update tasks, and demonstrate that the graph-based method to discover DDoS attack behaviors substantially outperforms the methods compared herein.

**An improved network security situation assessment approach in software defined networks**

Published in: Peer-to-Peer Networking and Applications
March 2019, Volume 12, Issue 2, pp 295–309

**Abstract**

Software Defined Network (SDN) is a network framework which can be controlled and defined by software programming, and OpenFlow is the basic protocol in SDN that defines the communication protocol between SDN control plane and data plane. With the deployment of SDN in reality, many security threats and issues are of great concern. In this paper, we propose a security situation awareness approach for SDN. This approach focuses on the attacks like network scanning attack, OpenFlow flooding attack, switch compromised attack and ARP attack in both data plane and control plane. Based on the features of these attacks, we use multiple observations hidden Markov model (HMM) to quantify the network status and then get the security situation assessment values for SDN. The proposed approach can also detect these four attacks and predict the network status based on HMM when given a sequence of observed feature values. We build a test

scenario to simulate our approach with Ryu controller and OpenFlow switch and prove the feasibility of this approach.

**A Distributed Social-Aware Location Protection Method in Untrusted Vehicular Social Networks**

Published in**:** IEEE Transactions on Vehicular Technology (Volume: 68, Issue: 6, June 2019)

**Abstract**

An original sender's location-disclosure is a major privacy issue in vehicular social networks when people are interested in location-aware services. In this paper, we first propose a basic social-aware location-privacy protection (B-SLP) method in vehicular social networks. This method enables trustworthy users to obfuscate an original sender's location with the help of their regions. Then, we provide an improved SLP (I-SLP) to reduce the size of the cloaking area by covering at least k - 1 trustworthy users, while maintaining a required level of privacy protection. Due to disclosure of their locations, selfish users may not help the original sender as they put themselves at risks. To stimulate more trustworthy users to join in the location obfuscation, we then propose encouraging SLP (E-SLP) where each trustworthy user can increase and/or decrease its social tie according to its behavior (cooperation or no-cooperation). Experiments show that B-SLP, I-SLP, E-SLP can improve the query success ratio compared to the existing method, while maintaining a required level of privacy protection.

**A Power-Efficient and Social-Aware Relay Selection Method for Multi-Hop D2D Communications**

Published in**:** IEEE Communications Letters (Volume: 22, Issue: 7, July 2018)

**Abstract**

Due to the short communication range, users are selected as relays to support multi-hop transmission for content sharing/downloading in D2D communications. In this letter, we first exploit social relationships from interacts and contributions, and then formulate an optimal relay selection problem to enhance cooperative multi-hop D2D communications. A Power-efficient and Social-aware Relay Selection (PSRS) algorithm is provided to solve the above problem. Simulation results show that our method has the lowest average power consumption compared to the existing methods.

**Characterization and Detection of Tail Energy Bugs in Smartphones**

Published in**:** IEEE Access (Volume: 6; October 2018)

**Abstract**

Smartphones are the most ubiquitous and popular hand-held devices because of their rich set of features and wide variety of services that require frequent battery recharging. In

smartphones, most energy issues are due to energy bugs (ebugs). These ebugs are said to be exist when smartphone software applications (apps) consume more power than expected while executing, or they continue to consume energy even after these apps are closed or terminated. In this research, we introduce the concept of application tail energy bugs (ATEBs) and provide an operational definition for it. Then, we discuss about the main potential causes of ATEBs and the user actions that can trigger them. To provide a proof of concept, we conduct experiments using real Android apps. To identify all the scenarios that can cause ATEBs, we develop a testing app and perform 32 experiments. The main goal of the experiments is to check the behavior of app components, such as activities and services in the presence/absence of four different types of wakelocks. Then, we discuss the relationship between software changes and energy consumption by tracing wakelocks that keep the device awake and services that might be engaging the CPU. The power consumption of the app is measured using the monsoon power meter. Because power meters are not often available to software developers, we design a tool to detect ATEBs. This tool utilizes Android debug bridge (adb) commands to extract system-related information. The tool effectiveness is evaluated using five Android apps.

**Modeling Handover Signaling Messages in OpenFlow-Based Mobile Software-Defined Networks**

Published in: Journal Computer Networks and Communications. 2018: 1543531:1-1543531:14 (2018)

**Abstract**

The software-defined networking (SDN) paradigm has become essential in tackling several issues and challenges in conventional networking, especially in mobile/cellular networks. In order to realize the benefits brought by SDN to mobility management, we study the effects of SDN in conjunction with OpenFlow protocol on the handover procedure. However, in this new setting, the handover still suffers from delay due to the exchange of OpenFlow signaling messages. In this paper, we focus on SDN in mobile networks and quantify the delays of handover-related OpenFlow messages in order to identify the performance measures as well as the underlying challenges. For our analysis, we provide an analytical model, using which we modeled two handover-related OpenFlow messages in such networks. To the best of our knowledge, no previous work has modeled OpenFlow messages other than Packet-in messages. In this paper, in addition to the Packet-in message, we model Port-status messages. Following our analysis, we propose a novel solution to make handover more efficient and less interruptive. Furthermore, we study our solution in an LTE architecture and compare it to an existing solution. We show that, in normal traffic conditions, our solution can decrease the handover delay as much as 20%.

# Possibility for Controlling Global Warming by Launching Nanoparticles into the Stratosphere

## by Shigenao Maruyama, Member EUAS

Short Biography

*Present Affiliation: President, National Institute of Technology, Hachinohe College, Hachinohe 039-1192, Japan*

***Academic Qualifications***

*B.Eng. 1977, Department of Mechanical Engineering II, Tohoku University, Japan*
*M.Sc. 1979, Department of Aeronautics, Imperial College, London University, UK*
*M.Eng. 1980, Department of Mechanical Engineering, Tohoku University, Japan*
*PhD 1983, Department of Mechanical Engineering, Tohoku University, Japan*

***Professional Carriers***

*1983 Assistant Professor, Institute of High Speed Mechanics, Tohoku University*
*1988 Visiting Scholar, School of Mechanical Engineering, Purdue University, USA*
*1989 Associate Professor, Institute of Fluid Science, Tohoku University*
*1997 Professor, Institute of Fluid Science, Tohoku University.*
*2005-2006 Specially Appointed Assistant to the President, Tohoku University*
*2006-2009 Councilor, Tohoku University*
*2006-2008 Special Advisor to President, Tohoku University*
*2006-2013* ***Special Advisor for Centenary Events and Alumni, Tohoku University***
***2008-2011, 2015-2017 Distinguished Professor of Tohoku University***
***2016 Visiting Professor, INSA de Lyon***
***2017- President, National Institute of Technology, Hachinohe College***

***Awards***

*Japan Society of Mechanical Engineers (JSME), Award for Young Engineers, 1989*
*Fluid Science Foundation, Award for Fluid Science, 1995*
*Heat Transfer Society of Japan (HTSJ), Award for Scientific Contribution, 1998, 2016*
*JSME Medal for Outstanding Paper, 1999, 2013*
*HTSJ, Award for Scientific Measurement, 1999*
*JSME Tohoku Division, Award for Technical Contribution, 2001*
*Japan Society of Applied Electromagnetic and Mechanics, Best Technical Contribution Award, 2001*
*JSME Thermal Engineering Division, Award for Academic Achievements, 2001*
*HTSJ, Award for Technical Contribution, 2002*
*Societe Francaise de Themique, 2002 International SFT Award, 2002*
*JSME Thermal Engineering Division, Award for Contribution, 2003*
*JSME Fellow, 2004*
*Government of Japan, Japanese Medal of Honor (Medal with Purple Ribbon), 2012*
*JSME Thermal Engineering Division, Award for Achievements (Research), 2012*

***Research Activities***

*Professor Shigenao Maruyama specializes in thermal engineering. He has published more than 10 books and 200 academic research papers, and has acquired 50 patents. He investigated various aspects of fluid flow and energy exchange. Based on the principle that conventional heat transfer and thermal control focuses on the enhancement of heat transfer and temperature control of equipment, he has proposed a novel concept of heat-transfer control, in which the heat transfer is actively enhanced or reduced. The proposed active thermal insulation system and a heat-transfer control device utilizes Peltier effects. His work is interdisciplinary utilizing knowledge from various academic disciplines. He has co-authored and edited Thermodynamics (JSME Text series) [1], one of the bestselling books on thermodynamics for mechanical engineering students in Japan. He has also published a book to educate the public*

*thermal science [2], and a novel describing accidents in Fukushima Daiichi nuclear plants [3].*
*Some aspects of his research activities are as follows:*
***Radiative heat transfer:*** *Detailed studies on radiative heat transfer, which is energy transfer by infrared or electromagnetic waves, has been carried out. A generalized analysis method to calculate radiative heat transfer was proposed [4], and this method was applied to analyze heat transfer in semi-conductor processes [5] and industrial furnaces. This method was also applied to large-scale environmental energy transfer processes, such as heat transfer in fogs and clouds [6]. Thermal emission from nano-scale structures was also investigated [7]. These results were published in a monograph [8] which is the first textbook on radiative heat transfer in Japan.*
***Natural convection:*** *Natural convection induced by temperature differences in fluid and the gravitational force was studied, and a generalized description was presented [9]. These results were applied to the cooling fins of electronic devices [10]. This research has been extended to understanding large-scale natural convection in oceanography. The up-welling velocity of deep seawater in the ocean which was proposed by Stommel to be a perpetual salt fountain, was successfully measured for the first time in the world [11].*
***Active heat-transfer control by Peltier elements:*** *Peltier elements, used as cooling equipment, have been applied to a heat-transfer control device. This device has been utilized to the heat-transfer control of equipment in a microgravity environment [12], in an active catheter, and in artificial heart muscles [13]. Furthermore, this heat-transfer control has been applied to the fields of oriental medicine and cryosurgery [14]. The concept of heat-transfer control has been expanded to fusion of thermal engineering and medical engineering [15].*

## Possibility for Controlling Global Warming by Launching Nanoparticles into the Stratosphere [16]

Global warming is one of the most serious problems faced by humans. One method to decrease the Earth's temperature is to reduce solar irradiation by dispersing nanoparticles in the atmosphere. Submicron-diameter particles or aerosols scatter solar irradiation, whereas they are transparent to long-wavelength infrared radiation emitted by the Earth. This phenomenon has received attention in the discussions of the nuclear winter, which is an uncontrolled cooling of the global temperature. The objective of the present work is to examine the first-order approximation of the feasibility of controlling the global temperature without reducing the emission of greenhouse gases. We propose the controlled dispersion of nanoparticles into the stratosphere at an altitude of 30 km. A precise analysis of the radiative properties of particles in the solar spectrum and IR regions is conducted, and radiative transfer through the stratosphere-dispersed nanoparticles is approximated using a one-dimensional single-scattering model. Several types of nanoparticles are considered. The optimum size of the nanoparticles determined using the model is 350-450 nm. The dispersion of nanoparticles with a total mass of $3\times10^7$ tons into the stratosphere will reduce 3% of the solar irradiation. The blockage can be maintained by launching 10-ton projectiles 19 times per day from 100 launch sites.

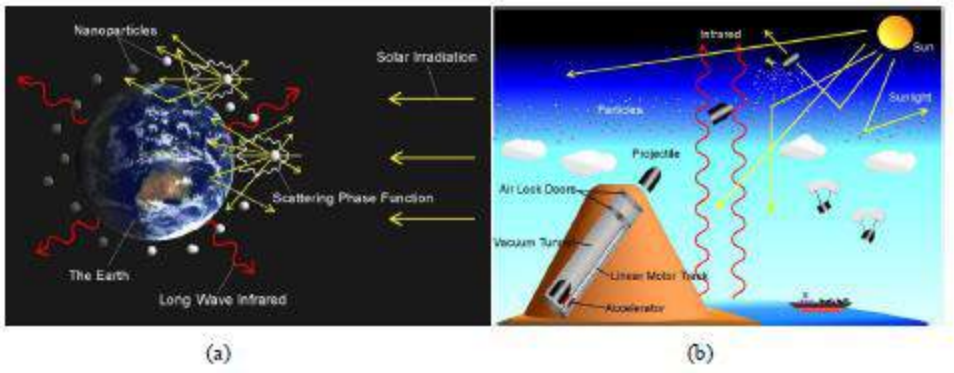



**Fig. 1** Sunlight is scattered by nanoparticles in the atmosphere and infrared emitted by the earth is transparent against the nanoparticle layer (a). Schematic of a system for launching nanoparticles into the stratosphere (b).

The particles will remain in the stratosphere for 5.6 years when they are dispersed at an altitude of 30 km. If we launch 10-ton projectiles 19 times a day from 100 launch sites, we can maintain the mass of the particles in the stratosphere.

## Concept Design of Linear-Motor-Accelerated Projectile for Nanoparticle Dispersion in Stratosphere [17]

Global warming is one of the most serious issues facing humans. The author has proposed dispersing calcite nanoparticles into the stratosphere to decrease solar irradiation without changing the earth's longwave infrared emission [16]. The previous work has shown the potential of the launch system; however, the actual length of the vacuum tunnel, the energy supply to the accelerator, and the flight trajectory of the projectile after being ejected obliquely from the vacuum tunnel have not been investigated. In this paper, a feasibility design of a projectile is introduced to disperse 10 tons of nanoparticles at an altitude of 30 km using a linear-motor accelerator. According to the simulation, a projectile weighing 15 tons can be accelerated up to 1000 m/s in a 34-km acceleration vacuum tunnel by using superconducting linear motors. When the projectile is launched at an altitude of 3.5 km, it can reach an altitude of 30 km. By unfolding sailwings at that altitude, the projectile maintains a level flight during dispersing of the nanoparticles in the stratosphere. The energy required for the launch is $2.55 \times 10^{10}$ J, and the maximum electrical power required is 0.8 GW. The energy cost for dispersing nanoparticles is small compared with other methods such as rockets and airplanes.

**Fig. 2** A conceptual image of projectile flying on the shore of Izu-Oshima dispersing nanoparticles at the altitude of 30 km above the sea.

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# In - Phase and Anti - Phase Synchronization in a Laser Frequency Comb

## by Erich Gornik, Member EUAS

Short Biography

***Erich Gornik*** *received his Ph.D. degree in Physics in 1972. He was a Postdoctoral Fellow at Bell Laboratories, Holmdel, USA, from 1975 to1977. In 1979, he has been appointed Professor for Experimental Physics at the University of Innsbruck. In 1988, he became Professor for Semiconductor Physics and Director at the Walter Schottky Institute of the Technical University Munich. From 1993 until 2012, he was Full Professor for Semiconductor Electronics and Director of the Micro-and Nanostructure Center (ZMNS) at the Technical University of Vienna and since then he is emeritus Professor. From 2003 to 2008 he was managing director of the Austrian Research Centers. Since 2012 he is emeritus Professor at the Technical University Vienna.*

*He has spent several Research Professorships at numerous international research institutions and has received various awards; among others, he is Fellow of the American Physical Society since 1995. In 1997 he received the "Wittgenstein Award" of the Austrian Government and in 2000 the "Erwin Schrödinger Award" of the Austrian Academy of Science. He has supervised more than 150 Master and PhD students. Further achievements are 523 refereed publications, 236 conference proceedings, 90 invited and plenary lectures at international conferences, 7 Patents, h-factor 46.*

**In-Phase and Anti-Phase Synchronization in a Laser Frequency Comb**
PhysRevLett.124.023901

**Abstract**

Coupled clocks are a classic example of a synchronization system leading to periodic collective oscillations. Already in 1665, Christiaan Huygens described this phenomenon as a kind of "sympathy" among oscillators. In this work, we describe the formation of two types of laser frequency combs as a system of oscillators coupled through the beating of the lasing modes. We experimentally show two completely different types of synchronization in a quantum dot laser—in-phase and splay-phase states. Both states can be generated in the same device, just by varying the damping losses of the system.

This modifies the coupling among the oscillators. The temporal laser output is characterized using both linear and quadratic autocorrelation techniques. Our results show that both pulses and frequency-modulated states can be generated on demand within the same device. These findings allow us to connect laser frequency combs produced by amplitude-modulated and frequency-modulated lasers and link these to pattern formation in coupled systems such as Josephson-junction arrays.

A frequency-comb laser simultaneously emits many wavelengths of light, with each being equidistant from the next in frequency space. Some emit an amplitude-modulated (AM) beam, which appears as pulsed rather than continuous light, others emit a frequency-modulated (FM) beam, where the light has a steady intensity but a modulated frequency. Because these two types of comb produce different outputs, researchers thought that their spectra arose from independent physical mechanisms. Now, in a new experiment, Benedikt Schwarz of the Technical University of Vienna and colleagues demonstrate a quantum-dot laser that produces both types of frequency combs.

The researchers produce the AM and FM frequency combs using a near-infrared laser, where the light comes from photons emitted by excited quantum dots. When they apply a negative voltage to the dots, they find that they can excite the dots more quickly, and the laser produces an AM beam. Without the negative voltage, the laser emits a FM beam.

To explain the finding, the team likens the AM and FM laser outputs to the motion of a group of metronomes. Metronomes are known to swing in either synchrony or antisynchrony when placed on a tabletop, the motion type depending on the table's damping. In the comb, each frequency couples to its neighbor to produce a so-called "beat note" whose frequency is equal to the spacing between the comb's teeth.

If all contributions to the beat note have the same phase—move in synchrony—the beat note intensity is maximized, and the result is an AM "pulsed" output. However, if the laser's gain medium is sufficiently damped, the phases antialign, and the beat note vanishes, leading to a FM output. Their theoretical work suggests that many semiconductor lasers can sustain both settings.

# Two-Drug Combinations as First-Step Antihypertensive Treatment

## by Giuseppe Mancia, Member EUAS

Short Biography

***PRESENT POSITION***. *GM is Professor Emeritus of the University Milano.-Bicocca. He is also Head of the Hypertension Center, university Institute, Verano, Policlinico di Monza, President of the Italian Foundation on "Ricerca e Innovazione su Ipertensione e Protezione Cardiovascolare" and Chairman of the Foundation of the European Society of Hypertension (ESH, Zurig, Switzerland). He serves since 2008 as Chairman of the Joint Board of the Italian Scientific Societies operating in the area of cardiovascular prevention.*

***DEGREES/DIPLOMAS***. *He trained at the University of Siena, Medical School, where he graduated in 1964 cum laude. He obtained in 1967 the Post-graduate Diploma (cum laude) of Specialist in Cardiology and Rheumatology while working at the Istituto di Patologia Medica of the University of Siena with a fellowship of the National Research Council. He obtained the Ph.D. (Libera Docenza) in Physiology in 1970 and worked as Post-graduate Fellow of the US Public Health Service and Associate Researcher at the Mayo Clinic (1972-1974).He has been Resident in the Postgraduate School of Cardiology of the Virginia Commonwealth University(1974)*

***ACADEMIC/HOSPITAL POSITIONS***.*GM has been Assistant and Associate Professor of Internal Medicine at the University of Milan from 1969 to 1985.From 1985 he has been appointed full Professor of Internal Medicine at the University of Milano first and the Milano-Bicocca University later. Between 1992 and 2012 he has been Head of the Division of Internal Medicine and Chairman of the University and Hospital Departments of Clinical Medicine at the S. Gerardo Hospital, Monza. He has also been Director of several Postgraduate Schools of Medicine (Cardiology, Internal Medicine, Emergency Medicine and Endocrinology),University Masters (Transplant Medicine, Electrophysiology and Cardiac Electro-Stimulation),and the Research Doctorate in Hypertension and Cardiovascular Risk of the Milano-Bicocca University. He has chaired the Interuniversity (Universities of Milano, Milano-Bicocca and Pavia) Center of Clinical Physiology and Hypertension from 2001 to 2012 .*

***SCIENTIFIC SOCIETES/TASK FORCES/COMMITTEES***. *GM has served as Member of the Scientific Council, Secretary and President of the International Society of Hypertension (ISH) between 1982 and 1992, President of the European Society of Clinical Investigation (1980-1982), Chairman of the Working Group on Hypertension and the Heart of the European Society of Cardiology (ESC,1994-1996), member of the Executive Scientific Committee of ESC (1986-1991), President of the Italian Society of Hypertension (1997-1999) and member of the Scientific Council of ESH between 1989 and 2003 (President, 1999-2001). He has been member ex-officio (only European) of the Executive Council of the American Society of Hypertension (1996-2008), Officer for the ISH Forum of National Societies, member of the Committee on Cardiovascular Drugs and Therapy of the World Heart Federation and member of the Writing Committee of the ESC guidelines on Prevention of Cardiovascular Diseases (1993, 1998, 2003),the WHO/ISH Guidelines on Hypertension (1993, 1999) and the Guidelines on Hypertension in the Elderly of the American College of Cardiology (2011,only European).He has co-chaired the Task Force on the ESH-ESC guidelines on Hypertension (2003,2007,2009 and 2013 and 2018) and the WHO/ISH Liaison Committee. He has chaired the Scientific and Organising Committees of various ESH Meetings (2001, 2003, 2005, 2007, 2009, 2011, 2013,2015,2017 and 2019). He has been Chairman of the Scientific Committee of the ISH Congress in Prague (2002) and Honorary President of the ISH Meeting in Montreal (1990), San Paulo (2004), and Athens (ESH/ISH meeting,2014).He is currently Chairman of the Educational Board of ESH.*

***AWARDS/HONORS***.*GM has received several Awards, among which the Heymans Award of the International Society of Pharmacology, the Wright International Award of the High Blood Pressure Council of Australia, the ISH Volhard and the Tigersted (MSD) Awards, the ESH Folkow Award, the Life Achievement Award of the Italian Society of Hypertension, the Peter Sleight Award of the World Hypertension League and the Alberto Zanchetti Life Achievement Award of ESH. He was appointed Lecturer of the Year by the Belgian Universities and Hypertension Leagues (1992) and was conferred the Talal Zein Foundation Award, the International Recordati Prize (2000), the 2001 Invernizzi Award for Medicine, the Gold Medal of the Lorenzini Foundation (2008),the Hariri Memorial Award (2009) and the Spinoza Award of the Amsterdam University. He has been appointed Honorary Member of ESH, the High Blood Pressure Council of Australia, the Latino-American Hypertension Society(LASH) and the Japanese Circulation Society. He is honorary member of many other Scientific Academies or Societies, among which the British Hypertension Society, the German Hypertension League ,the Spanish Hypertension Society, and the Hellenic Cardiology Society . He has received the highest Award of the Lombardy Region (Rosa Camuna) and the title of Commander of the Order of the Italian Republic in 2014.He has recently been awarded as one of the 100 Italian excellences in various areas of human activities (Award ceremony in the Italian Parliament ,December 2015).He is member of the 2003 Group for Research (the Group of the highly cited*

*Italian scientists in the world) and member of the European Academy of Sciences*
*He has been invited to give state-of-the-art, keynote, debates or special and plenary lectures in more than 700 international meetings. He has also been guest lecturer at meetings of many national societies of hypertension, cardiology awarded as one and internal medicine, among which the Pickering Lecture (British Hypertension Society), the Tigersted Lecture (Finnish Hypertension Society), the Merck Frosst Lecture (Canadian Society of Cardiology), the Saeb Salam Memorial Lecture (Beirut University), the Brian Bronte Steward Memorial Lecture (Glasgow University) the Leloir Nobel Laureate Lecture (Buenos Aires),the Mac Donald Lecture (Hamilton),the Gavras Life Achievement Award Lecture (Athens),and the Population Health Lecture (Mac Master University, Hamilton).*
***HONORARY DEGREES/ACADEMIC RECOGNITIONS**. GM has received the Honorary Professorship of the University of Cordoba. He is Honorary member of the Academy of Science of Cordoba, and has been conferred the Degree Honoris Causa in Medicine from the University of Gdansk and the Carol Davila University of Bucharest. He has also received the Degree Honoris Causa (Doctor of Science) from the University of Glasgow..*
***EDITORIAL ACTIVITY**. GM has edited more than 90 Special issues or Supplements to international cardiovascular and internal medicine Journals. He has written or edited more than 20 books on hypertension, metabolic diseases and cardiovascular diseases edited by international Publishers, among which several Manuals, including the official ones of ESH. He is or has been member of the Editorial Board, Guest Editor and Reviewer of many important international journal on hypertension, cardiovascular disease and internal medicine. He is Editor-in-Chief of the Journal of Hypertension, the official ISH/ESH Journal*
***SCIENTIFIC ACTIVITY**. GM's research interests focus on epidemiology pathophysiology, diagnosis and treatment of hypertension, heart failure, and coronary disease, as well as on the clinical aspects of diabetes, obesity and other metabolic abnormalities. His expertise includes ambulatory blood pressure monitoring, neurohumoral control of the circulation, large artery mechanics, hemodynamic changes of cardiovascular drugs, cardiovascular regulation during stress and sleep as well as epidemiology and intervention trials in hypertension and diabetes. He has been member or chairman of the steering committees of several clinical trials. He has published more than 2000 original papers, reviews and editorials in peer-review journals.*
***BIBLIOMETRIC DATA**. GM is since many years in the list of the Highly Cited scientists of ISI and Clarivate Analytics. One of his papers has been the most highly cited article in the world medical literature in the years 2004-2005 (Ref. The Scientist) and three have been included among the most widely quoted hypertension papers ever (Ref. Hypertension,2014).In 1995 he was classified as the most widely quoted cardiologist in Italy and in 2013 has been included among the 400 most influential biomedical investigators in the world ( Ref. EJCI).In 2019 he has been classified as the first expert in Europe and the second in the world for the area Hypertension-Cardiovascular(2008-2018 publications, Baltimore University, Ref. Expertscape). Recently, a career assessment of 6 million scientists from all research areas (Ref. Plos Biology, 7 million papers analysed )has ranked him among the first 300 scientists in the world (1st in Italy) as well as the 12$^{th}$ world cardiologist and 1st hypertensiologist. GM's publications have received, up to December 2019, more than 201.000 citations in the international medical literature, with a H-index of 170 ( Ref. Microsoft Academy), the highest among Italian cardiologists and internists.*

## Two-Drug Combinations as First-Step Antihypertensive Treatment.

Mancia G, Rea F, Corrao G, Grassi G
Circulation Research 2019,124.1113-1123

## Abstract

Blood pressure (BP) control in patients with hypertension is variable worldwide, and in general, it results largely unsatisfactory. Factors responsible for this phenomenon include insufficient national cardiovascular healthcare policies for prevention, poor patient compliance with prescribed treatment schedules, and the reluctance of physicians to modify treatment strategies when BP is still elevated, that is, the so-called therapeutic inertia. A further important factor favoring poor BP control is the limited use of combination drug treatment, despite evidence of its superior ability to control BP in patients with difficult-to-treat hypertension. In addition, combination treatment allows to achieve BP control more easily (and more quickly) as compared with monotherapy. This article, after briefly examining the main features of BP control, will review the importance in the treatment of hypertension of the drug combination strategy, based on the

recommendations of the 2018 European Society of Cardiology/European Society of Hypertension guidelines. Empahsis will be given to the drug combination treatment as first step of the antihypertensive therapeutic intervention. The potential drawbacks and barriers to combination drug treatment as initial therapeutic strategy will also be briefly discussed.

## Limited reproducibility of MUCH and WUCH: evidence from the ELSA study.

Giuseppe Mancia, Rita Facchetti3, Cesare Cuspidi3, Michele Bombelli3, Giovanni Corrao4, and Guido Grassi

## Abstract

**Aims**
To evaluate the long-term reproducibility of masked (MUCH) and white-coat uncontrolled hypertension (WUCH), an information crucial for determining the long-term prognostic impact of these conditions.
**Methods and Results**
Reproducibility of MUCH and WUCH was assessed in 1664 hypertensive patients recruited for the European Lacidipine Study on Atherosclerosis and treated with atenolol or lacidipine (±additional drugs) during a 4-year period. Office and 24 h blood pressure (BP) was measured at baseline and every year during treatment, allowing repeated classification of either condition. After 1 year of treatment 21.1% and 17.8% of the patients were classified as MUCH and WUCH, respectively. For both conditions the prevalence was similar in the following years, although with a large change in patients composition because only about 1/3 of patients classified as MUCH or WUCH at one set of office and ambulatory BP measurements maintained the same classification at a subsequent set of measurements. In only 4.5% and 6.2% MUCH and WUCH persisted throughout the treatment period. MUCH and WUCH reproducibility was worse than that of patients showing control or lack of control of both office and ambulatory
BP, i.e. controlled and uncontrolled hypertension, respectively.
**Conclusion**
Both MUCH and WUCH display poor reproducibility over time. This should be taken into account in studies assessing the long-term prognostic value of these conditions based on only one set of BP measurements.

## Effects of renal denervation on kidney function and long-termoutcomes: 3-year follow-up from the Global SYMPLICITY Registry

Felix Mahfoud, Michael Bo¨hm, Roland Schmieder, Krzysztof Narkiewicz, Sebastian Ewen, Luis Ruilope, Markus Schlaich, BryanWilliams, Martin Fahy, and Giuseppe Mancia

## Abstract

**Aims**
Several studies and registries have demonstrated sustained reductions in blood pressure (BP) after renal denervation (RDN). The long-term safety and efficacy after RDN in real-world patients with uncontrolled hypertension, however, remains unknown. The objective

of this study was to assess the long-term safety and efficacy of RDN, including its effects on renal function.

**Methods and Results**

The Global SYMPLICITY Registry is a prospective, open-label registry conducted at 196 active sites worldwide in hypertensive patients receiving RDN treatment. Among 2237 patients enrolled and treated with the SYMPLICITY Flex catheter, 1742 were eligible for follow-up at 3 years. Baseline office and 24-h ambulatory systolic BP (SBP) were 166 ± 25 and 154 ± 18 mmHg, respectively. SBP reduction after RDN was sustained over 3 years, including decreases in both office (-16.5 ± 28.6 mmHg, P < 0.001) and 24-h ambulatory SBP (-8.0 ± 20.0 mmHg; P < 0.001). Twenty-one percent of patients had a baseline estimated glomerular filtration rate (eGFR) <60 mL/min/1.73m2. Between baseline and 3 years, renal function declined by 7.1 mL/min/1.73m2 in patients without chronic kidney disease (CKD; eGFR >_60 mL/min/1.73 m2; baseline eGFR 87 ± 17 mL/min/1.73m2) and by 3.7 mL/min/1.73m2 in patients with CKD (eGFR <60 mL/min/1.73m2; baseline eGFR 47 ± 11 mL/min/1.73 m2). No long-term safety concerns were observed following the RDN procedure.

**Conclusion**

Long-term data from the Global SYMPLICITY Registry representing the largest available cohort of hypertensive patients receiving RDN in a real-world clinical setting demonstrate both the safety and efficacy of the procedure with significant and sustained office and ambulatory BP reductions out to 3 years.

## High Normal Blood Pressure and Left Ventricular Hypertrophy Echocardiographic Findings From the PAMELA Population.

Cuspidi C, Facchetti R, Bombelli M, Tadic M, Sala C, Grassi G, Mancia G
Hypertension. 2019 Mar;73(3):612-619

## Abstract

Cross-sectional and longitudinal data analysis of the PAMELA (Pressioni Monitorate E Loro Associazioni) population was performed to assess the association between prehypertension and left ventricular hypertrophy (LVH) at entry and the risk of new-onset LVH associated to this condition in the subset of participants with normal LV mass index (LVMI). A total of untreated 1397 participants with measurable echocardiographic parameters at baseline were considered in the cross-sectional analysis. The longitudinal analysis included 880 participants without LVH at baseline and with measurable LVMI at follow-up examination performed 10 years later. At entry, after adjustment for major confounders LVH prevalence rates (LVM/body surface area) showed a significant, progressive increase from the normotensive (2.1%), to prehypertension (6.7%), and hypertension group (18.3%). The incidence of LVH increased progressively from the normotensive to prehypertension and hypertension group (9.0%, 23.2%, and 36.5%, respectively). The risk of new LVH was significantly greater in prehypertension who progressed to sustained hypertension (odds ratio, 4.21; CI, 1.64-10.83; P=0.003) than in those with persistent prehypertension (odds ratio, 1.89; CI, 0.77-5.11; P=0.21) compared with persistent normotensive participants after adjustment for age, sex, baseline LVMI, obesity, glucose, creatinine, total cholesterol and the use of antihypertensive drugs at follow-up. Further adjustments for changes in body mass index, metabolic variables, and

creatinine during the follow-up did not modify the strength of association between prehypertension and new-onset LVH. Our findings offer a new piece of evidence on the association of prehypertension with LVH and support the view that preventive actions for this condition affecting a large fraction of the general population should be intensified.

## Blood Pressure Non-Dipping and Obstructive Sleep Apnea Syndrome: A Meta-Analysis

Cesare Cuspidi, Marijana Tadic,, Carla Sala, Elisa Gherbesi, Guido Grassi and Giuseppe Mancia

## Abstract

We examined the reduced blood pressure (BP) nocturnal fall in patients with obstructive sleep apnea (OSA) by a meta-analysis including studies that provided data on prevalence rates of non-dipping (ND) pattern during 24-h ambulatory blood pressure monitoring (ABPM). Design: The PubMed, OVID-MEDLINE, and Cochrane CENTRAL literature databases were searched for appropriate articles without temporal restriction up to April 2019 through focused and sensitive search methods. Studies were identified by crossing the search terms as follows: “obstructive sleep apnea”, “sleep quality”, “non dipping”, “reduced nocturnal BP fall”, “circadian BP variation”, “night-time BP”, and “ambulatory blood pressure monitoring”. Results: Meta-analysis included 1562 patients with OSA from di_erent clinical settings and 957 non-OSA controls from 14 studies. ND pattern prevalence in patients with OSA widely varied among studies (36.0–90.0%). This was also the case for non-OSA controls (33.0% to 69.0%). Overall, the ND pattern, assessed as an event rate in the pooled OSA population, was 59.1% (confidence interval (CI): 52.0–65.0%). Meta-analysis of the seven studies comparing the prevalence of ND pattern in participants with OSA and controls showed that OSA entails a significantly increased risk of ND (Odds ratio (OR) = 1.47, CI: 1.07–1.89, $p < 0.01$). After the exclusion of patients with mild OSA, OR increased to 1.67 (CI: 1.21–2.28, $p < 0.001$). Conclusions: The present meta-analysis, extending previous information on the relationship between OSA and impaired BP dipping, based on single studies, suggests that this condition increases by approximately 1.5 times the likelihood of ND, which is a pattern associated with a greater cardiovascular risk than normal BP dipping.

# Advances in Water Microbiology, Water Quality and Public Health Safety

## by Joan Rose, Member EUAS

Short Biography

*Dr. Joan Rose serves as the Homer Nowlin Chair in Water Research at Michigan State University, the Co-Director of the Center for Advancing Microbial Risk Assessment (CAMRA) a 10 million dollar grant funded by the EPA and US Department of Homeland Security. She is also the Director of the Center for Water Sciences (CWS). Dr. Rose received her B.S., in 1976 from University of Arizona, her MS from University of Wyoming in 1980 and Ph.D. in Microbiology from the University of Arizona in 1985. She served as a Professor in the College of Marine Science, University of South Florida (USF) from 1998-2002 and Associate Professor, Department of Marine Science, USF from 1994-1997. In 1995, she was an Assistant Professor, Department of Environmental and Occupational Health, USF, and from 1986-1989, she served as Research Associate/Lecturer, Department of Microbiology and Immunology, UAZ.*

*Dr. Rose is an international expert in water microbiology, water quality and public health safety publishing more than 300 manuscripts. She has been involved in the investigation of numerous waterborne outbreaks world-wide. Her work has examined new molecular methods for waterborne pathogens and zoonotic agents such as Cryptosporidium and enteric viruses and source tracking techniques. She has been involved in the study of water supplies, water used for food production, and coastal environments as well as water treatment wastewater treatment, reclaimed water and water reuse and quantitative microbial risk assessment. She specifically interested in microbial pathogen transport in coastal systems and has studied the impact of wastewater discharges and climate on water quality. She was named as one of the 21 most influential people in Water in the 21st Century by Water Technology Magazine in 2000 and won the Clarke Water Prize ($50,000. prize) (one of 5 international awards for contributions to water science and technology).*

*She current serves on a number of advisory committees include 1) Chair of the Drinking Water Committee for the Science Advisory Board for the U.S. Environmental Protection Agency 2) Vice-Chair of USA National Committee for the International Water Association, 2002-05, 4) Member of the Strategic Council for IWA 2005-08, 3) Chair of the Specialist Group Health-Related Water Microbiology (IWA). 4) She is currently advisory to the Governments of Singapore and Queensland, Australia, serving as chair of the audit committee for the Public Utilities Board in Singapore for the last 4 years.*

*She was appointed to Water Science and Technology Board of National Academy of Science, National Research Council, 1998-2004 and served as Vice Chair of the Board from 2002-04. Professional society memberships include American Academy of Microbiologists, American Public Health Association, American Society of Microbiology,, American Water Works Association (AWWA), Society for Risk Analysis, International Water Assoc. and Water Environment Federation.*

*Sources of recent grant and/or contract support include NOAA, EPA, Water Environ. Research Foundation, and NSF,*

***Positions and Honors***

***Positions and Employment***

*1986-1989: Research Associate/Lecturer, Department of Microbiology and Immunology, and Nutrition and Food Science, University of Arizona*

*1989-1994: Assistant Professor, Department of Environmental and Occupational Health, University of South Florida*

*1994-1997: Associate Professor, Department of Marine Science, University of South Florida*

*1995: Courtesy Appointment, Associate Professor, Department of Civil and*

*Environmental Engineering, University of South Florida*
*1998-2002: Professor, College of Marine Science, University of South Florida*
*2005-2014: Co-Director, Center for Advancing Microbial Risk Assessment (CAMRA), Michigan State University (Center of Excellence DHS/EPA)*
*2003-present: Homer Nowlin Endowed Chair for Water Research, Michigan State University*
***Honors** (Most Recent)*
*Member of the National Academy of Engineering, inducted 2011*
*Awarded the KWR Water Fellow, Netherlands, October, 2016*
***Stockholm Water Prize 2016***
*Recipient of The Michigan Environmental Council's Helen & William Milliken Distinguished Service Award, 2018*

Dr. Rose has been studying the water virome. Pathogenic viruses are of great concern because they are more environmentally stable as compared to bacteria, display resistance to various conventional methods used for controlling bacterial pathogens and cause high probability of infection at low doses. The actual burden of waterborne infections caused by pathogenic viruses is likely underestimated because they are not routinely monitored for both in clinical and environmental samples. There is currently no established method to fully describe the broad diversity of human viral pathogens in environmental samples despite the increasing importance of environmental viral infections in global public health. The advent of high throughput sequencing technologies coupled with metagenomics offers an opportunity to identify human viral pathogens in various environmental samples without a priori knowledge of what viruses may be present. Moreover, environmental surveillance for the presence of pathogenic viruses is important for development of rational disease control strategies. The advances in high-throughput next-generation sequencing (NGS) have greatly enhanced our understanding of the water microbiome. While viruses are the most abundant entities on earth we know very little about viral abundance and diversity. Engineered systems that move water around including ship ballast, aquaria and sewage were examined using NGS. In aquaria, viromes were dominated by DNA phages of the order Caudovirales and aquarium viromes were associated with controlled system parameters, including nitrate, salinity, and temperature as well as resident animal profiles, indicating the close interaction of viromes with aquarium management practice. Emerging human viruses including human picobirnavirus, novel astrovirus MLB strains, cosavirus, cardiovirus, bocavirus, Aichi virus, parechovirus and salivirus, were detected in sewage. Metagenomic analysis of the ballast water samples revealed viral communities that were dominated by dsDNA bacteriophages (mainly Myoviridae, Podoviridae, and Siphoviruses) as well as dsDNA algal viruses, Phycodnaviridae and ssDNA bacteriophages, Microviridae. Of the contigs with similarity to animal viruses, emerging viral pathogens of fish and shrimp were detected that included European catfish virus and Singapore grouper iridovirus infecting fish and White spot syndrome virus and Infectious myonecrosis virus infecting shrimp. Implications for the biohealth of the planet using new technology will be further explored the water virome.

She has also been involved with the study of non-point source pollution and the

landscape. Water is one of the most critical of all the world's life support systems on which the Blue Planet depends upon. Water quantity and quality (access and management) are interlinked with our global biohealth servicing a sustainable plant, animal and human network.The understanding of water quality at larger scales, ground and surface water interactions impacted by land and climate is essential to our future investments for protection and restoration. In the last 60 years we have seen a great acceleration of population growth (in people and animals), landuse change, use of fertilizers, and water. This has led us into the anthropocene where continued water quality degradation as demonstrated by increased eutrophication and fecal contamination associated with microbial hazards along with antibiotic resistance which is a global phenomenon. This is exacerbated by climate change and extreme events. Despite our investment in infrastructure and better environmental protection policies, water pollution shows a continual and dramatic impact on health. In order to address remediation efforts fecal pollution sources at the watershed scale and water quality across the entire lower peninsula of Michigan have been investigated. New technology that allows greater precision, droplet digital PCR (ddPCR) was used for microbial source tracking (MST) for bovine and human markers along with data on E. coli . Results were able to identify non-point sources including septic tanks and animal manure and showed a relatively high number of sites contaminated during different flow regimes (45 – 75% of samples). Higher spatial and temporal water samples (n=136) were collected from 17 sites from 5 watersheds in Michigan's Lower Peninsula during eight sampling events, between April 2017 and May of 2018, representing the growing season, fall/winter baseflow and spring snow melt. Spatial clusters were consistent with land use and tillage practices at each watershed, whereas temporal clusters were mainly explained by hydrological conditions. We identified two major spatial clusters of sampling locations, which resembled the difference in the percentage of the developed area within each watershed. The animal and human contamination were not correlated with E. coli. Different mechanisms were shown to be associated with the various fecal pollution sources including ground water and overland runoff impacts on surface waters in Michigan. Key watersheds were identified for further assessment and restoration.

For more than 20 years Dr. Rose has been involved in drinking water investigations of water-borne outbreaks and she well known for my work on the waterborne outbreak of *Cryptosporidium* in Milwaukee. She served as the Co-Director of the Center for Advancing Microbial Risk Assessment (CAMRA, Dept of Homeland Security and EPA sponsored 10 million dollar center) as well as the QMRA wiki which houses all the pathogen specific data for risk assessment http://qmrawiki.org/

**International Activities**

Professor Rose has quietly pursued her two passions over the last 30 years: i. assessing pathogenic microorganisms in water through engaged community

research and ii. global water science networking and education. In fact she began her PhD work in Mexico evaluating a full-scale drinking water treatment system for enteric virus removal for over two years. Dr. Rose has been a key global leader involved in the evolution of the field of health-related water microbiology and she works at full-scale focusing on new methods and their use in the field, surveillance, water treatment control and risk assessment. She has brought the new methods, new frameworks, the biology-math approaches to programs around the world. From the start she worked broadly in Central and South America, but then shifted and is now additionally working in Asia.

Professor Rose began her studies in environmental virology but quickly embraced and developed testing methods for enteric protozoa including *Giardia* and was the first to publish on methods and surveillance of water for *Cryptosporidium* as it emerged dramatically and globally in the 80s.

**Central and South America**

From 1988 to 2001, she organized and ran 9 workshops for transferring the technology for monitoring viral and protozoan pathogens in Argentina, Brazil, Chile, Guatemala, Mexico, Panama and Venezuela. This included hands on training and collection of local samples. The unique aspect of these workshops was that the audience was always a mixture of academics (including students), government workers (including public health officials; laboratory scientists) and policy makers. As her work on risk assessment progressed Professor Rose began working with her international colleagues providing workshops at their request to train scientists and students from engineering, public health and water microbiology.

**Asia**

Professor Rose began her work in Asia when she was asked to join the PUB NEWater Expert Study Panel from 2000 – 2002, where she provided independent advice, reviews and evaluation of the results and findings of the study that evaluated the suitability of NEWater for potable use. This was critical in ensuring that the NEWater Study was robust. The NEWater Expert Study Panel eventually concluded that NEWater was consistently of a safe, high quality, well within the international drinking water requirements, and recommended that NEWater could be considered for indirect potable use (IPU).

Following that, Professor Rose went on to chair PUB's External Audit Panel since its inception in 2003, and continues to do so even till today. The panel conducts an independent audit and review of the sampling and analysis of water quality covering PUB's entire water supply system from source to tap, including NEWater, desalinated water, tap water and reservoir water. In addition, Professor Rose actively engages local undergraduates and researchers, providing guidance

and education in local universities through visiting professorship programmes.

An example of the effort and help that Professor Rose has always been willing to give was demonstrated during the Asian Tsunami tragedy. During her time in Singapore she met Dr. Mayuna Srisuphanunt from Faculty of Public Health, Mahidol University in Thailand. Mayuna spent several months in Professor Rose's laboratory learning the methods for protozoan parasites. After the Tsunami hit, 20 days later Professor Rose was there and joined the Thailand public health team from the School of Public Health where they sampled for source tracking markers and pathogens in addition to indicators to help in identifying water sources that were highly polluted due to the disruption of the sanitation systems.

This work continued and resulted in key work presented in Asian conferences. Professor Rose began her work in Africa after moving to Michigan State University in 2004. Working with a team with long term relationships with Malawi she started assisting with water quality issues initially as part of an NSF grant on water and climate.

**Global Efforts**

Special mention must be made of her efforts internationally leading the professional group in Health Related Water Microbiology. She chaired this group from 2003 to 2010. The respect she has gained and the leadership she has displayed has culminated into her directing her latest effort the Global Water Pathogens Project. http://www.waterpathogens.org/. Here 140 authors thus far have agreed to assist her in producing an online resource. She envisioned and developed this program almost single-handedly, creating the collaborations (including with UNESCO and WHO), establishing the network and taking on the fundraising.

To improve sustainable access to basic sanitation and safe drinking water, GWPP will update knowledge on water pathogens using advanced information technologies by publishing and disseminating a state-of-the-art reference resource on water-related disease risks and intervention measures (replacing Sanitation and Disease Health Aspects of Excreta and Wastewater Management by Feachem, Bradley, Garelick and Mara. 1983) and create an online open-access data base and knowledge platform. GWPP will provide an updated review of the efficacy of sanitation technologies and serve as a compendium of waterborne pathogen information and quantitative data to support risk assessment to protect water safety. Work will also be conducted with the World Health Organization to support its Sanitation Guidelines.

Professor Rose continues to open her laboratory and give of her time to train the next generation of scientists and students who have then gone onto their respective institutions to build water pathogen diagnostic capabilities.

# Drug-drug Interaction Extraction based on Transfer Weight Matrix and Memory Network

## by Fuji Ren, Member EUAS

Short Biography

*Prof. Fuji Ren received his B.E. and M.E. degrees from Beijing University of Posts and Telecommunications, Beijing, China, in 1982 and 1985, respectively. He received his Ph.D. degree in 1991 from Hokkaido University, Japan. He is a professor in the Faculty of Engineering of Tokushima University, Japan. His research interests include information science, artificial intelligence, language understanding and communication, affective computing, and Intelligent robot. He is a member of The Engineering Academy of Japan, a fellow of IEICE and CAAI. He is a fellow member of the Japan Federation of Engineering Societies. He is the president of the International Advanced Information Institute. He is the author/co-author/editor of eight books and over 500 research publications.*

### Drug-drug Interaction Extraction based on Transfer Weight Matrix and Memory Network

Fuji Ren

***Digital Object Identifier 10.1109/ACCESS.2017.Doi Number***

Abstract

Extracting drug–drug interaction (DDI) in text is the process of identifying how two target drugs in a given sentence interact. Previous methods, which were limited to conventional machine learning techniques, were susceptible to issues, such as '*vocabulary gap'* and unattainable automation processes in feature extraction. Inspired by deep learning in natural language preprocessing, we addressed the aforementioned problems based on word embedding and a recurrent neural network (RNN). A TM-RNN method is proposed by adding the transfer weight matrix in RNN to improve robustness and introduce a memory network for feature fusion. We evaluated our TM-RNN model on the DDIExtraction 2013 Task. Our model achieved an overall F-score of 72.43, which outperforms the latest methods based on support vector machine and other neural networks. Meanwhile, the experimental

results also indicated that our model is more stable and less affected by negative samples.

Conclusions

In this study, we propose a multilayer bidirectional LSTM with transfer weight matrix and memory network to solve the DDI classification problem. Results highlight the following points: RNN with transfer weight and attention mechanism should be considered as a powerful structure in a DDI task. The transfer weight matrix is an effective means to prevent overfitting, whereas the memory network, which decomposes input information into memory and attentive spaces, ensures that the proposed model can completely access all stored memory. In addition, our model is less sensitive to negative samples compared with other methods, considering that many irrelevant samples exist in drug–drug relation extraction tasks. This advantage helps us discard artificial features completely (or pretreatments). Although our proposed TM-RNN has been able to achieve comparable results, a reliable and precise DDI classification system should be further improved from the following aspects: (1) Although the LSTM can encode any sentence length, an extremely long sentence and two target drug entities that are too far from each other will still introduce noise information. This aspect will hinder the performance of the TM-RNN. To solve this problem, the most straightforward way is to introduce parser tree information, because drug entities may be structurally close to each other although far away in word sequence. (2) A typical error is that the input sample will be misclassified as 'Other', which is equivalent to noise in the datasets. Punishing the 'Other' label or modifying the loss function to release the problem will be the next step in our future work.

## Feature Reuse Residual Networks for Insect Pest Recognition

Fuji Ren, WenJie Liu and GuoQing Wu

***Digital Object Identifier 10.1109/ACCESS.2017.Doi Number***

Abstract

Insect pests are one of the main threats to the commercially important crops. An effective insect pest recognition method can avoid economic losses. In this paper, we proposed a new and simple structure based on the original residual block and named as feature reuse residual block which combines feature from the input signal of a residual block with the residual signal. In each feature reuse residual block, it enhances the capacity of representation by learning half and reuse half feature. By stacking the feature reuse residual block, we obtained the feature reuse residual network (FR-ResNet) and evaluated the performance on IP102 benchmark dataset. The experimental results showed that FR-ResNet can achieve significant

performance improvement in terms of insect pest classification. Moreover, to demonstrate the adaptive of our approach, we applied it to various kinds of residual networks, including ResNet, Pre-ResNet, and WRN, and we tested the performance on a series of benchmark datasets: CIFAR-10, CIFAR-100, and SVHN. The experimental results showed that the performance can be improved obviously than original networks. Based on these experiments on CIFAR-10, CIFAR-100, SVHN, and IP102 benchmark datasets, it demonstrates the effectiveness of our approach.

Conclusions

In our work, we proposed the feature reuse residual network (FR-ResNet) for insect pest recognition. The central idea of the structure was described in this paper involves learning half and reuse half feature in each Feature Reuse Residual block. Based on the simple structure, we constructed the FR-ResNet and evaluate the classification performance on IP102 dataset which is a challenging insect pest recognition benchmark dataset. The experimental results on IP102 showed that FR-ResNet can achieve better accuracy recognition performance compared with the baseline models. We also demonstrated that our approach can be adopted by other residual networks and outperform the original networks on CIFAR-10, CIFAR-100, and SVHN datasets. Through these empirical studies, the effectiveness of our approach was demonstrated, and this approach can be easily implemented in other residual networks.

In future work, we will try to extend the proposed network to different technical fields and explore more effective feature reuse network structure.

# Mechanics of Compliant Materials

## by Alan D. Freed, Member EUAS

Short Biography

*Professor*
*J. Mike Walker '66 Department of Mechanical Engineering*
*Texas A&M University, College Station, TX 77843-3123, USA*
*Joint Faculty Appointment as a Mechanical Engineer*
*Impact Physics Branch, Protection Division, Weapons and Materials Research Directorate*
*Army Research Laboratory, Aberdeen Proving Ground, Aberdeen, MD 21005, USA*

***Education***

*PhD 1985 University of Wisconsin, Madison, WI, USA, Engineering Mechanics*
*minors Computer Science and Material Science*
*advisor Prof. Bela I. Sandor*
*committee Profs. Arthur S. Lodge, Millard W. Johnson, Jr., and Terry Richards*
*MS 1980 University of Wisconsin, Madison, WI, USA, Engineering Mechanics*
*BS 1978 University of Wisconsin, Madison, WI, USA, Engineering Mechanics*

***Employment***

*2018-present Joint Faculty Appointment, U.S. Army Research Laboratory, Aberdeen Proving Ground*
*2014-present Professor of Mechanical Engineering, Texas A&M University, TX, USA*
*2007-2014 Clifford H. Spicer Endowed Chair of Engineering, Saginaw Valley State University, MI, USA*
*2003-2007 Adjunct Staff, Lerner Research Institute, The Cleveland Clinic, Cleveland, OH, USA*
*1996-2007 Senior Research Engineer, NASA John H. Glenn Research Center, Cleveland, OH, USA*
*1989 Sabbatical at Office National d'Etudes et de Recherches Aérospatiales, Châtillon, Cedex, France. Mentored by Dr. Jean-Louis Chaboche*
*1985-1996 Research Engineer, NASA Lewis Research Center, Cleveland, OH, USA*
*1984-1985 Assistant Professor, Department of Mechanical Engineering, University of New Hampshire, USA*
*1978-1984 Graduate Teaching and Research Assistant, University of Wisconsin, Madison, WI, USA*
*1972-1974 Self-Employed Motorcycle Mechanic*

***Honors/Awards***

*2019 Member of the EU Academy of Sciences*
*2016 Brittan Undergraduate Teaching Award, Texas A&M University*
*2006 Cleveland Clinic Innovator Award*
*2004 NASA Exceptional Service Medal*
*2000 Fellow of the American Society of Mechanical Engineers (ASME)*
*1995 Chair of the Materials Division of ASME*
*1990-1995 Member of the Executive Committee of the Materials Division of ASME*
*1982 Sigma Xi*
*1978 Tau Beta Pi*

Dr. Freed is best known for his research in the field of nonlinear solid mechanics, and in the development of some enabling technologies. His research focus resides mostly with the science of engineering, rather than with the applications of engineering. Nevertheless, most of his scientific work was done under the guise of one project or another. Funding for pure mechanics research is nearly impossible to secure in the States. Dr. Freed has a stronger reputation in Europe than he does in the States, due largely to past collaborations that he has formed with researchers from England, France and Germany. He spent 22 of his 40 or so years of research working for NASA as a research engineer, with the remainder being spent working in academia. A chronological listing of what Dr. Freed considers to be some of his more influential papers is appended as a bibliography.

Upon his arrival at NASA, Dr. Freed was teamed with a small group of research engineers tasked to improve the life of the nozzle in the Space Shuttle Main Engine (SSME), at that time the most costly part in the engine. To better prepare him for this work, Dr. Freed went to Europe to work under the tutelage of Dr. Jean-Louis Chaboche at ONERA in Châtillon France. An outcome of that collaboration was the creation of a thermodynamic foundation for a class of viscoplastic models [1]. Out of that framework, Dr. Freed developed a material model to describe the thermo-mechanical response of the SSME rocket nozzle liner during its eight minutes of burn from launch to orbit. To be able to handle such a thermal shock event that takes the nozzle from near absolute zero to near melting in a fraction of a second placed severe constraints on the material model being developed. Two outcomes that came from that research were the creation of an asymptotic link between his viscoplastic model with Odqvist's model for creep under steady state conditions [2], and thereby an ability to incorporate Odqvist's creep parameters directly into his viscoplastic model [3].

During the time when Dr. Freed was working in the area of viscoplasticity, it became apparent to him that the kinetics of evolution for the kinematic variables were not first order; rather, they obey fractional-order kinetics. Consequently, he proposed the first viscoplastic model whose internal state variables evolved at a fractional rate; specifically, a fractional derivative of the Caputo type was proposed to describe the evolution of back stress that, because of dislocation dynamics, lead to a system of nonlinear, fractional-order, differential equations that needed to be solved. At that time, only methods capable of solving linear, fractional-order, differential equations existed. There was no method whereby Dr. Freed could solve his differential equations. It was Prof. Rudolf Gorenflo from the Free University of Berlin that introduced Dr. Freed to Dr. Kai Diethelm, then a recent graduate in mathematics from the Universität Hildesheim, Germany, starting his career at the Technische Universität Braunschweig. Soon thereafter, Prof. Neville Ford from the University of Chester, England joined our collaboration out of which many papers were written. Our numerical method for solving nonlinear, fractional-order, differential equations [4] has had broad impact across the sciences.

It was because of an executive order signed by President Clinton that NASA paired Dr. Freed with The Cleveland Clinic, where he adjuncted during his last seven years with NASA. At this time, Dr. Freed began his research in biomechanics, first creating a fiber model for crimped collagen, which was modeled after the idea of stretching a spring straight [5]. This 1D model was then implemented into tissue models via splayed fiber archetectures [6]. Biologic tissues are inherently viscoelastic, and during his tenure at the Clinic he also collaborated with Prof. Diethelm in developing a fractional operator that incorporates the same kernel found in Caputo's derivative, but with an objective forcing function [7]. (The Caputo derivative of a tensor field, as defined, is not an objective operator.)

It was during a fishing trip to Canada with some friends from the Air Force that lead to Dr. Freed's return to academia in 2007. Professor Ronald Bagley's (retired Air Force, and of fractional calculus renown) Jeep had broken down. Dr. Freed and Prof. Kullgren (retired Department Head from the Air Force Academy, and then Dean of Engineering and Science at Saginaw Valley State University (SVSU)) drove to a nearby town, bought parts, and some tools sufficient for Dr. Freed to fix the broken down vehicle. We made it to fishing camp six hours late, but we made it. Shortly thereafter, Prof. Kullgren recruited Dr. Freed from NASA to come teach at SVSU, stating that this was the kind of professor he wanted for teaching his students. This was Dr. Freed's strangest interview. He held the Clifford H. Spicer endowed chair in engineering during his seven years at SVSU. It was there that he began developing material models using an implicit theory of elasticity [8]. This work was first done in collaboration with Dr. Daniel Einstein, then from Pacific Northwest National Laboratory, who was interested in lung mechanics. Also during this time frame, Dr. Freed wrote a textbook for introducing his students to the continuum modeling of compliant materials [9].

Professor K. Rajagopal was on the editorial board for the series through which Dr. Freed's book was published, and it was from this interaction that lead Texas A&M University to recruit Dr. Freed to join their faculty in 2014. He and Prof. Rajagopal promptly collaborated on what has become a promising model for biologic fibers, derived from an implicit theory and incorporating a viscoelastic kernel of fractional origin [12]. During Dr. Freed's interview trip, Prof. Arun Srinivasa gave him a recent paper of his where a QR decomposition was applied to the deformation gradient instead of the commonly employed polar decomposition. Having recently worked on Hencky (logarithmic) strain [10], it was a natural continuation that they collaborate on establishing the logarithm of this stretch tensor that arises from a triangular decomposition of the deformation gradient [11], a stretch tensor that Drs. Freed and Rajagopal now call the Laplace stretch [14]. Continuing to establish the theoretical and physical foundations for the use of Laplace stretch in mechanics has been Dr. Freed's primary research topic since arriving in Texas. Examples from this developing body of literature include the derivation of a metric tensor that convects with the motion of deformation, derived from an elongation/shear decomposition of the Laplace stretch [13], and an elastic-

plastic decomposition of Laplace stretch that draws heavily upon the fact that Laplace stretch belongs to the group of real upper-triangular matrices with positive diagonal elements under an operation of matrix multiplication. (The commonly used symmetric measures for stretch do not belong to such a group; specifically, there is no closure.)

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# A Sputtered Nanocrystalline Coating For High Temperature Applications On The Nickel-base Single Crystal Superalloy René 5

**by Fuhui Wang, Member EUAS**

Short Biography

*Prof. Fuhui Wang was born in 1960, received his B.S. degree in Materials Science from the Harbin Engineering University in 1983 and M.S. degree in Materials Sciences from Institute of Metal Research, Chinese Academy of Sciences in 1986 and Ph.D. degree in Corrosion and Protection from Institute of Corrosion and Protection of Metals, Chinese Academy of Sciences in 1992. Prof. WANG has been a full professor in the Institute of Corrosion and Protection of Metals since 1994, and was Deputy Director of the institute from 1998 to 1999. In 1999, he was appointed as the director of the State Key Lab for Corrosion and Protection, Institute of Metal Research, CAS, and as the Chairman of High Temperature Committee of Chinese Society for Corrosion and Protection in 2001. Prof. Fuhui WANG worked in Technical University of Munich, Germany for one year and in University of New South Wales, Australia for six months. He was appointed as members of Editorial Advisory Board of Anti-Corrosion Methods and Materials and International Journal of Materials and Product Technology, UK and Editor in-chief of Corrosion Science and Protection Technology, China in 2004. His main research interests are both on fundamental and application research of corrosion at high temperatures including oxidation and hot corrosion resistant nanocrystalline coatings, synergistic effect of solid NaCl and water vapor on corrosion of materials at intermediate high temperatures(300-600$^{o}$C), protective coatings for turbine blades such aluminide, MCrAlY, TiAlN and enamel coatings. Now he opens his new research directions of corrosion and protection of magnesium alloys and organic nano-paints. Prof. WANG received Young Scientists and Engineers Award presented by International Union of Materials in 1993 in Japan, Young Expert Title of Outstanding Achievements, CAS in 1994 and Innovation Award of Science and Technology for Young Scientists, CAS in 2001.In 2014, Prof. Wang was elected to be President of Chinese Society for Corrosion and Protection. In 2016 he moved to the Northeastern University, Shenyang China. So far, he has authored and co-authored more than 400 scientific publications in peer-reviewed journals.*

## A Sputtered Nanocrystalline Coating For High Temperature Applications On The Nickel-base Single Crystal Superalloy René 5

With increasing performance and oxidation resistance of a second generation single-crystal nickel-base superalloy N5, has attracted interests in advanced thrust-weight ratio and potentially using as blade material. To prolong the lifetime of the superalloy, high temperature protective coating is frequently used for protecting the substrate alloy under extremely harsh environment. Usually, the coated samples show great improvement on oxidation and hot corrosion resistance. However, a series of problems were reported in

using the traditional protective coatings, such as serious spallation of the oxide scales and interdiffusion between the coating and substrate, resulting in harmful effects on the oxidation performance and decreasing the mechanical properties under high temperature environment. Recently, sputtering nanocrystalline coating was designed as a new protective coating with better performance on oxidation resistance and perfectly avoided the interdiffusion between coating and substate alloy causing by differences amount of the intrinsic elements.

The oxidation and interdiffusion behavior of NiCrAlY and sputtered nanocrystalline coatings on a single-crystal superalloy were studied. Results indicated that the superalloy substrate already possessed a high oxidation resistance. However the spallation resistance of oxide scale was very low. NiCrAlY coating enhanced the spallation resistance to some extent of the superalloy substrate at the expense of elevating oxidation rate and occurrence of severe interdiffusion. Sputtered nanocrystalline coating enhanced substantially the spallation resistance of the superalloy substrate meanwhile avoided elements interdiffusion. Its oxidation rate was lower than the superalloy substrate at 1000◦C but a little higher at 1100◦C.

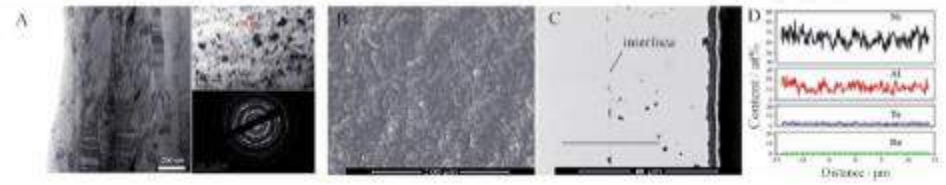


**Fig. 1** The plan-view and cross-sectional TEM bright field images (A) and corresponding electron diffraction pattern of the as-sputtered nanocrystalline coating. Microstructure of the sputtered nanocrystalline coating after oxidation at 1000◦C for 1000 h in air: (B) surface morphology; (C) cross-sectional view; (D) EDS line scan at interface for elements Ni, Al, Ta and Re

Oxidation behavior of a Ta-containing nanocrystalline coating with different contents of Y and Al on the N5 single-crystal superalloy is investigated at 1050 and 1150 °C. Results indicate that the refractory element, Ta, is very active during oxidation. It diffuses easily from the interior of the nanocrystalline coating to the interface of coating/scale in the form of γ′-$Ni_3$(Al, Ta), where it is oxidized and ruins the compactness of oxide scale. Adding moderate amount of Y retards the movement and oxidation of Ta, thus increases oxidation resistance. Such retarding effect is strengthened by increasing Al content, while weakened by increasing temperature.

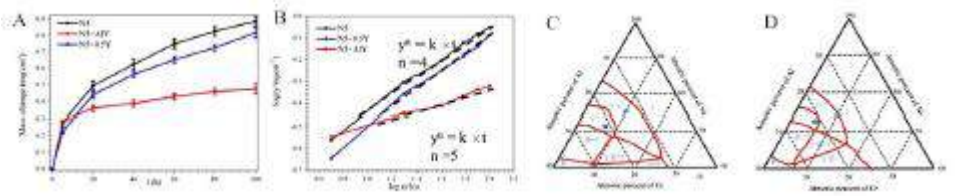


**Fig. 2** Isothermal oxidation kinetics of the three nanocrystalline coatings (N5, N5+0.5Y, N5+AlY) at 1150 °C in air: (A) y vs. t, and (B) log (y) vs. log (t) (the dashed lines fit the linear relationship of these three curves). Ni-Cr-Al phase diagrams at different temperatures and the composition location of the three nanocrystalline coatings: (C) 1050 $^{o}$C, and (D) 1150 $^{o}$C (▲: N5 and N5+0.5Y, ★: N5+AlY)

The above work has been published in ***Corrosion Science*, 98 (2015) 530-540, *Corrosion Science*, 126 (2017) 344-355**.

## Corrosion and Protection for Magnesium Alloy

Magnesium (Mg) and its alloys are promising engineering materials for transportation, aerospace, and electronics industries. However, their relatively low corrosion resistance is the main issue limiting Mg from having a wide range of applications. Therefore, many anti-corrosion coatings have been increasingly developed to improve the corrosion performance of Mg alloys. Among these, phosphate conversion coatings (PCCs) have attracted immense attention from both the academia and industry owning to their highly protective performance of Mg alloys. The corrosion resistance of phosphate conversion coatings depends on the composition of the treatment solution. Based on the state-of-the-art methodologies used in the relevant studies, technical challenges are required to be dealt with for the preparation of high-quality PCC systems to meet the needs for corrosion protection. With the aid of thermodynamic equilibrium calculations, a crucial contributor, i.e. total acidity/pH value (TA/pH), was proposed for the first time to guide the design of the chemical formulation of metal-phosphate-based conversion coatings having excellent corrosion resistance for Mg alloys. A solution with a low TA/pH facilitated the formation of an Mn-PCC with a homogeneous microstructure and improved corrosion performance, whereas a high TA/pH led to a porous layer with a poor corrosion resistance. Our study and published works were compared to validate the proposed theory and correlation between the TA/pH and corrosion resistance of the resulting coatings. A significant contribution of this work was the elucidation of the kinetic role of the buffering nature of chemical bath in regulating the formation of corrosion resistant phosphate conversion coatings.

Cracking and low thickness are major obstacles to the high corrosion performance of conversion coating on magnesium alloy. Based on TA/pH, a new principle regarding the design of conversion bath was proposed in order to overcome this obstacle. The conversion bath should contain two categories of species: G-I species and G-II species. G-I species reacts directly with Mg substrate, forming a cracked inner layer. The pH will be increased due to the reaction of G-I species, promoting the nucleation of supersaturated G-II species. The rapid nucleation of G-II species will form a compact and refined PCC. Due to the high density of nucleation, the PCC will be rich with grain boundaries, which will release the local stress and mitigating the formation of cracks. The ionic product ($J_{sp}$) and the critical ionic product ($J_{C,sp}$) of G-II species are crucial to the designing of conversion bath. The closer $J_{sp}$ to $J_{C,sp}$, the bigger nucleation density and the smaller grain size one can obtain on Mg substrate, and the better quality PCC one can acquire. The nature of tuning TA/pH is to increase $J_{sp}$ to the level of $J_{C,sp}$, thus promoting the cluster size of G-II species to its critical nucleus size. This is very similar to the concept of constitutional supersaturation and critical nucleus size. The adjustment of TA/pH should be accompanied by the addition of complexing agent; the acceleration of reaction rate should be achieved by adding oxidizing agent and catalysts.

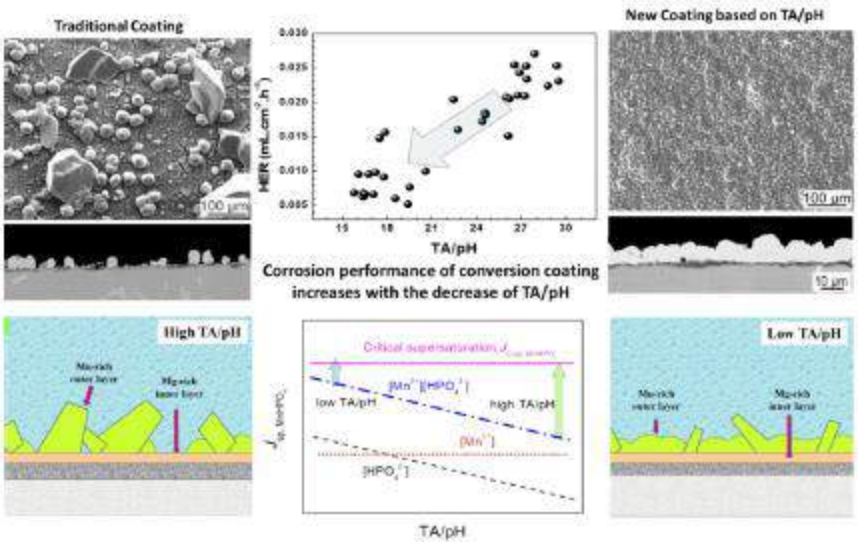


**Fig. 3** The comparison of the surface (left) and cross-sectional morphology (right) of conversion coating based on the indicator of TA/pH (middle). The traditional conversion coating presents a typical non-uniform coating with numerous cracks (left), while the conversion coating based on the indicator of TA/pH exhibits a significant improvement concerning the drawback of non-uniformity and cracking (right).

The above work has been published in ***Surface & Coatings Technology*, 359 (2019) 414-425, *Corrosion Science*, 150 (2019) 279-295, *Journal of Magnesium and alloys*, (2020).**

## Failure Behavior and production of Anticorrosive Coatings in Deep Sea Environment

With the development of oceanic and deep sea in China's marine industry, the study on corrosion protection of materials under shallow sea environment can no longer meet the needs. The failure of anticorrosive coatings under the deep-sea environment has already been caused people's attention and needs urgent solution. At present, the biggest obstacle to research and development of high-performance anticorrosive coating in this environment is that the failure mechanism is not clear, and then there is no targeted R & D.

The work reveals: the alternating pressure in the deep-sea environment is the most important for organic coatings. Alternating pressure causes failure of the coating by breaking the interface between the coating/metal and the pigment/base resin. The FEM simulation method was used to simulate the bubble formation and fracture process at the coating/metal interface, and to establish a theoretical model for the non-Fick transport of water molecules in the coating under deep-sea conditions. The deep-sea organic anti-corrosion coating was constructed to include the filler size, shape, and content, and the organic resin. The theoretical design model for factors such as cross-link density and resin type. On this basis, an overall theoretical life prediction model is established, which achieves accurate life prediction of the active coating.

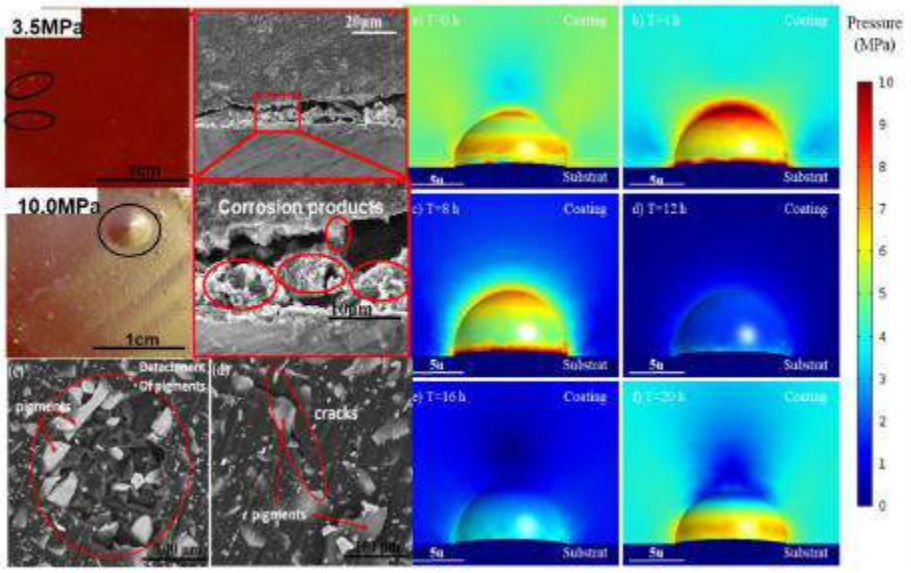


**Fig. 4** Macro morphology pictures of a commercial anticorrosive coating serving 240 hr under 3.5MPa and 10MPa, and micro cross section (a), (b) and mirco surface (c), (d) morphologies of this coating after serving 240 hr under 3.5MPa. The results show that the larger the hydrostatic pressure is, the more serious the failure of coating is. Both interfaces between coating and based metals, and filers and resin have been destroyed seriously by hydrostatic pressure. FEM modified the interface between coating and based metals and reveal that alternating pressure destroy this interface.

The above work has been published in ***Corrosion Science*, 74 (2013) 59–70, *Corrosion Science*, 86 (2014) 81-92, *Progress in Organic Coatings*, 82 (2015) 101-112, *Corrosion Science*, 101 (2015) 139–154, Progress in Organic Coatings, 123 (2018) 168-175, Progress in Organic Coatings, 131 (2019) 346–356, Surface & Coatings Technology, 361 (2019) 188–195, Coatings, 9 (2019) 852-865, Journal of Materials Science & Technology, (2020).**

# Viruses in the Brain...? Any Connections to Parkinson's and other Neurodegenerative Diseases?

**by Alain L. Fymat, Member EUAS**

Short Biography

*DR. ALAIN L. FYMAT is a medical-physical scientist and an educator. He is the current President/ CEO and Institute Professor at the International Institute of Medicine & Science with a previous appointment as Executive Vice President/Chief Operating Officer and Professor at the Weil Institute of Critical Care Medicine, California, U.S.A. He was formerly Professor of Radiology, Radiological Sciences, Radiation Oncology, Critical Care Medicine, and Physics at several U.S. and European Universities. Earlier, he was Deputy Director (Western Region) of the U.S. Department of Veterans Affairs (Office of Research Oversight). At the Loma Linda Veterans Affairs Medical Center, he was Scientific Director of Radiology, Director of the Magnetic Resonance Imaging Center and, for a time, Acting Chair of Radiology. Previously, he was Director of the Division of Biomedical and Biobehavioral Research at the University of California at Los Angeles/Drew University of Medicine and Science. He was also Scientific Advisor to the U.S. National Academy of Sciences, National Research Council, for its postdoctoral programs tenable at the California Institute of Technology. He is Health Advisor to the American Heart & Stroke Association, Coachella Valley Division, California. He is a frequent Keynote Speaker and Organizing Committee member at several international scientific/medical conferences. He has lectured extensively in the U.S.A, Canada, Europe, Asia and Africa. He has published ~ 475 scholarly scientific publications and books. He is also Editor-in-Chief, Honorable Editor or Editor of numerous medical/scientific Journals to which he regularly contributes. Dr. Fymat is a Board member of several institutions, a member of the New York Academy of Sciences and the European Union Academy of Sciences, and a reviewer for the prestigious UNESCO Newton Prize, United Kingdom National Commission for UNESCO.*

***RESEARCH INTERESTS***

*DR. FYMAT's current research interests are focused on neurodegenerative diseases (Alzheimer's, Parkinson's, epilepsy, dementias and others), oncology (glioblastoma), molecular/ precision/ personalized medicine, and nanomedicine & nanobiotechnology. These are represented in part in his latest books "**From the Heart to the Brain**: My Collected Works in Medical Science Research (2016-2018)" pp 592 and "**Alzhei ...Who?** Demystifying the disease and what you can do about it" pp 235, Tellwell Talent Publishers, 2019.*

## Viruses... in the brain? Any connections to Parkinson's and other neurodegenerative diseases?

The connection between influenza infection and psychosis had been reported in Europe as early as 1835. It became more apparent during the Spanish flu epidemic of 1918. As we recall, that epidemic, caused by the H1N1 virus (a subtype of the H1N5 virus), correlated with an epidemic of Parkinson's disease a few decades later. In the U.S., between the 1940s and early 1950s, the diagnosis of Parkinson's disease increased abruptly from 1-2% to 2.5-3% (that is, about 50% more people were diagnosed with the disease) before falling back to its previous rate of 1-2%. However, because of the unexplained geographically-distant and delayed-onset of Parkinson's disease by several decades, that connection was cast aside.

Bacteria, viruses, fungi, and other microbes are part of a growing list of pathogens found in the brains of patients with neurodegenerative diseases. Generally, brain infections by pathogens can lead to transient or permanent neurologic or psychiatric dysfunctions. Microbes in the brain may indicate meningitis or encephalitis, two diseases that are active infections with inflammation. For neurodegenerative diseases like Parkinson's, Alzheimer's and others that were not thought to be infectious, finding pathogens in the brain is both surprising and concerning.

Evidence has since continued to accumulate linking the brain to various pathogens. But, how do these organisms get into the brain since it is protected by the blood-brain barrier? They do so when the barrier looses some of its impermeability. Other avenues for reaching directly the brain are the intra-nasal and sinus access, the mouth through the lingual nerve, the gut through the vagus nerve, and even the eye through the olfactory bulbs, all of which connect to the brain by replicating and spreading. Thus, in 1974, Gamboa *et al.* found viral antigens in the brains of deceased people affected by *encephalitis lethargica*. It was associated with (and some thought caused by) the 1918 Spanish flu epidemic. It was even speculated that the condition could be a precursor to Parkinson's. Other scientists had also noted the connection between influenza and neural dysfunction. In 1997, Ogata *et al.* reported that rats exposed to the Japanese encephalitis virus developed symptoms similar to human Parkinson's.

At that time, this connection between viral infection and brain disease had been hotly contested because of other conflicitng experiments. In 2001, utilizing the technology known as polymerase chain reaction to look for the genome of the H1N1 virus in the preserved brain tissue of victims of *encephalitis lethargica*, researchers at the U.S. Armed Forces Institute of Pathology found no sign of the virus. In 2003, Heiko Braak proposed the widely accepted hypothesis that Parkinson's starts in the gut and moves into the brain, a process that may take place over 25-30 years over the life of the infected individual. However, in 2006, researchers at the U.S. Centers for Disease Control & Prevention, studying the effects of the influenza strain that caused the 1918 Spanish flu epidemic, did not see any signs of inflammation in the brains of infected mice. The above conflicting results suggested that more work was needed to link viral infection and neurodegenerative diseases.

Then, seminal experiments were conducted by Richard Smeyne. In 2008, observing ducks infected by the H5N1 virus, he wondered whether a connection existed between the viral infection and the extensive neurodegeneration he observed (devastation of the *substantia nigra*, which is often damaged in Parkinson patients, and obliteration of all the neurons). It seemed that the virus was inducing inflammation and death into the parts of the brain that degenerate in Parkinson's. He further remarked that in rodents, which have a much shorter lifetime than humans, the same travel from the gut to the brain, as hypothesizd by Braak, may take only a few weeks as opposed to decades in humans. Even if they cannot reach the brain, the viruses can still play a role in neurodegeneration by

triggering severe inflammation. In 2009, in other mice experiments, Smeyne also observed that H5N1 not only is not blocked by the blood-brain barrier from entering the brain but it can easily infiltrate nerve cells in the brain and kill them, especially targeting the dopamine-producing neurons in the *substantia nigra*. While H1N1 could not penetrate the barrier, it still caused central nervous system immune cells (the microglia) to flow into the *substantia nigra* and the hippocampus, causing inflammation and cell death in the area. Interestingly, we have here two different flus, two different mechanisms, but the same effect - inflammation and death in that part of the brain that degenerates into Parkinson's.

Other experiments than Smeyne's suggested that viral infections can contribute to neurodegenerative diseases. The connection is not limited to influenza but extended to several different viruses, including measles and herpes that can give rise to symptoms of multiple sclerosis in rodents. In addition, levels of herpes virus were found to be higher in the brains of people who died from Alzheimer's than in those without the disease. Also, some HIV patients developed dementia that appears to be associated with the infection. Lately, in 2017, after administering the toxin MPTP (a byproduct of a bad batch of synthetic heroin that led users to develop Parkinson's), Smeyne *et al.* additionally observed that the treated mice developed signs of Parkinson's, losing 25% more neurons in the *substantia nigra* than uninfected mice treated with the toxin. He, then, concluded that whereas the H1N1 viral infection alone may not cause Parkinson's, it primed the nervous system to be sensitive to other things that would. All of the above experiments are prompting a reconsideration of the pathogen connection to the brain.

Now, infections of the brain often also involve other parts of the central nervous system including the spinal cord. They can cause inflammation of the brain (encephalitis) and of the layers of tissue (meninges) that cover the brain and the spinal cord (meningitis). Often, bacterial meningitis spreads to the brain itself, causing encephalitis. Similarly, viral infections that cause encephalitis often also cause meningitis. Usually in encephalitis and meningitis, infection is not confined to one area but may occur throughout the brain, within the meninges, along the entire length of the spinal cord and over the entire brain. Infection may also be confined to one area (empyema in an existing space in the body; abscess). Bacteria and other infectious organisms can reach the brain and meninges in several ways by being carried by the blood, entering the brain directly from the outside (for example, through a skull fracture or during surgery on the brain), or spreading from nearby infected structures (for example, sinuses or middle ear). Sometimes a brain infection, a vaccine, cancer, or another disorder may trigger an autoimmune reaction as a result of which the brain becomes inflamed. Encephalitis is most commonly due to viruses (herpes simplex, herpes zoster, cytomegalovirus, West Nile virus, HIV and prion disease).

However, the flu-Parkinson connection is not the only link between viruses and neurological problems. The broader link between viruses and neurodegeneration can be seen from the following developments that took place in the late 1980s-early 1990s. Mice infected with viruses such as measles and herpes suffered the same kind of damage to their oligodendrocytes as patients with multiple sclerosis do. It is unclear whether the viruses invaded the oligodendrocytes directly or simply provoked the mice's immune systems to attack the cells (an autoimmune reaction), but the end result was demyelination of neurons. One of the viruses that induced multiple sclerosis symptoms in mice was herpes virus 6 which has also been tentatively associated with the onset and development of Alzheimer's. Indeed, over the past few decades, tentative links have been documented between viral infections and Alzheimer's disease. From a review of data from brain banks and published studies, Joel Dudley *et al.* found that Alzheimer patients had elevated levels of viruses such as human herpes viruses 6 and 7 in four key brain regions. Based on genetic and proteomic

data, they also found that human herpes virus 6 may induce gene expression that spurs the development of the protein amyloid β which forms plaques – one of the hallmarks of Alzheimer's. While viruses may not cause the disease, their presence suggests that pathogens may play a part in neurodegenerative diseases after all.

Compared to previous musings on the pathogen hypothesis, we now have more powerful genetic and other sequencing methods that can take a more unbiased look at the microbial DNA/RNA landscape of brain tissue. Further, in the case of HIV, beginning in the 1990s, it was shown that it could traverse the blood-brain barrier, infiltrate the brain, and spur neuronal death and a loss of synaptic connections. In late 2010, it was further shown that patients with HIV developed dementia and loss of brain matter that mirrors what is seen in Alzheimer's. More recently, other studies showed that HIV patients develop plaques of amyloid β (like in Alzheimer's) and can also develop slowness in movement and tremors (like in Parkinson's). Lastly, in 2019, Korte *et al.* reported that the brains of mice infected with certain strains of the flu virus suffered memory deficits even after they seemingly recovered. It turned out their brains were full of microglia even 30-60 days after the infection first took hold and can remain high for up to 120 days (equivalent to more than 10 years in human time).

More recently, Smeyne *et al.* conducted another experiment on mice in which (a) one group of mice received an H1N1 vaccine 30 days before infecting the animal with the virus and (b) another group of mice were treated with Tamiflu for the week after they were infected. Both groups were allowed to recover before being given a low dose of a toxic material (MPTP), and (c) a control group received neither the vaccine nor the flu treatment. They determined that while (c) developed Parkinson-like symptoms, (a) and (b) developed no neurodegenerative effects. In other words, mice were protected against Parkinson-like symptoms by either prophylactic treatment (with a vaccine) or by early treatment (with Tamiflu). Extrapolating these results from mice to humans, if valid, the logical conclusion would be that if a person gets a pathogen infection, vaccination or at least treatment with Tamiflu may treat the influenza but also help prevent the complications of influenza infection such as neurodegeneration.

The long time lag between viral infection and the development of neurodegenerative diseases is exactly the reason why scientists have had (and continue to have) trouble accepting that viruses could cause the diseases. The link is difficult to demonstrate except perhaps in rodent studies. We need to better understand how the brain responds to viral infection long after our immune system has cleared the infection from our bodies. This will help us develop ways to mitigate the neurological effects. Further, understanding how infections trigger the immune system could lead to ways to down-regulate glia-driven inflammation in hope of preventing long-term damage.

In summary, the pathogenic hypothesis remains a hypothesis whose rigorous testing is long overdue. Notwithstanding the several instances of the link between viruses and neurodegenerative diseases, even if a definitive link were established, it may only be correlative not causal. While the cause(s) of the major neurodegenerative disorders (Alzheimer's, Parkinson's, epilepsy, and others) remain unknown, I have posited earlier that they are the consequence of a runaway brain autoimmune system that is unable to maintain homeostasis between opposing synaptoblastic and synaptoclastic pressures. At this juncture, this runaway autoimmune disease explanation remains the only plausible one and the root cause of neurodegenerative diseases, everything else amounting to consequences of risks and correlations.

# Supercritical Hydrothermal Reactions for Material Synthesis

## by Tadafumi Adschiri, Member EUAS

Short Biography

*Prof. Adschiri graduated from The University of Tokyo in 1981, and received his Doctorate in Engineering from the same institution in 1986. He worked as a Special Research Fellow of JSPS (Japan Society for the Promotion of Science), following which he was appointed as an Assistant Professor in The University of Tokyo in 1987. As a visiting scholar, he has had the opportunity to carry out research work at the University of Waterloo (1991, Canada), University of Hawaii (1996, US), and University of Delaware (1997, US). Prior to joining Tohoku University, the primary focus of his research was on coal conversion technology. In 1989, he moved to Tohoku University and began studying reactions in supercritical fluids for biomass conversion, chemical recycling of wastes, new organic reactions, and materials synthesis. He has published nearly 300 papers, with over 10,000 citations, and has an h-index of over 50. He has been invited more than forty times to major international conferences in a variety of research fields as a plenary/keynote/invited lecture. For his research excellence, he has been awarded many prizes, including awards from the Chemical Society Japan (Science Award), Society of Chemical Engineering of Japan (Best Research Award, and SCEJ Society Award), Japan Energy Society (Progress Award), etc. In addition to the academic societies, he is the recipient of the honorable Japan Invention Award from the Japanese government and three-time winner of the Minister's awards of MEXT (Ministry of Education, Culture, Sports, Science and Technology) as well. Ten years ago, the Japanese government selected five (now nine) distinguished research teams as part of the World Premier Research Center Initiative (WPI), and he had the honor to be selected as a principal researcher for the Advanced Institute of Materials Research (WPI-AIMR) in Tohoku University. Currently, Prof. Adschiri serves as the President of ISHA (International Solvothermal Hydrothermal Association) from 2018, Vice President of IASCF (International Society for Advancement of Supercritical Fluids) from 2014, Chairman of the Asian Society of Supercritical Fluids, and President of the Society of Chemical Engineering of Japan (2018). In 2014 he was assigned as a member of Science Council of Japan (six-year appointment followed by a conjuncted membership for an additional twelve years). In 2016, he became a member of the Engineering Academy of Japan (life time). This year Doctor Honoris Causa was given from University of Bordeaux, and Distinguished Professorship from Tohoku University. What is even more noteworthy is the Medal with Purple Ribbon from the Emperor of Japan.*

### Supercritical Hydrothermal Reactions

Industrial materials manufacturing is classified into gas-, liquid-, or solid-phase reaction processes. In addition to the gas, liquid, and solid phases, there is another "phase" called "supercritical", which exhibits both gas and liquid characteristics. Dr. Tadafumi Adschiri

conceived the idea of "supercritical water" as a reaction solvent for the synthesis of new materials that cannot be done in conventional processes. The phase-change behavior near the critical point and the anticipated significant solvent effects on the kinetics and the reaction equilibrium due to the change in physical properties would make this possible. (Fig. 1)

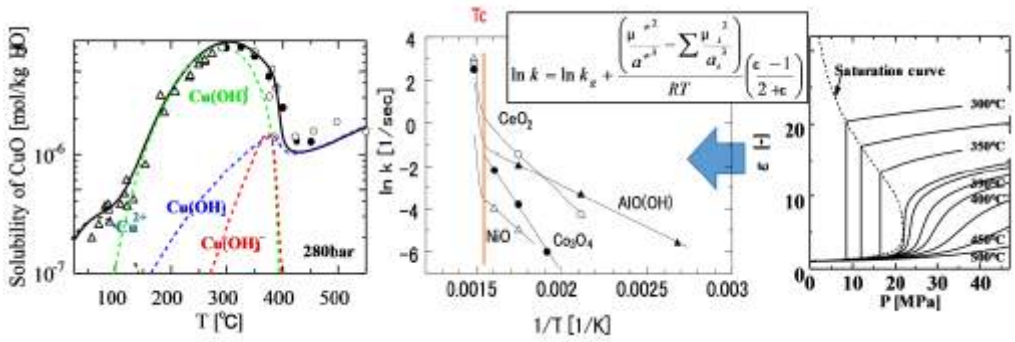


**Fig.1** Because of the drastic change of dielectric constant (right figure) around the critical point, both solubility of metal oxides (left) and the reaction rate (middle) drastically varied.

Dr. Adschiri, therefore, explored a wide range of reactions in supercritical water. Since the early 1990s, in addition to the basic study of the mechanisms of the unusual behaviors of supercritical hydrothermal reactions (kinetic and equilibrium), he has performed research on the use of supercritical water in diverse applications, including heavy oil reforming, waste polymer decomposition and chemical raw materials recovery, cellulose hydrolysis and sugar recovery, lignin decomposition and chemical raw materials recovery, relevant organic reactions, and nanoparticle synthesis, all without using any catalysts. The aforementioned research and developments have been done based on the understanding of the unique feature of supercritical water to dissolve organic molecules, and the ability of water molecules to function as an acid or base catalyst in promoting hydrolysis. That fundamental research led to the commercial process for the first supercritical chemical recycling process in Japan, in which the distillation bottom residue of the toluene diisocyanate (TDI) production process (raw material for polyurethane) was hydrolyzed in supercritical water without any catalyst to recover toluene diamine, which can be re-used in the TDI production process.

## The Invention of Supercritical Hydrothermal Synthesis and Nanoparticle Synthesis

Dr. Adschiri invented "supercritical hydrothermal synthesis" for the continuous preparation of metal oxide nanoparticles, which has already found worldwide industrial applications. In supercritical water, especially near the critical point, both the dielectric constant and density change significantly. Under constant pressure, the dielectric constant greatly decreases from near the critical point with increasing temperature. This change in the dielectric constant greatly affects the reaction. For example, in hydrothermal synthesis, which is the formation of a metal oxide by hydrolysis of the corresponding metal salt, a decrease in the dielectric constant greatly increases the rate of hydrolysis while substantially decreasing the solubility of the metal oxide product.

He proposed the two-fluid mixing type flow system, where an aqueous metal salt solution was mixed with supercritical water to heat the solution to the supercritical state

with a very short mixing time constant, that could never be achieved by conventional reactor systems. This is the "supercritical hydrothermal synthesis" method, which became widely known worldwide. A great number of researchers around the world are currently performing research in this field. (Fig. 2)

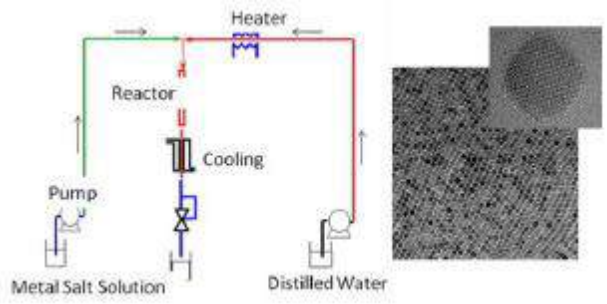


**Fig.2** Continuous flow reaction system that achieves rapid heating of metal salt solution to the supercritical state and thus nano particle synthesis.

Outside of academia, nanoparticle synthesis by this method has been applied in the industry. In South Korea, cathode materials for Li-ion batteries are produced at 1,000 t/year. In the UK, large-scale processes that produce various high-performance nanomaterials are now in operation while pilot plants for similar applications are being constructed in France.

**Organic-Modified Hybrid Nanoparticles and their Applications**

Dr. Adschiri found that the homogeneous phase of water and organic matter in supercritical water could be used to synthesize hybrid nanoparticles consisting of inorganic nanoparticles chemically bonded with organic molecules.

In the application of nanomaterials, one of the big challenges is the difficulty in the dispersion of nanomaterials in polymers and solvents. It could be possible to improve the affinity between nanoparticles and their carrier media (either polymer or solvent) by binding organic molecules to the surfaces of nanoparticles. A solution to this problem would be to form chemical bonds between a nanoparticle and an organic molecule. However, while nanoparticles are hydrophilic and disperse well in water, organic molecules targeted for binding with nanoparticles can only dissolve in organic solvents. Such organic modification is therefore not possible at high concentrations of organic molecules.

Equipped with an understanding of both inorganic nanoparticle synthesis and of organic reactions in supercritical water, both explained above, Dr. Adschiri conceived and investigated the idea that these reactions could occur simultaneously under supercritical conditions. As a result, he succeeded in demonstrating that organic-inorganic hybrid nanoparticles could be synthesized in a supercritical state. Because organic molecules at high concentrations can form a homogeneous phase with water only under the supercritical condition, this material represents a new class of nanomaterials that can only be prepared in the supercritical phase.

**Fig. 3** Organic reagents and aqueous solution for a homogeneous at a high temperature and organic-inorganic reaction takes place.

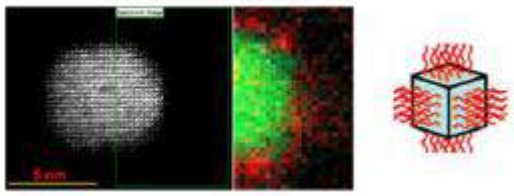

**Fig.4** Red color indicated the organic molecules that are attached on the surface of $CeO_2$ nanoparticles.

Using this method of modification with organic compounds has led to the fabrication of nanoparticles with high affinity for organic solvents and polymers, and has thus allowed high concentration dispersions of these nanoparticles into those media (solvent or polymer) to be achieved. This achievement led to the successful synthesis of nano inks (highly concentrated nanofluids) for 3D inkjet printing and printed electronics. New hybrid polymers with nanoparticles demanded by the industry have also been developed, including transparent high-refractive-index flexible film materials, and materials with high thermal conductivity, high insulation, high adhesion, and modality. Additionally, it is now possible to synthesize nanoparticle crystals via self-assembly of these modified nanoparticles.

**New Catalyst**

Dr. Adschiri has also expanded his research to the field of catalysis. Recent research in catalysis revealed that high catalytic activity can be achieved by controlling exposure of the active face of the catalyst. However, since the most active face is also typically the least stable face, the synthesis of crystals with the active face exposed is considered impossible in principle. This is the case especially for nanoparticles with high surface energy. However, in the case of organic-modified nanoparticle synthesis, an unstable face exhibits higher reactivity with the organic molecules, and thereby the most reactive face will be selectively modified and protected during nanoparticle synthesis. Using this organic-modified nanoparticle synthetic method, nanoparticles bearing an exposed reactive face were successfully synthesized. In the evaluation of the catalytic activity, extremely high oxygen mobility and oxidative catalytic activity were obtained, even at low temperatures. Metal oxides are ceramics, and in general, high oxygen mobility in such materials is only observed at high temperatures of 400 ˚C or higher. In contrast, for the nanoparticles with the most active face exposed, high oxygen mobility was observed even at 150 ˚C, suggesting its high catalytic activity for oxidation. Indeed, it is demonstrated that steam reforming of heavy waste in water can occur even at low temperatures. It is anticipated that this technology could also be applied to hydrogen synthesis using low-temperature waste heat, a process that until now has been considered impossible.

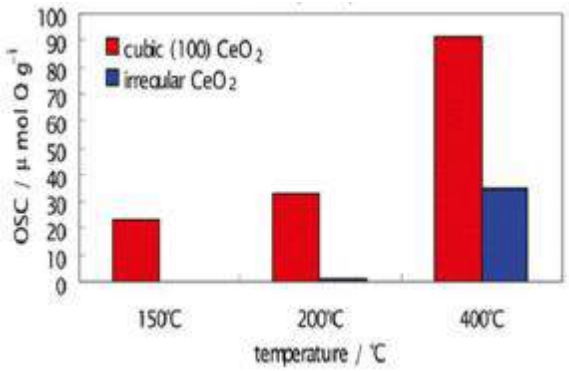


**Fig.5** Oxygen strage capacity of $CeO_2$ (oxygen mobility) was found even at very low temperature.

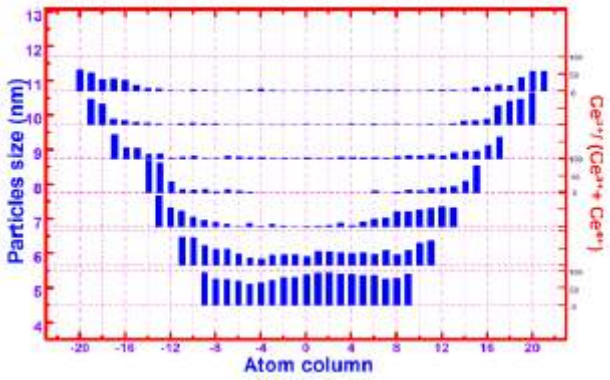


**Fig.6** Size-dependent valence state distribution inside $CeO_2$ NCs,which suggests the high oxygen mobility deep inside the particles for 5nm nanoparticles.

# Vehicle Scanning Method for Bridges

## by Yeong-Bin Yang, Member EUAS

Short Biography

*Honorary Dean, School of Civil Engineering, Chongqing University, Chongqing 400045, China*

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*Dr. Yeong-Bin Yang received his Ph.D. degree from Cornell University in 1984. He is a member of Chinese Academy of Engineering, foreign member of Austrian Academy of Sciences, and member of EU Academy of Sciences. Currently, he is Honorary Dean of Civil Engineering, Chongqing University, Feng Tay Chair Professor of National Yunlin University of Science and Technology (YunTech), and Professor Emeritus of National Taiwan University (NTU). Also, he is Editor-in-Chief of International Journal of Structural Stability and Dynamics, former President of Asian-Pacific Association of Computational Mechanics, and former Chairman of International Steering Committee of East Asia-Pacific Conference on Structural Engineering and Construction.*

*Previously, he was YunTech's President, Dean of College of Engineering, NTU, Chairman of Civil Engineering Department, NTU, and President of four societies in Taiwan: Institute of Engineering Education Taiwan, Chinese Institute of Civil and Hydraulic Engineering, Society of Theoretical and Applied Mechanics, and Chinese Society of Structural Engineering. He has published over 245 referred journal papers, focused on the following areas: structural nonlinear theory and analysis, vehicle-bridge interaction dynamics, train-induced wave propagation, and vehicle scanning method for bridges. In each area he has published a monograph.*

Bridges constitute an essential part of transportation systems such as highways, railways, city rail systems, and highspeed railways. Regardless of their irreplaceable role in ensuring the free and safe passage of passengers and cargoes, bridges often suffer from varying degrees of damages due to degradation in stiffness of structural members, connections, supports, or material strength, caused by vehicles' overloading, weathering, or natural disasters, such as earthquakes, typhoons, deluges, etc. The amount of bridges that have been built in the past three decades has increased tremendously. For example, in China there is a total of some 800,000 highway bridges built in this period. Many of them have been ranked the top tens in the world in terms of span length, bridge type, and column height. Perhaps, the most fantastic is the newly built record-breaking Hong Kong-Zhuhai-Macao Bridge system that connects Hong Kong, Zhuhai and Macao, totaling a length of 55 km including seabed tunnels of some 35 km. From the global picture, there is clearly an urgent need to develop efficient and mobile techniques for the damage detection of bridges so as to enhance the quality of maintenance and possibly rehabilitation.

To monitor the operational and/or damage conditions of bridges, vibration-based methods have been adopted for half a century or longer. Most of the methods require the

installation of quite a number of sensors on the bridge for detecting the modal properties, such as frequencies, mode shapes, and damping coefficients. They were referred to as the direct approach in that the modal properties were retrieved from the vibration data taken directly from the bridge. An enormous volume of research has been carried out along these lines using the ambient vibration, traffic vibration, forced vibration, impact vibration, etc. One drawback with the direct approach is that it usually requires numerous sensors to be installed on the bridge along with data acquisition systems, for which the deployment and maintenance cost is generally high. Another drawback is that the vast amount of data generated, the so-called sea-like data, may not be effectively digested. It should be added that the monitoring system tailored for one bridge can hardly be transferred to another bridge and to work there, a problem known as the lack of mobility.

The vehicle scanning method (VSM) for bridge measurement was proposed by the senior author and coworkers in 2004 mainly to circumvent the drawbacks of the direct approach. This method was known in the early days of development as the indirect approach, to distinguish it from the direct approach conventionally used. However, the term "indirect approach" is not self-explanatory, since it can only be explained along with the direct approach. Recently, we started to use the term "vehicle scanning method for bridges" instead, for its better conveyance of the meaning implied. With this technique, the vibration data collected by one or few sensors installed on the moving test vehicle are used to retrieve the modal properties of the sustaining bridge. No sensors are needed on the bridge. Compared with the direct approach, the vehicle scanning method shows great potential in economy, mobility and efficiency, although further research in software and hardware is required to enhance its robustness in field applications.

To our knowledge, this book is the first one on the subject of VSM for bridges. After some 15 years of research on the VSM, we believe it is timely, and indeed necessary, to present an in-depth coverage of the technique, at least based on the works by the senior author and coworkers. The contents of the book have been arranged such that they are reflective of the progressive advancement of the technique, which is also good for pedagogical reasons. By and large, each chapter can be comprehended by readers with little reference to the previous chapters, since a minimum amount of background information is provided in the introductory section. The following is a summary of the key contents of each of the eleven chapters.

In Chapter 1, a state-of-the-art review is given of the works known to the authors up to roughly 2018 on the subject of the VSM. Among these, a substantial part is the series of papers published by the senior author and coworkers. It can be seen that research has been extended from the original goal of bridge frequency extraction to a variety of applications, including damage detection, modal identification and damping estimation of the bridges. Aside from the theoretical explorations, small-scale lab experiments and field tests have also been attempted.

In Chapter 2, the vehicle-bridge interaction (VBI) model used for extracting the bridge frequencies is introduced. For the first time, the feasibility of extracting bridge frequencies from the passing vehicle's response is theoretically investigated. For simplicity, only the first mode of vibration of the bridge is considered. From the closed-form solution derived for the passing vehicle, the key parameters involved in the VMS technique are unveiled.

Chapter 3 differs from Chapter 2 in that all the modes of vibration of the bridge are included in the formulation. The general theory presented in this chapter confirms the validity of the simplified theory presented in Chapter 2. Besides, the parameters involved in the VBI are evaluated with potential applications identified.

The first field test of the technique is presented in Chapter 4 for scanning the frequencies of vibration of a bridge in northern Taiwan. The device used is a single-axle test cart towed by a light tractor. This test confirms that the bridge frequencies can be successfully retrieved from the response recorded of the test cart during its passage over the bridge by the fast Fourier transformation (FFT).

Chapter 5 is aimed at enhancing the visibility of bridge frequencies from the vehicle's response. Firstly, the vehicle response is processed by the empirical mode decomposition (EMD) to yield the intrinsic mode functions (IMFs). Then the IMFs are processed by the FFT to yield bridge frequencies not restricted to the first mode.

Chapter 6 deals with road roughness of the bridge, a polluting factor that may render bridge frequencies unidentifiable from the vehicle's response. Both numerical and closed-form solutions are used to physically interpret the effect of road roughness on the retrieval of bridge frequencies. Then a dual vehicle model is proposed for reducing such an effect by deducting the response of one vehicle from the other.

In Chapter 7, three filtering techniques are assessed for removing the (undesired) vehicle frequency from the vehicle's spectrum, so as to enhance the visibility of the (desired) bridge frequencies. The singular spectrum analysis with band-pass filter is demonstrated to be most effective among the three schemes.

Chapter 8 is aimed at tuning the various parameters of the test vehicle for field use. As such, a hand-drawn single-axle cart is extensively tested in the lab and in the field. The qualitative guidelines drawn from this part of study using the handy test cart serve as a useful reference for the design of practical test vehicles.

Chapter 9 presents a theoretical framework for retrieving the mode shapes of a bridge from the passing vehicle's dynamic response. By the Hilbert transform, the mode shape is recognized as the envelope of the instantaneous amplitude of the component response of the moving test vehicle. Factors that may affect such a procedure are studied.

In Chapter 10, the contact point of the vehicle with the bridge, rather than the vehicle body itself, is proposed as a better parameter for use in the VSM technique. The contact-point response, back calculated from the vehicle response, is free of the vehicle frequency that may overshadow the bridge frequencies. The relatively better performance of the contact-point response is demonstrated in the numerical simulations.

As a sequel to Chapter 10, the capability of the contact-point response for damage detection of the bridge is presented in Chapter 11. By the Hilbert transform, the instantaneous amplitude squared (IAS) calculated of the driving component of the contact-point response is demonstrated to be effective for detecting bridge damages for scenarios including the presence of ongoing traffic.

In the Appendix, the derivation of the VBI element is given in details based on Chang et al. (2010), a modification from Yang and Yau (1997). Also given is the procedure for assembling the VBI elements (acted upon by vehicles) and non-VBI elements (free of vehicles) for a bridge. The main reason for placing this material in the appendix rather in the main text is not to bring unnecessary intrusion to the main flow of presentation.

We are indebted to a number of friends in preparation of this book. Our work would not be complete without an acknowledgement of this debt and a particular offering of thanks by the senior author to the following:

To the late Professor William McGuire, Cornell University, for introducing him to the interesting field of structural stability and dynamics and for inspiring him to conduct researches that have eventually led to the outcome of this book.

To Professor J. D. Yau, Tamkang University, for the collaboration of research on vehicle-bridge interaction problems that lays partially the foundation of this book.

To Dr. C. W. Lin, CECI Engineering Consultants, Inc., Taiwan for his first and successful attempt on the vehicle scanning method for bridges, which has pathed the way for future research along these lines.

To Dr. C. S. Chan, National Yunlin University of Science and Technology, Taiwan for his skills in designing the hand-drawn cart, which forms an essential part of the experimental study presented in Chapter 8.

To the following former students whose graduate study has contributed to the development of material in the book: Dr. K. C. Chang (now in Kyoto University), Mr. Y. C. Li, Dr. W. F. Chen, and Mr. H. W. Yu from National Taiwan University, and Mr. Y. Qian from Chongqing University.

As for the Wiley side, we would like to express our appreciation to Ms. Anne Hunt for her handling of the book proposal in the initial stage, to Ms. Jemima Kingsly for serving a while as the contact point of Wiley, and to Mr. Steven Fassioms, project editor, and Mr. Hari Sridharan, production editor, for their timely and efficient editorial assistance in making the book come true.

# University Education in Crisis Transdisciplinary Approaches in the Arts, Humanities and Sciences

## by Marcel Van de Voorde, Member EUAS

Short Biography

***Studies at the Catholic University Leuven (B), University of Technology Delft (NL), Nancy University/School of Mines (F):***

*Industrial Engineer, Engineer in Chemistry, Physicist, Degree in Nuclear Engineering*
*PhD in Natural & Technical Sciences*

***Academic Career: now "Emeritus professor " (1975 - …)***

** Professor University of Technology DELFT (NL)*
** Visiting & Honorary Professor: State University Ghent (BE), La Sapienza University(I), Cracow (PL), Columbia University (NY), Tsinghua University Beijing (China), Tokyo University (Japan)*

***Scientific - Professional Career "Emeritus status "(1970 - …..)***

*Direction/Senior Research management functions:*

** CERN (European Organisation for Nuclear Research), Geneva (CH), I*
** European Commission Research (B)*
** Distinguished Visiting Professor Max Planck Institute Stuttgart (D),*
** Science Council of the French Senate and National Assembly, Paris (F)*
** Co-Founder and Executive Advisor to CEO's & President of IMEC-Technology Institute*

***(Former & Present: "Member, Chairman & President of Science Research Councils/Governing Boards (1975 - …)***

****** *NATO & von KARMANN: Research & Technology, Brussels -Paris*
** ESA (European Space Agency), Hermes Programme, Noordwijk (NL) & Paris*
** CNRS (Conseil National pour la Recherche Scientifique), FR*
** CEA (Commissariat de l'Energie Atomique), FR*
** CNR (Consiglio Nazionale Delle Ricerche), IT*
** CSIC (Consiglio Superior de Investigaciones Cientificas), ES*
** JST (Japan Science& Technology), Tokyo – Japan*

***The main topics and achievements in my career are summarized***

*40 years' experience in European & Worldwide Academic & Research & Innovative institutions: Professor – Scientist – Research manager – Director - Councillor.*

** Disciplines: Physics: nuclear, low & high temperature, health; Polymer & Chemistry and Biochemistry, Materials & Aeronautics; Engineering; Medicine: Physical/medical imaging, Cancer treatment technology, Nanomedicine*

***University professor at multiple Universities, worldwide:***

- *Radiation chemistry, nuclear physics & engineering, radiation safety and protection*
- *High temperature materials for gas turbines for aeroengines and space applications*
- *Nanoscience and nanotechnology*

***Research and technology:***

- *Radiation damage studies, dosimetry, radiation chemistry, health physics*

- *Materials sciences. Metals, ceramics and polymers*
- *Nanoscience & nanotechnology: nanomedicine, nanoelectronics,*
- *Accelerator engineering*
- *Proton-therapy technologies for cancer treatments*

***Spin-off technologies***

- *Pioneering work in the foundation of IMEC – Leuven: institute where after 30 years existing 4.000 scientists/engineers/technicians from 100 different countries are employed.*

***Promotion of University Education in Europe-active role in:***

*° The Ministerial Conference in Bologna – Uniformity of the Education throughout all European countries with the result of BSc, MSc and PhD programmes*

*° Pioneering work in the preparation on the EC: ERASMUS programme which lead to the mobility of students through Europe.*

*° The classification of Excellency of Universities in Europe has never been successful….a most critical subject which is still on the table.*

***Recent published science (study) books & encyclopaedia***

**** Engineering, Medicine, and Science at the Nano-scale Study book for MSc and PhD students, WILEY Publ. Co November 2018; co-author with Prof. S. FONASH, PEN STATE University & Director US-NSF Nanoscience*

**** Nano cosmetics: SPRINGER Publ.in July 2019: co-authors Dr J. CORNIER & Prof. dr. Cornelia KECK*

**** Nanoscience and Nanotechnology: Advances and developments in Nano-sized Materials, DE GRUYTER Publ. Co June 2018*

**** Nanotechnology, Innovations & Applications.: Encyclopedia-15 Volumes WILEY Publ. Co in May 2017, series editor and author of chapters.: Nano Health Care, Nano Information and Communication, Nano Industry*

**** The Nano-Micro Interface, 2 Volumes WILEY publ. Co 2015 co-author with Prof. H.J. FECHT and Matthias WERNER*

**** Nanotechnology in a Nutshell, From Simple to Complex Systems, SPRINGER Publ. 2014 co-author with Dr C. NGO – CEA Paris*

**** GENNESYS White Paper: A new European partnership between nanomaterials science and technology and synchrotron radiation and neutron facilities, Max Planck Gesellschaft, 2011, Co-author with Prof. Dosch DG DESY (D)*

**** European White Book on Fundamental Research in Materials Sciences, Max Planck Institute, Stuttgart 2005, Co-author with MPI Colleagues*

# University Education in Crisis
# Transdisciplinary Approaches in the Arts, Humanities and Sciences

One of the main concerns to day of the University Education in Europe is the specialization which will result in:

- studies for jobs which will not exist anymore in the future and
- problems of mobility during its career which may lead to catastrophic situations e.a. loss of job at ages of 40 &50 years.

This topic will be elaborated in this paper.

## I. INTRODUCTION

This millennium will see us enter an era of revolutions in a range of technologies from medicine to transport that will have transformational effects on society. With new tools, new insights and understanding, and a developing convergence of the disciplines of physics, chemistry, materials science, biology and computing, we will realize novel and superior products and systems that were, until the 21st Century, the stuff of science fiction. This will not be possible without collaborative links between disciplines.

Up to now, academic education has been strongly oriented towards specific academic disciplines. In this, it is often overlooked that most of the problems that research and education are supposed to help us solve are not defined in terms of disciplines, and these problems are precisely the ones that are particularly urgent: examples are the environment, energy, and health. There is an disconnect between the development of problems and the development of disciplines, and this disconnect is growing to the extent that disciplinary development is increasingly determined by specialisation.

In this context, the need for an inter-disciplinarily approach is often mentioned. But inter-disciplinarity, a cooperation between disciplines with a finite duration, is not enough. The development of the problems tackled by today's science assumes that inter-disciplinarity is more a short-term approach to a specific issue rather than a fundamental new instrument of science and research.

"It is not enough to value the links between experiences, disciplines, creativity and ideas. One has to develop methods, strategies and practices that will transform those links into real connections. We have to recognize interdependence in order to actualise it and we have to know how to act once we have developed that recognition."

The University has to change: because its environment (social as well as institutional and regulatory) is changing, and because science and research, that shape internal structures and processes, are changing. Similarly, many conventional jobs will disappear in the near future, by the time that children currently in primary education have graduated. Others will transform radically and many new jobs will be created. Hence industry, government, and the services sector will, in the future, look to recruit candidates with flexibility and an open mind.

The historical development of the universities has been greatly influenced by government intervention in the last fifty years. Fifty years ago, governments showed little interest or interference in universities, unless they propagated anti-government views. Governments were content that universities should be seats of learning, pure research, and scholarship; and would provide funding if affordable. Universities around the world had similar structures, with essentially independent departments.

In the last fifty years the world has fundamentally changed. Many governments now realise that new scientific knowledge holds the key to our future wealth and health: many new medical drugs and industrial products are based upon discoveries made in universities. The industrial hubs in the USA have moved away from the steel centre of Pittsburgh and the car centre of Detroit to high-technology companies based around MIT and Silicon Valley companies based around Stanford University and the University of California. If Europe is to compete successfully with China and the USA then it has to focus on high-technology products and the ideas and materials for many of these will originate in our universities. Hence governments around the world are now intensely interested in their universities.

However, the structure of our universities has changed little in the past fifty years. The majority of Universities still tend to have relatively small, independent departments. A key feature of the university-of-the-future must be flexibility: we must make it easy for an engineer to learn Chinese or an Indian language, history and culture without this being an additional burden. Concerning research, we must acknowledge that much of the most exciting and useful research is occurring at the boundaries between traditional disciplines. Many biologists who design new medical drugs to attach to specific protein molecules have been trained as physicists. Many new materials for next generation mobile phones, computers, cars and planes are designed and developed by materials scientists working with chemists, physicists and engineers. However, University departmental structures often impede rather than facilitate multidisciplinary research.

A major concern is the increased administrative burden being placed on Universities by government regulation and reporting. There is often a disconnect between the administrative functions of a University and the primary activity of research and teaching.

## II. ENHANCING THE EDUCATION, RESEARCH, AND INNOVATION BASE

The social, scientific and technological conditions for the development of ideas, knowledge, and solutions to problems have changed dramatically over recent decades. The globalisation of information, of work, of ecological considerations, to mention just a few, have made a tremendous impact on our life. Problems have become more complex and their solutions require new thinking that has to consider influences from multiple sources in our world.

University education plays a vital role in the welfare and well-being of global society, and it is recognized that good education systems underpin prosperity and stability. The challenges are to provide a trans-disciplinary education that is recognised and transferable around the world.

### *A. Multi- Inter- and Transdisciplinary Education*

A *Discipline* is a sub-field of science, engineering, humanities, etc. with a specific approach, fundamental concepts, language, methods, and tools, that aims to analyse, understand, and describe parts of Nature.

*Multi- disciplinarity* is where several disciplines come together in parallel to tackle one subject.

*Interdisciplinarity* is where the concepts and methods of one discipline are used in the work of another discipline.

*Transdisciplinarity* is a holistic approach that sees all aspects of the world inter-related through patterns of interdependent systems. These include natural, social, economic and political systems. Transdisciplinary integrates knowledge and methods from any source that can be of value in addressing a particular problem or research question. Essential requirements for any transdisciplinary work are curiosity and patience; and understanding of other disciplines and their languages takes time and commitment. Transdisciplinary research and teaching do not respect traditional boundaries.

### *B. Challenges for Inter- and Trans-disciplinary activities*

- *Language*: Each discipline creates its own jargon. I/T-disciplinarity requires the appropriation and accommodation of different languages, meaning communication of I/T-disciplinary research and teaching can be difficult since it requires the use of technical terms borrowed from one discipline but that are not well understood by the specialists from the other discipline.
- *Methods*: Disciplines are often devoted to their own methods of investigation. This may lead to misunderstanding and opposition.
- *Institutional constraints*: Institutions are mostly disciplinarily organised, creating barriers for I/T- disciplinarity; though strong, well-defined disciplines are necessary as any interdisciplinary activity starts with a deep understanding of single disciplines.
- *Cognitive constraints*: It is very difficult for an individual to become expert in two or more disciplines. An in-depth knowledge of different disciplines is however the requirement for genuine I/T-disciplinary research. This raises the question of the impact of these difficulties on education and on the institutionalisation of interdisciplinary training programs.
- *Assessment*: Experts (reviewers) for evaluating the results of M/I-disciplinary research and education are lacking. Standardised bibliometric information is scarce and not representative. New ways of quality assessment need to be developed.
- I/T-disciplinarity requires mastering of more than one discipline in depth. Superficial learning of several disciplines does not lead to meaningful I/T-disciplinary research and corresponding solutions of complex problems.
- Experience has shown that learning the essentials of several disciplines has to be done consecutively, not in parallel: for example, doctoral studies in one discipline and post-doctoral work in another.

### *C. Importance of Inter-Trans disciplinarily for Universities*

Inter/Trans-disciplinarity matters because, in the real world, most scientific, technological, and social problems do span different disciplines: so in future, graduates have to operate in a multi-disciplinary environment, very different from what has existed in the past. The present generation of students must be convinced that they will have good careers if they take a research route in their early years, and that University research leads to careers other than in academia. Whilst today, someone with inter/trans-disciplinary expertise might be viewed as a generalist, in the future this could be regarded as a specialism. For example, a graduate with three Master's degrees in biology, informatics, and engineering, may, in future, be better off than with one PhD in biology etc. Interdisciplinary degrees need to be defined in a sensible way that does not simply double the workload and content. It should be possible to opt for a full MSc inter-disciplinary degree enveloping various Faculty disciplines. This change in culture to an inter/trans-disciplinary approach can be created only during the training of researchers and must be part of their curriculum. University courses must be broader and open to related disciplines thus giving to the students the predisposition to interdisciplinary work after Graduation. Industry will be keen to hire graduates who have mastered the challenge of studying different fields with success and who will also be able to perform trans-disciplinary work and research

The real need is for the next generation of scientists to know how to move forward when faced with a real-world problem on a technical topic they have never met before, on a realistic time-scale, and with a realistic budget. Future research is aimed to solve problems where many traditional disciplines are involved and where an interdisciplinary approach is essential. For example, the rapidly emerging field of biomimetic, intelligent, nano-materials and systems will form possibly the most important technologies of the 21$^{st}$ Century. They will require the input of researchers from solid state and organic chemistry, biology and medicine, physics and mathematics, informatics, and engineering if their potential is to be fully realized.

In Universities, inter-departmental barriers are often very high, particularly in "traditional" institutions based on small Departments of 10-20 academics focused on a single narrow discipline. A modern approach, that has been shown to be more useful, flexible, and efficient, is to have teaching activity based in larger Schools, of up to 100 academics, that can be broadly based and allows for the development and delivery of curriculum from a range of discipline specialists. Research can then be focused either within the School around particular themes, or linked to cross-cutting University Research Centres that can span Schools and Faculties and further exploit the opportunities for cross-disciplinary collaboration.

The primary functions of universities are to educate students, perform innovative and horizon-broadening research, and transfer new knowledge for the benefit of society. Universities need to be flexible enough in their structures, management and culture to establish new interdisciplinary, interdepartmental Centres for working on the scientific fields of tomorrow.

### *D. The roadmap for the Inter-Trans disciplinary Universities of the Future*

There is a need for a change in approach, and a revisitation of recent trends, in fully enabling Universities to become incubators of successful inter/trans-disciplinary research.

For University Leaders, there needs to be:

- Recognition that teaching is primarily for students who will not become future academics, and who will be pursuing careers that do not exist yet;
- Recognition that research and teaching must be closely linked, so that students will benefit from the new ideas of knowledge that research will provide;
- Recognition that research changes very rapidly. It is therefore good practice to develop teaching within large Departments with strong vision for curriculum and continuity, and have research institutes into which it is easy to bring people from various departments for the span of a project.

For Funding Agencies, there needs to be:

- A diversity in approach to funding at all levels, since the challenges of interdisciplinary science are so diverse.
- Better integration between funders and those who conduct the research, so that funding decisions are informed by current challenges.
- Successful models that reward and encourage success, and have a low management burden.
- Active encouragement of interdisciplinary approaches in the solution of research challenges.

### *E. Global University Mobility*

In ensuring the move towards globalisation is meaningful and successful, University education plays a vital role. To facilitate collaboration between universities worldwide, it is important that the curriculum and degrees of the various universities is unified. Europe, with its 30 countries and multiple University systems with different curricula succeeded in realising a uniform University education system called the "BOLOGNA Minister's declaration". The United States have a system quite similar to Europe, and other continents as South America and Asia should move towards a global unified system in the future.

An intercontinental University education system demands great efforts from Universities and governments. A global, uniform education system which facilitates contact between students and academics from universities and nations on a global scale will result in multiple benefits in education quality, mobility, and cultural understanding. The mobility of young students and scientists demands knowledge of foreign languages and cultures and this should form part of the curriculum.

### *F. Mobility of Students and Scientists*

It is important to encourage greater exchange of students and scientists between disciplines and countries. This would be aided by standardised qualification recognition procedures, world-wide training courses, and official exchange programmes. An interdisciplinary culture must be implanted through educational and funding initiatives. It must also be realised that the heterogeneity of world cultures is an asset, not a hindrance, with the potential to provide imaginative ideas and diverse skills. As an example, in the European Union the ERASMUS programme was developed in which possibilities were offered to students and scientists from all countries throughout Europe to study at the faculties of universities of their choice with recognition of their obtained degrees all over Europe.

Employers in the future will be looking for candidates with broad experience and flexibility of thinking. Employers often bemoan that the graduates they recruit are unprepared for the jobs that they are asked to do. The modern economy places an enormous premium on brainpower, and there is not enough to go around. The best evidence of "talent shortage" can be seen in high tech firms: companies such as Yahoo! And Microsoft are battling for the world's best computer scientists. Many firms now have some form of talent-management.

## III. CONCLUSIONS

Universities have historically focussed their education and research towards specific academic disciplines. It is often overlooked that most of the problems that research and education are supposed to help us solve are not defined in terms of disciplines, and these problems are precisely the ones that are particularly urgent: examples are the environment, energy, and health.

In ensuring a broad-based education, that is globally-recognised and allows for global mobility of students, there is a need to develop a World University System that promotes networks of universities with shared qualifications and close research collaborations.
Governments, Ministries for Education, Research and Innovation together with Presidencies of universities, all over Europe, should have the courage and the goodwill to take action to reform the university systems for the future welfare of the economy and society.

# PST TiAl Single Crystals - High-Strength Low-Alloy Steels

**by Guang Chen, Member EUAS**

Short Biography

*Prof. Guang Chen is currently a distinguished professor at Nanjing University of Science and Technology, China. He is well known internationally for his outstanding contributions to the design and development of advanced metallic and intermetallic materials. He did pioneer work on deriving new theories of controlling crystallographic orientation based on interfacial anisotropy, developing a new preparation technique with the combination of directional solidification and directional solid-state phase transformation, and mechanistically solving the intrinsic brittleness of bulk metallic glass via introducing in-situ spherical crystalline phases. All his innovative research has significantly promoted the development of structural materials with superior mechanical and metallurgical properties for engineering applications. He has published more than 200 technical papers in archival journals, textbooks, and encyclopedia chapters. His papers have been highly cited by the materials community. He has received numerous honors and recognitions from academia, government, industry, and professional societies, including special allowance of the State Council in 2018, the State Innovation Pioneer Award in 2017, the State Technological Invention Award in 2016, the State Innovative Achievements Award of Industry-University-Research Institute Collaboration in 2014, two Ministry of Education Technological Invention Awards in 1997 and 2012, the Jiangsu Province Patent Inventor Award in 2018, six Province Scientific and Technological Awards in 1995, 2002, 2006, 2007, 2010 and 2013, the Distinguished Award of the 9$^{th}$ International Workshop on Advanced Materials (IWAM) in 2016, and many other awards and citations from state ministries, province government agencies, and Nanjing University of Science and Technology.*

## 1. PST TiAl Single Crystals

Currently, TiAl alloy is the only lightweight metallic material which can be used for longtime service in oxidative environment above 600 ℃. The theoretical density of TiAl alloy is only 3.9 g/cm$^3$, which is less than half of that of nickel-based superalloys. It will deliver a significant weight reduction to substitute nickel-based superalloys with TiAl alloys. Therefore, TiAl alloys have shown great potential of application in the field of aeronautics, aerospace, automobile and energy industry.

However, two dominant defects of polycrystalline TiAl alloys severely limit the engineering application. The first one is low ductility at ambient temperature (<2%), which brings much cost and difficulty in processing and assembling. It also brings risk in the design of aeroengine and thus cannot be used in compressor blades. The second one is limited service temperature. The high temperature strength starts to decrease rapidly from ~650 ℃ and microstructure instability occurs at 700 ℃/3000 h, which means longtime

service temperature cannot exceed 700 ℃.

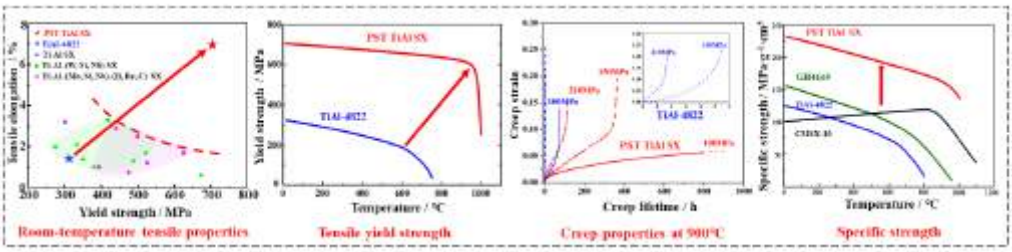


**Fig.1** Microstructure and mechanical properties of PST TiAl single crystals

We have developed a novel seedless single-crystal fabrication technique with the combination of directional solidification and directional solid-state phase transformation. For the first time, polysynthetic twinned (PST) TiAl single crystals with controlled lamellar orientation and excellent performance are fabricated. The well-aligned PST TiAl single crystals exhibit a combination of substantially enhanced ductility of >6% and yield strength of >700 MPa at ambient temperature. Creep lifetime and minimum creep rates at 900℃ are superior to commercial TiAl-4822 alloy by more than one order of magnitude. Its specific strength is higher than all kinds of nickel-based superalloys, including single-crystal superalloys (Fig. 1). This could provide expanded opportunities for higher-temperature applications, such as in aeronautics and aerospace.

## 2. High-Strength Low-Alloy Steels

High-strength low-alloy (HSLA) steels strengthened by Cu-rich precipitates have broad engineering structural applications, from bridges, mining and dredging equipment, to critical naval and offshore applications. Minute addition of Ni and Cu is sufficient to bring in a high density of ultrafine coherent BCC Cu precipitates, which leads to high yield strength over 1000 MPa while maintaining satisfactory ductility of 10%. It implies a significant cost reduction due to only minute alloying for a large strength improvement without sacrificing the ductility. However, the steel requires a peak aging at 550 ℃ that falls within the temper-embrittlement regime of 300-600 ℃. The embrittlement is even worse in the presence of Cu, Cr, Ni, and Mn which are commonly used in HSLA steels. Therefore, the temper embrittlement remains an unsolved issue in HSLA steels, limiting their widespread in various engineering applications.

We have successfully produced a low-C-Ni-Cu HSLA steel with a combination of high strength, satisfactory ductility, and superior low-temperature (-40 ℃) impact toughness by a careful control of grain size, Cu-rich precipitates, tempered martensite, and fresh martensite (or carbides) at a heat treatment temperature beyond the temper-embrittlement regime. These results have been published in the article, *Hardening mechanisms and impact toughening of a high-strength steel containing low Ni and Cu additions*, *Acta Materialia*, 172 (2019): 150-160.

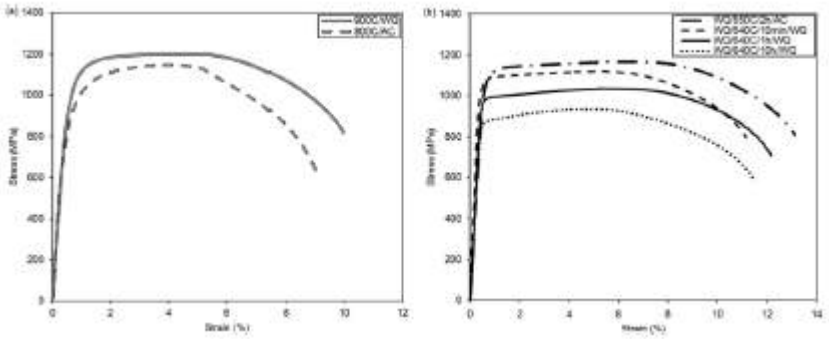

**Fig. 2** Room temperature stress-strain curves of (a) 900℃/WQ and 900℃/AC samples and (b) WQ/550℃/2h/AC, WQ/640℃/10min/WQ, WQ/640℃/1h/WQ, and WQ/640℃/10h/WQ samples

The steel is insensitive to heat-treat temperatures such that the YS and UTS can be maintained at over 1000 MPa even at a heat-treat temperature of 640 ℃ due to multiple strengthening mechanisms (Fig. 2). Besides, the UTS strength of the steel is insensitive to cooling rate and maintains at over 1000 MPa when it is air cooled from the 90 ℃ solution treatment. It is also demonstrated that, by a prolonged 10 h aging at 640 ℃, the steel can achieve a low YS of 800 MPa with low work hardening which is beneficial for manufacturing. Such superior mechanical properties are obtained through the fine grain size (~2.5 mm), large overaged Cu-rich precipitates (~30-50 nm, Fig. 3) and the formation of fresh martensite (or carbides) during the 640 ℃ water quenching.

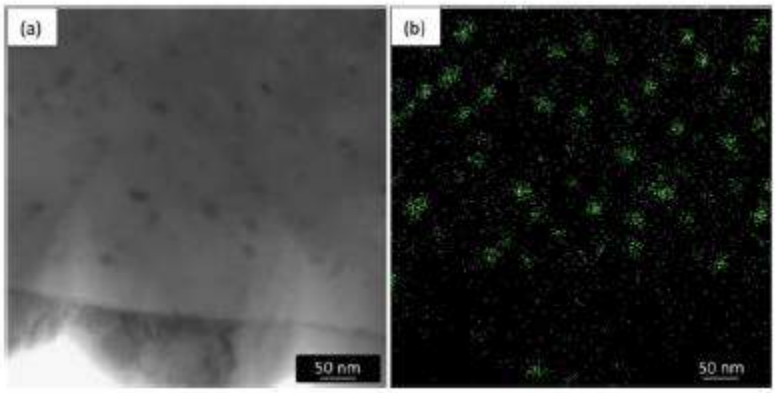


**Fig. 3**. STEM images of WQ/640℃/10h/WQ sample showing the presence of (a) overaged Cu-rich precipitates and (b) EDX elemental mapping of the Cu-rich precipitates. The size and the number density of the Cu-rich precipitates are approximated to be around 30-50 nm and $5.2\times10^{20}/m^3$, respectively.

## 3. Light Element Doped BiCuSeO Thermoelectric Materials

Thermoelectric (TE) materials are capable of direct conversion between thermal and electrical energy, and provides an alternative solution for power generation, solid-state cooling, and air conditioning. The performance of TE materials is determined by the dimensionless figure of merit ZT, which is determined by Seebeck coefficient, the electrical conductivity, the total thermal conductivity, and the absolute temperature. Layered oxyselenide BiCuSeO with ZrSiCuAs like structure is a recently reported potential superior TE material which exhibits an intrinsically low thermal conductivity. However, the Seebeck coefficient and carrier mobility in reported doped BiCuSeO system are too small, which limits the improvement of thermoelectric performance.

We successfully discover that light element Li doping boosts carrier mobility (7.39 $cm^2$

$V^{-1}$ $s^{-1}$) due to largely reduced carrier scattering, which results in about 2-fold increase in carrier mobility as compared with reported $Bi_{0.875}Ba_{0.125}CuSeO$ through modulation doping or microstructure texturing (Fig. 4). Moreover, the Seebeck coefficient remarkably increases by contribution of spin entropy induced by magnetic ions Mn incorporation. The enhancement of Seebeck coefficient coupled with enhanced electrical conductivity result in high power factor. Furthermore, nanoprecipitates and dual-atom point defect leads to a significant reduction of lattice thermal conductivity. Therefore, a high ZT value of 0.9 was achieved at 873 K through optimizing power factor while maintaining low thermal conductivity (Fig. 5). Our findings provide a new perspective for designing prospective thermoelectric materials, and have been published in the article, *Light element doping and introducing spin entropy: an effective strategy for enhancement of thermoelectric properties in BiCuSeO*, *ACS Applied Materials & Interfaces*, 11.17 (2019): 15543-15551.

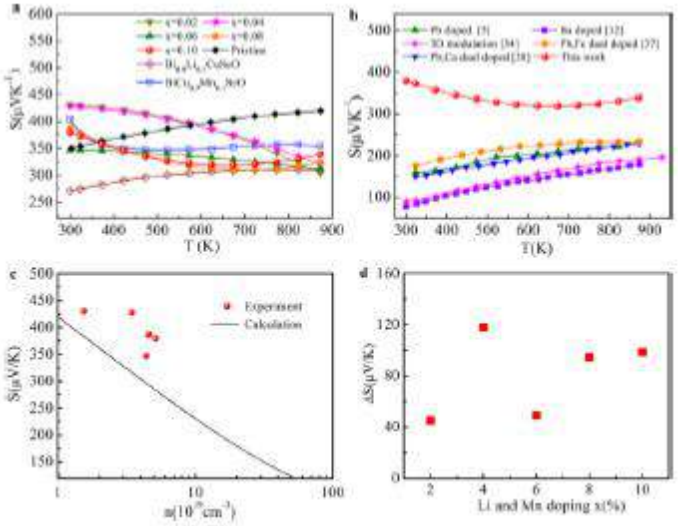


**Fig. 4** (a) Temperature dependence of Seebeck coefficient (*S*). (b) Seebeck coefficient of $Bi_{0.9}Li_{0.1}Cu_{0.9}Mn_{0.1}SeO$ compared with results of references. (c) Hole concentration dependence of the Seebeck coefficient of BiCuSeO at room temperature. (d) Seebeck coefficient difference, $\Delta S$, as a function of Li and Mn doping level *x*.

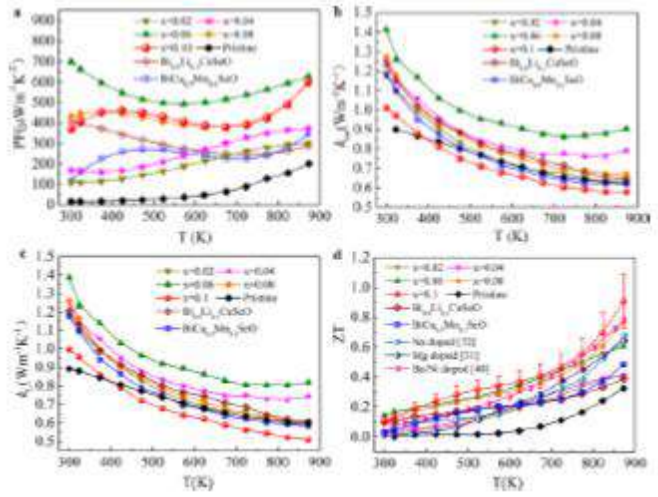


**Fig. 5** Temperature dependence of (a) power factor (PF), (b) total thermal conductivity, (c) lattice thermal conductivity, and (d) ZT for $Bi_{0.9}Li_{0.1}CuSeO$, $BiCu_{0.9}Mn_{0.1}SeO$, and $Bi_{1-x}Li_xCu_{1-x}Mn_xSeO$. Data on the temperature-dependent transport reported for $Bi_{1-x}Na_xCuSeO$, $Bi_{1-x}Mg_xCuSeO$, and $Bi_{0.875}Ba_{0.125}Cu_{1-x}Ni_xSeO$ are shown for comparison.

# Conversion of Mg-Li Bimetallic Alloys to Magnesium Alkoxide and Magnesium Oxide Ceramic Nanowires

**by Gleb Yushin, Member EUAS**

Short Biography

***EDUCATION AND TRAINING:***

| | | | |
|---|---|---|---|
| *Saint-Petersburg Polytechnic Institute* | *Physics* | *MS (with Honors)* | *1999* |
| *North Carolina State University* | *Materials Science* | *PhD* | *2003* |
| *Drexel University* | *Materials Science* | *Postdoctoral training* | *2003-2004* |

***PROFESSIONAL APPOINTMENTS:***

| | | |
|---|---|---|
| *Graduate Research Assistant* | *Ioffe Institute (Russia)* | *1997-1999* |
| *Graduate Research Assistant* | *North Carolina State University* | *1999-2003* |
| *Postdoctoral Fellow* | *Drexel University* | *2003-2004* |
| *Research Assistant Professor* | *Drexel University* | *2004-2007* |
| *Co-Founder and BoD Member* | *Y-Carbon, Inc.* | *2005-2007* |
| *Assistant Professor* | *Georgia Institute of Technology* | *2007-2012* |
| *Co-Founder, CSO and BoD Member* | *Streamline Nanotechnologies, Inc.* | *2008-2011* |
| *Co-Founder, CTO and BoD Member* | *Sila Nanotechnologies, Inc.* | *2011-present* |
| *Associate Professor (early promotion)* | *Georgia Institute of Technology* | *2012-2015* |
| *Professor (early promotion)* | *Georgia Institute of Technology* | *2015-present* |
| *Editor-in-Chief* | *Materials Today* | *2016-present* |

***SELECTED PERSONAL HONORS & AWARDS:***

| | |
|---|---|
| *Soros (International Science Foundation) Student Scholarship* | *1997* |
| *Polytechnic Institute Fellowship Award for Excellence in Graduate Studies* | *1997-1999* |
| *Saint-Petersburg City Scholarship for Best Graduate Students and Young Scientists* | *1998* |
| *Roland B. Snow Award from the American Ceramic Society* | *2005* |
| *NASA Nanotech Briefs® Nano 50™ Award in the Technology category* | *2006* |
| *Roland B. Snow Award from the American Ceramic Society* | *2007* |
| *Petroleum Research Fund Young Investigator Award* | *2008* |
| *Honda Initiation Award* | *2008* |
| *Air Force Office of Scientific Research Young Investigator Program Award* | *2009* |
| *R&D 100 Award (Y-Carbon, Inc.'s application)* | *2009* |
| *National Science Foundation (NSF) Young Investigator CAREER Award* | *2010* |
| *Invited talk at a Gordon Research Conference (GRC)* | *2012* |
| *NASA Inventions and Contributions Board Tech Brief Award* | *2012* |
| *Invited talk at the 2012 International Meeting of Li Ion Batteries (IMLB)* | *2012* |
| *Emerging Investigator and Invited Participant in the special Emerging Investigators issue "Materials for Energy and Sustainability", Journal of Materials Chemistry A* | *2014* |
| *Kavli Fellow Award* | *2014* |
| *Invited Participant at the German-American Kavli Frontiers of Science symposium, co-organized by the Alexander von Humboldt Foundation and the U.S. NAS* | *2014* |
| *Invited Participant at the Japan-America Frontiers of Engineering symposium, co-organized by the Engineering Academy of Japan and the U.S. NAS* | *2016* |
| *Finalist and Honoree of the Blavatnik Award for Young Scientists, NYAS* | *2017, 2018* |
| *"Leading and Most Cited Researchers in Sciences Around the World", Clarivate Analytics* | *2017-2019* |
| *Sigma Xi Best Faculty Paper Award* | *2018* |
| *Hall of Fame, North Carolina State University, College of Engineering, MSE* | *2018* |
| *Fellow, EU Academy of Sciences* | *2018* |
| *Outstanding Achievement in Research Innovation Award, Georgia Tech* | *2019* |
| *Fellow, National Academy of Inventors* | *2019* |

***SELECTED HONORS & AWARDS OF MENTORED STUDENTS:*** *three TiGER Fellowship Awards (two years long entrepreneurial projects); Women of Distinction Award; Outstanding Graduate Student Award at*

*the Georgia Tech Women's Leadership Conference; MRS Gold Graduate Student Award; Outstanding Student Achievement Award from Georgia Section of the Electrochemical Society; Phi Kappa Phi Award; College of Engineering Outstanding Undergraduate Researcher Award; Henry Ford II Scholar Award; Boeing Fellowship Award; NASA Graduate Student Researcher Program Award; Robert G. Shackelford Fellowship Award; NSF Graduate Fellowship Award; 23 Presidential Undergraduate Research Awards; multiple best poster awards at local, national and international meetings, among others.*

1**) "Conversion of Mg-Li Bimetallic Alloys to Magnesium Alkoxide and Magnesium Oxide Ceramic Nanowires"**
by Shunrui Luo, Kostiantyn Turcheniuk, Ah-Young Song, Aashray Narla, Doyoub Kim, Alexandre Magasinsky, Gleb Yushin.

**Abstract:** Technologically important composites with enhanced thermal and mechanical properties rely on the reinforcement by the high specific strength ceramic nanofibers or nanowires (NWs) with high aspect ratios. However, conventional synthesis routes to produce such ceramic NWs have prohibitively high cost, thus making them unsuitable for most industrial applications. Here we demonstrate a revolutionary direct transformation of bulk Mg-Li alloys into Mg alkoxide NWs without the use of catalysts, templates, expensive or toxic chemicals or any external stimuli. This mechanism proceeds through the minimization of strain energy at the boundary of phase transformation front leading to the formation of ultra-long NWs with tunable dimensions. Such alkoxide NWs can be easily converted in air into ceramic MgO NWs with similar dimensions. We discuss the impacts of the alloy grain size and Li content, synthesis temperature, inductive and steric effects of alkoxide groups on the diameter, length, composition, ductility, and oxidation of the produced NWs. The reported approach opens new avenues for multiple low-cost synthesis routes of NWs with tunable composition and morphology for their use in nanofiber-reinforced composites and other applications.

2) **"Cycle Stability of Conversion-Type Iron Fluoride Lithium Battery Cathode at Elevated Temperatures in Polymer Electrolyte Composites"**
by Qiao Huang, Kostiantyn Turcheniuk, Xiaolei Ren, Alexandre Magasinski, Ah-Young Song, Yiran Xiao, Doyoub Kim, Gleb Yushin.

**Abstract:** Metal fluoride (MF) conversion cathodes offer a pathway towards developing lower cost Li-ion batteries (LIB). Unfortunately, such cathodes suffer from extremely poor performance at elevated temperatures, which may prevent their use in large-scale energy storage applications. Here we report that replacing commonly used organic electrolytes with solid polymer electrolytes (SPEs) may allow one to overcome such a hurdle. We demonstrate long-cycle stability for over 300 cycles at 50 °C attained in high-capacity (> 450 mAh g-1) FeF2 cathodes. The absence of liquid solvents reduced electrolyte decomposition, while mechanical properties of the SPE enhanced cathode structural stability. Our findings suggest that the formation of elastic, thin and homogeneous cathode electrolyte interphase (CEI) layer on active particles is likely a key for the stable performance. The successful operation of MFs at elevated temperatures opens a new avenue for their practical applications and future successful commercialization.

3) **"Mechanisms of Transformation of Bulk Aluminum-Lithium Al-loys to Aluminum Metal-Organic Nanowires"**

by Fujia Wang, Kostia Turcheniuk, Baolin Wang, Ah-Young Song, Ashok Vallamattam, Angela Park, Kolby Hanley, Donghui Long, Ting Zhu, Gleb Yushin.

**Abstract**: Fabrication and applications of light-weight, high load-bearing, thermally stable composite materials would benefit greatly from leveraging the high mechanical strength of ceramic nanowires (NWs) over conventional particles or micron-scale fibers. However, conventional synthesis routes to produce NWs are rather expensive. Recently we discovered a novel method to directly convert certain bulk bimetallic alloys to metal-organic NWs at ambient temperature and pressure. This method was demonstrated by a facile transformation of polycrystalline aluminum-lithium (AlLi) alloy particles to aluminum alkoxide NWs, which can be further transformed to mechanically robust aluminum oxide (Al2O3) NWs. However, the transformation mechanisms have not been clearly understood. Here, we conducted advanced materi-als characterization (via electron microscopy and nuclear magnetic resonance spectroscopies) and chemo-mechanical modeling to elucidate key physical and chemical mechanisms responsible for NWs formation. We further demonstrated that the content of Li metal in the AlLi alloy could be reduced to about 4 wt.% without compromising the success of the NWs synthesis. The new mechanistic understanding may open new avenues for large-scale, low-cost manufacturing of NWs and nanofibers for a broad range of composites and flexible ceramic membranes.

4**) "Understanding Li-ion Dynamics in Lithium Hydroxychloride (Li2OHCl) Solid State Electrolyte via Addressing the Role of Protons**"
by Ah-Young Song, Kostiantyn Turcheniuk, Johannes Leisen, Yiran Xiao, Lamartine Meda, Oleg Borodin, and Gleb Yushin.

**Abstract**: A low melting point solid-state electrolytes (SSE) are critically important for low cost manufacturing of all solid-state batteries. Lithium hydroxychloride (Li2OHCl) is a promising material within the SSE domain due to its low melting point (mp <300 °C), cheap ingredients (Li, H, O, Cl), and rapid synthesis. Another uniqueness of this compound is the presence of Li-vacancies and rotating hydroxyl groups which promote Li-ion diffusion, yet the role of the protons in the ion transport remains poorly understood. To examine lithium and proton dynamics, we conducted a set of solid-state NMR experiments, such as magic-angle spinning (MAS) 7Li NMR, static 7Li and 1H NMR and spin-lattice T1(7Li)/T1(1H) relaxation experiments. We determined that only Li+ contributes to long-range ion transport, while H+ dynamics is constrained to an incomplete isotropic rotation of the OH group. Our results uncovered detailed mechanistic understanding of the ion transport in Li2OHCl. We showed that two distinct phases of ionic motions appear at low and elevated temperatures, and that the rotation of the OH group controls Li+ and H+ dynamics in both phases. Our model based on the NMR experiments is fully consistent with crystallographic information, ionic conductivity measurements, and Born–Oppenheimer molecular dynamic (BOMD) simulations.

5) **"Anatase TiO2 Confined in Carbon Nanopores for High-Energy Li-Ion Hybrid Supercapacitors Operating at High Rates and Subzero Temperatures"**
by Wenbin Fu, Enbo Zhao, Ruiying Ma, Zifei Sun, Yang Yang, Marta Sevilla, Alexandre Magasinski and Gleb Yushin.

**Abstract**: Li-ion hybrid supercapacitors (Li-HSCs) hold great promise in future electrical energy storage due to their relatively high power and energy density. However, a major

challenge lies in the slow kinetics of Li-ion intercalation/extraction within metal-oxide electrodes. Here, we show that ultrafast charge storage is realized by confining anatase TiO2 nanoparticles in carbon nanopores to enable a high-rate anode for Li-HSCs. The porous carbon with interconnected pore walls and open channels not only works as a conductive host to protect TiO2 from structural degradation but also provides fast pathways for transport of both ions and electrons. As a result, the assembled cells based on the composites can exhibit remarkable rate capabilities with a specific capacity of ~140 mAh g-1 at a slow charge and ~60 mAh g-1 at a 3.5 sec fast charge. While the charge/discharge process can be completed as fast as that of state-of-the-art electrical double-layer capacitors (EDLCs), the produced nanoporous TiO2-C nanocomposites show 2–5 times higher volumetric capacitance than activated carbon electrodes used in commercial EDLCs with acetonitrile (AN)-based electrolytes (280 F cc-1 vs. 55-90 F cc -1). Equally important for some applications in cold climates or the space, the Li-HSCs can operate at subzero temperatures as low as −40 °C, which is likely only limited by thermal properties of the AN (melting point of −45 °C). In addition to energy storage devices, the described synthesis approach is expected to find use in catalysis and other applications.

6) **"Transformation of Bulk Alloys to Oxide Nanowires"**
by Danni Lei, Jim Benson, Alexandre Magasinski, Gene Berdichevsky, and Gleb Yushin.

**Abstract:** One dimensional (1D) nanostructures offer prospects for enhancing electrical, thermal and mechanical properties of a broad range of functional materials and composites, but their synthesis methods are typically elaborate and expensive. We demonstrate direct transformation of bulk materials into nanowires under ambient conditions without use of catalysts, or any external stimuli. The nanowires form via minimization of strain energy at the boundary of a chemical reaction front. We show transformation of multi-micron particles of Al or Mg alloys into alkoxide nanowires of tunable dimensions, which are converted into oxide nanowires upon heating in air. Fabricated separators based on Al2O3 nanowires enhanced the safety and rate capabilities of Li-ion batteries. The reported approach allows ultra-low cost scalable synthesis of 1D materials and membranes.

# Optimizing Analysis of Spectral Data

## by David Aspnes, Member EUAS

Short Biography

*D. E. Aspnes was born in Madison, Wisconsin, US. He obtained Bachelors and Masters Degrees in Electrical Engineering from the University of Wisconsin, Madison, in 1960 and 1961, respectively. He obtained a Ph.D. in Physics from the University of Illinois Urbana-Champaign in 1965. After a year as a postdoctoral research assistant at the UIUC in 1965-1996 and a second year at Brown University 1966-1967, he joined the Surface Science Department at Bell Laboratories, Murray Hill, NJ, as a Member of the Technical Staff, where is most important contribution is probably the development of spectroscopic ellipsometry, a diagnostic tool now widely used in science and integrated-circuits technology. In 1984 he became Head of the Interface Physics Department of Bell Communications Research in Red Bank, N.J. In 1992 he joined the Department of Physics of North Carolina State University, and was named Distinguished University Professor of Physics in 1998.*

*Professional recognition includes being named a Fellow of the American Physical Society, the Optical Society of America, the Society of Photo-Optical Instrumentation Engineers, the American Vacuum Society, the World Innovation Foundation, and the American Association for the Advancement of Science. Recognition includes numerous awards, the Wood Prize of the Optical Society of America in 1987, the John Yarwood Memorial Medal of the British Vacuum Council in 1993, the Frank Isakson Prize of the American Physical Society in 1996, the Medard W. Welch Award of the American Vacuum Society in 1998, and the Mentor Award of the Society of Vacuum Coaters in 2011. He was elected to the National Academy of Sciences in 1998, and became a Fellow of the National Academy of Inventors in 2013. He has served in various professional capacities, including a term as President of the American Vacuum Society in 1995. He is presently an Associate Editor of the Journal of Applied Physics. He has over 500 publications in various journals. Current research interests include the application of electrodynamics to understand resonant enhancement of optical measurements, and advancing capabilities of extracting information from spectra, optical and otherwise, by linear and nonlinear techniques. The work described below is done in collaboration with co-workers Long V. Le and Y. D. Kim at Kyung Hee University, Seoul, Korea.*

## Previous year's Research

The motivation for the work described in refs. 1-3 is that spectra, optical and otherwise, are a primary source of information about surfaces, interfaces, thin films, materials, nanostructures, and other physical systems. Consequently, it is of primary interest in spectral analysis to establish optimal methods of eliminating noise while preserving information. In the last year we have addressed three topics of interest: (a) establishing linear and nonlinear methods that eliminate noise as much as possible while preserving information to the maximum extent possible; (b) combining filtering with interpolation, thereby allowing efficient processing of data obtained linear in wavelength to equivalent data linear in energy, as needed by theory, and (c) improving methods of removing principal components in Fourier analyzing data, allowing Fourier coefficients to be accessed that are several orders of magnitude smaller than possible by direct Fourier analysis.

The ultimate limit determining access to information is usually set by noise. The challenge is not simply to eliminate noise, which is relatively easy to do, but to do it

intelligently in a way that does not compromise information. This concern is hardly new: in 1977 Kaiser and Reed[4] noted that filtering algorithms are usually "applied blindly to the data and the results are simply inspected to see if they 'look good'". In 1995 Barak[5] pointed out that all too often filtering is "hit or miss". Because limits to achievable accuracy in modeling depend in part on keeping the information while reducing noise as much as possible, approaches more systematic than simple inspection or hit-or-miss are required.

Common methods of filtering include direct-space convolution, for example with a running average such as $(1/3,1/3,1/3)$. This is equivalent to multiplying the reciprocal-space (RS) Fourier coefficients $C_n$ of the data by the coefficients $C_n'$ of the convolving function, then back-transforming the result to direct space (DS). Obviously, to establish whether a filter is appropriate one must first verify that the cutoff of the selected filter matches the boundary between the low-order coefficients that contain the information and the high-order coefficients that are dominated by noise, and second, that the low-order coefficients are preserved as much as possible.

We find that the best approach is the Gauss-Hermite procedure initially described by Hoffman et al.[6] in a work that has never received the attention that it deserves. While a strong argument can also be made for binary methods,[4] Gaussian filtering is preferred because the Fourier transform of a Gaussian is a Gaussian, hence this function minimizes the uncertainty product of the widths in direct and reciprocal spaces. In addition, Gaussians avoid cutoffs that are too rapid, thereby inhibiting the appearance of Gibbs oscillations (ringing).

To preserve low-order coefficients, the RS filter should multiply them by 1 as far as possible up to the white-noise cutoff. Hoffman et al. accomplish this by multiplying $e^{-x^2}$ by Hermite polynomials, where *x* is a scaled version of *n*. We use an equivalent but more intuitive and more general approach, noting that according to the Butterworth criterion, a "flat" RS filter is obtained by eliminating terms in a Taylor-series expansion of the RS filter function about $n=0$ as far as necessary. For the Gaussian, this can be done by multiplying $e^{-x^2}$ by $[e^{x^2}]_n$, where $[e^{x^2}]_n$ denotes the first *n* terms of the Taylor-series expansion of $e^{x^2}$. Example applications and closed-form expressions for Gaussian DS convolutions based on this approach are provided in Ref. 1.

Reference 3 addresses an issue that needed to be solved before the methods of Ref. 1 could be applied most successfully. Because Fourier analysis assumes periodicity, and spectra or spectral segments rarely start and end with the same value and first derivative, at some index *n* the $C_n$ become dominated by the contributions from the value and slope discontinuities at endpoints, masking the desired information. This problem was addressed many years ago by Yoo and Aspnes,[7] who showed that if a line and a parabola are added to the segment with scaling coefficients determined by minimizing the Fourier coefficients in the white-noise region, endpoint-discontinuity artifacts are essentially eliminated. They successfully unmasked coefficients by up to three orders of magnitude. Because information content varies as $\ln(C_n)$, where $C_n$ is the magnitude of the $n^{\text{th}}$ coefficient, the improvement in the capability to extract information is significant.

Reference 3 extends this procedure by placing the false data outside the spectral range of the segment. This results in less distortion of the data and generates new Fourier coefficients that are accurate interpolations of the originals. While these new coefficients

add no information, they improve our capabilities to recognize trends. Using model lineshapes, previous and new procedures were compared, investigating effectiveness and accuracy for X-ray photoelectron spectroscopy (XPS) data as an example.

Finally, many data are now obtained with photodiode-array detectors, which return spectral data equally spaced in wavelength instead of energy. Data equally spaced in wavelength are incompatible with standard methods of analysis, which are based on data equally spaced in energy. The usual approach for dealing with this conflict is interpolation, defined as any method where the interpolating function passes through the data themselves, leaving them unchanged. Intermediate values are then constructed according to a predefined rule. The most common is linear interpolation, where intermediate values are proximity-weighted averages of the nearest two values. Unfortunately, data typically include noise, so noise is interpolated as well.

Consequently, there is a need for a conversion method that is simple, convenient, accurate, and delivers noise-reduction effects that are quantified. The method presented in Ref. 2 meets these criteria, allowing interpolation, scale change, noise reduction, and additional processing such as differentiation (if desired) to be combined in a single step. It is based on the numerical integration of the data weighted locally by a Gaussian kernel.[1] Gaussian kernels are analytic, as well as having the advantages listed above. Analyticity confers significant advantages here because it allows the approach to be extended to operations such as differentiation or other forms of data processing. In addition, approximations are limited entirely to the numerical evaluation of a single integral. In this regard, the authors show that, owing to cancelling nonlinearities, the trapezoidal rule is accurate to fourth order in the ratio of point spacing to Gaussian width when evaluating Gaussian integrals. Hence, and counterintuitively, in this application the simplest and most convenient of the many available numerical-integration methods is also the most accurate.

The approaches described above are general, applicable not only to the ellipsometric spectra for which they were originally developed, but also to those obtained by infrared spectroscopy, X-ray photoemission spectroscopy, Raman scattering, etc. Interpolation is particularly important for XPS spectra, where Gaussian or near-Gaussian lineshapes cause RS coefficients to decrease as Gaussians, so relatively few are available for analysis.

**References**

1. D. E. Aspnes, V. L. Le, and Y. D. Kim, Linear and nonlinear filtering of spectra, J. Vac. Sci. Technol. B37, 051205 (2019). doi: 10.1116/1.5118230.
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3. V. L. Le, T. J. Kim, Y. D. Kim, and D. E. Aspnes, External removal of endpoint-discontinuity artifacts in the reciprocal-space analysis of spectra, Current Appl. Phys. 20, 232-236 (2019). doi: 10.1016/j.cap.2019.11.004.
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# Oral Peptide Delivery using Intestinal Permeation Enhancers and Nanoparticles

## by David J. Brayden, Member EUAS

Short Biography
*Full Professor of Advanced Drug Delivery at University College Dublin (UCD), Ireland*
*Room 231, Veterinary Sciences Centre, UCD Belfield, Dublin 4.*
*Home page: https://people.ucd.ie/david.brayden*

***Education***

| | |
|---|---|
| *Ph.D. 1989* | *Department of Pharmacology, University of Cambridge, UK* |

***Employment***

| | |
|---|---|
| *2001-present* | *Full Professor, UCD School of Veterinary Medicine* |
| *1991-2001* | *Senior Scientist, Elan Biotechnology Research, Dublin* |
| *1989-1991* | *Post-Doctoral Fellow, Cystic Fibrosis Laboratory, Stanford University, CA, USA* |

***Selected Honours/Awards***

| | |
|---|---|
| *2006* | *Board of Scientific Advisors of the Controlled Release Society (CRS)* |
| *2009* | *Distinguished service award from the CRS* |
| *2012* | *Elected to the College of Fellows of the CRS* |
| *2013* | *Appointed Senior Fellow, UCD Conway Institute of Biotechnology* |
| *2014* | *Reappointed to Editorial Advisory Board of Advanced Drug Delivery Reviews* |
| *2015* | *Distinguished service award from the CRS Annual Meeting Programme Committee* |
| *2017* | *Recipient of Marquis Who's Who® Albert Nelson Lifetime Achievement Award* |
| *2017* | *Appointed Senior Associate Editor "Therapeutic Delivery"* |
| *2017* | *Elected as Fellow of the American Association of Pharmaceutical Scientists (AAPS)* |
| *2019* | *Lead organiser for Keystone Conference on drug delivery (Dublin)* |
| *2020* | *Keynote speaker: Gordon Research Conference on Molecular Structure Elucidation* |

David Brayden studies the interaction of drugs with epithelia in order to help design dosage forms that cross biological barriers. Much of the research is on how to convert injectable peptides to oral forms, by using nanotechnology and intestinal permeation enhancers to orally deliver anti-diabetic peptides. He also works on oral delivery of peptide bioactives identified via bioinformatics from hydrolysates from food in collaboration with Nuritas Ltd, which is co-funded by the Science Foundation Ireland (SFI) BiOrbic Centre for Bioeconomy. Other strengths are in developing formulations that can be attached to the cheek in order to promote delivery of peptides, i.e. buccal delivery. Another project is in the area of intra-articular injection of protein-based nanoparticles containing celecoxib to offset joint inflammation in knee arthritis. These two projects are co-funded by the Science Foundation Ireland (SFI) Centre for Medical Devices (2014-

2021), where Prof. Brayden is a co-lead PI.

## Selected peer-reviewed publications from Brayden lab (2019)

**1. Hristov, D., McCartney, F. Beirne, J., Mahon, E., Reid, S., Bhattacharjee, S., Penarier, G., Werner, U., Bazile, D., Brayden, D. J. Silica-coated nanoparticles with a core of zinc, L-arginine and a peptide designed for oral delivery.** ***ACS Applied Materials & Interfaces*****. doi: 10.1021/acsami.9b16104.**

Nanoparticle constructs for oral peptide delivery at a minimum must protect and present the peptide at the small intestinal epithelium in order to achieve oral bioavailability. In a reproducible, scalable, surfactant-free process, a core was formed with insulin in ratios with two established excipients and stabilizers, zinc chloride and l-arginine. Cross-linking was achieved with silica, which formed an outer shell. The process was reproducible across several batches, and physicochemical characterization of a single batch was confirmed in two independent laboratories. The silica-coated nanoparticles (SiNPs) entrapped insulin with high entrapment efficiency, preserved its structure, and released it at a pH value present in the small intestine. The SiNP delivered insulin to the circulation and reduced plasma glucose in a rat jejunal instillation model. The delivery mechanism required residual l-arginine in the particle to act as a permeation enhancer for SiNP-released insulin in the jejunum. The synthetic process was varied in terms of ratios of zinc chloride and l-arginine in the core to entrap the glucagon-like peptide 1 analogue, exenatide, and bovine serum albumin. SiNP-delivered exenatide was also bioactive in mice to some extent following oral gavage. The process is the basis for a platform for oral peptide and protein delivery.

**2. McCartney, F., Jannin, V., Chevrier, S., Boulghobra, H., Hristov, D. R., Ritter, N., Miolane, C., Chavant, Y., Demarne, F. & Brayden, D. J. (2019). Labrasol® is an efficacious intestinal permeation enhancer across rat intestine: ex vivo and in vivo rat studies.** ***J. Controlled Release,*** **310: 115-126. http://hdl.handle.net/10197/10965**

Labrasol® ALF (Labrasol®), is a non-ionic surfactant excipient primarily used as a solubilising agent. It was investigated here as an intestinal permeation enhancer in isolated rat colonic mucosae in Ussing chamber and in rat in situ intestinal instillations. Labrasol® comprises mono-, di- and triglycerides and mono- and di- fatty acid esters of polyethylene glycol (PEG)-8 and free PEG-8, with caprylic (C8)- and capric acid (C10) as the main fatty acids. Source components of Labrasol® as well as Labrasol® modified with either C8 or C10 as the sole fatty acid components were also tested to determine which element of Labrasol® was responsible for its permeability-enhancing properties. Labrasol® (4, 8 mg/mL) enhanced the transport of the paracellular markers, [14C] mannitol, FITC-dextran 4000, and FITC-insulin across colonic mucosae. The enhancement was non-damaging, transient, and molecular weight-dependent. The PEG ester fraction of Labrasol® also had enhancing properties. When insulin was administered with Labrasol® in instillations, it had a relative bioavailability of 7% in jejunum and 12% in colon. C8- and C10 versions of Labrasol® and the PEG ester fraction also induced similar bioavailability values in jejunal instillations: 6, 5 and 7% respectively. Inhibition of lipases in instillations did not reduce the efficacy of Labrasol®, suggesting that its mechanism as a PE is not simply due to liberated medium chain fatty acids. Labrasol® acts as an efficacious intestinal permeation enhancer and has potential for use in oral formulations of

macromolecules and BCS Class III molecules.

**3. Twarog C, Fattah S, Heade J, Maher S, Fattal E, Brayden DJ. (2019). Intestinal permeation enhancers for oral delivery of macromolecules: a comparison between salcaprozate sodium (SNAC) and sodium caprate ($C_{10}$).*Pharmaceutics.*;11(2). pii: E78. doi: https://doi.org/10.3390/pharmaceutics11020078**

Salcaprozate sodium (SNAC) and sodium caprate (C10) are two of the most advanced intestinal permeation enhancers (PEs) that have been tested in clinical trials for oral delivery of macromolecules. Their effects on intestinal epithelia were studied for over 30 years, yet there is still debate over their mechanisms of action. C10 acts via openings of epithelial tight junctions and/or membrane perturbation, while for decades SNAC was thought to increase passive transcellular permeation across small intestinal epithelia based on increased lipophilicity arising from non-covalent macromolecule complexation. More recently, an additional mechanism for SNAC associated with a pH-elevating, monomer-inducing, and pepsin-inhibiting effect in the stomach for oral delivery of semaglutide was advocated. Comparing the two surfactants, we found equivocal evidence for discrete mechanisms at the level of epithelial interactions in the small intestine, especially at the high doses used in vivo. Evidence that one agent is more efficacious compared to the other is not convincing, with tablets containing these PEs inducing single-digit highly variable increases in oral bioavailability of payloads in human trials, although this may be adequate for potent macromolecules. Regarding safety, SNAC has generally regarded as safe (GRAS) status and is Food and Drug Administration (FDA)-approved as a medical food (Eligen®-Vitamin B12, Emisphere, Roseland, NJ, USA), whereas C10 has a long history of use in man, and has food additive status. Evidence for co-absorption of microorganisms in the presence of either SNAC or C10 has not emerged from clinical trials to date, and long-term effects from repeat dosing beyond six months have yet to be assessed. Since there are no obvious scientific reasons to prefer SNAC over C10 in orally delivering a poorly permeable macromolecule, then formulation, manufacturing, and commercial considerations are the key drivers in decision-making.

**4. McCartney, F., Rosa, M., & Brayden, D. J. (2019). Evaluation of sucrose laurate as an intestinal permeation enhancer for macromolecules: ex vivo and in vivo studies. Pharmaceutics, 11, (11) 565; https://www.mdpi.com/1999-4923/11/11/565/pdf**

Oral delivery of macromolecules requires permeation enhancers (PEs) adaptable to formulation. Sucrose laurate (SL) (D1216), a food grade surfactant, was assessed in Caco-2 monolayers, isolated rat intestinal tissue mucosae, and rat intestinal instillations. Accordingly, 1 mM SL increased the apparent permeability coefficient (Papp) of [$^{14}$C]-mannitol and reduced transepithelial electrical resistance (TEER) across monolayers. It altered expression of the tight junction protein, ZO-1, increased plasma membrane potential, and decreased mitochondrial membrane potential in Caco-2 cells. The concentrations that increased flux were of the same order as those that induced cytotoxicity. In rat colonic tissue mucosae, the same patterns emerged in respect to the concentration-dependent increases in paracellular marker fluxes and TEER reductions with 5 mM being the key concentration. While the histology revealed some perturbation, ion

transport capacity was retained. In rat jejunal and colonic instillations, 50 and 100 mM SL co-administered with insulin induced blood glucose reductions and achieved relative bioavailability values of 2.4% and 8.9%, respectively, on a par with the gold standard PE, sodium caprate (C10). The histology of the intestinal loops revealed little damage. In conclusion, SL is a candidate PE with high potential for emulsion-based systems. The primary action is plasma membrane perturbation, leading to tight junction openings and a predominant paracellular flux.

**5. Stuttgen, V. & Brayden, D. J. (2020). Investigations of piperazine derivatives as intestinal permeation enhancers in isolated rat intestinal tissue mucosae. AAPS Journal 22, Article number: 33. (doi: 10.1208/s12248-020-0416-9. https://rdcu.be/b0QFt**

A limiting factor for oral delivery of macromolecules is low intestinal epithelial permeability. 1-Phenylpiperazine (PPZ), 1-(4-methylphenyl) piperazine (1-4-MPPZ) and 1-methyl-4-phenylpiperazine (1-M-4-PPZ) have emerged as potential permeation enhancers (PEs) from a screen carried out by others in Caco-2 monolayers. Here, their efficacy, mechanism of action and potential for epithelial toxicity were further examined in Caco-2 cells and isolated rat intestinal mucosae. Using high-content analysis, PPZ and 1-4-MPPZ decreased mitochondrial membrane potential and increased plasma membrane potential in Caco-2 cells to a greater extent than 1-M-4-PPZ. The Papp of the paracellular marker, [$^{14}$C]-mannitol, and of the peptide, [$^{3}$H]-octreotide, was measured across rat colonic mucosae following apical addition of the three piperazines. PPZ and 1-4-MPPZ induced a concentration-dependent decrease in transepithelial electrical resistance (TEER) and an increase in the Papp of [14C]-mannitol without causing histological damage. 1-M-4-PPZ was without effect. The piperazines caused the Krebs-Henseleit buffer pH to become alkaline, which partially attenuated the increase in Papp of [14C]-mannitol caused by PPZ and 1-4-MPPZ. Only addition of 1-4-MPPZ increased the Papp of [3H]-octreotide. Pre-incubation of mucosae with two 5-HT$_4$ receptor antagonists, a loop diuretic and a myosin light chain kinase inhibitor, reduced the permeation enhancement capacity of PPZ and 1-4-MPP for [$^{14}$C]-mannitol. 1-4-MPPZ holds most promise as a PE, but intestinal physiology may also be impacted due to multiple mechanisms of action.

**6. Maher, S. Brayden, D. J., Casettari, L, & Illum, E. (2019). Application of permeation enhancers in oral delivery of macromolecules: an update. *Pharmaceutics*, 11(1). pii: E41. https://www.mdpi.com/1999-4923/11/1/41**

The application of permeation enhancers (PEs) to improve transport of poorly absorbed active pharmaceutical ingredients across the intestinal epithelium is a widely tested approach. Several hundred compounds have been shown to alter the epithelial barrier, and although the research emphasis has broadened to encompass a role for nanoparticle approaches, PEs represent a key constituent of conventional oral formulations that have progressed to clinical testing. In this review, we highlight promising PEs in early development, summarize the current state of the art, and highlight challenges to the translation of PE-based delivery systems into safe and effective oral dosage forms for patients.

**7. Maher, S., Walsh, S.J., Takyi, J., Wakai, A., Brayden, D. J., Hayden, J.C. (2018). Effect of over-encapsulation on the disintegration and dissolution of licensed formulations for blinding in randomised controlled trials. *J. Pharm. Sci.* 108 (3); 1227-1235. doi: https://doi.org/10.1016/j.xphs.2018.10.035**

Over-encapsulation is a technique used to conceal tablet products for blinding in randomized controlled trials. A tablet is inserted in an opaque capsule shell with backfill excipient to prevent rattling. Regulatory authorities require evidence that such modification does not materially alter drug release to approve their use in trials. The objective of this study was to assess impact of over-encapsulation on disintegration and dissolution of 4 immediate-release drug products (penicillin V, gemfibrozil, ciprofloxacin, and furosemide). Each unmodified tablet was compared to 3 over-encapsulated tablets with differing backfill excipient (colloidal silica, lactose monohydrate, or microcrystalline cellulose). All 12 over-encapsulated tablets met disintegration and dissolution acceptance criteria. Dissolution acceptance was dependent on apparatus as only 4/12 formulations met specifications using the rotating basket compared to 12/12 using the rotating paddle. Significant differences in release were observed at early time points (T5-T15). No correlation was observed between aqueous solubility and release, although dissolution of the lipophilic drug gemfibrozil was least impacted by over-encapsulation. There was evidence that type/quantity of backfill delays release at early time points. These findings indicate that under the specified conditions, over-encapsulated formulations of 4 drugs, 1 from each class of the Biopharmaceutics Classification System, met compendium requirements for release testing.

# Recent Developments in Ion-Solid Interactions

## by William J. Weber, Member EUAS

Short Biography

***Governor's Chair Professor, Department of Materials Science and Engineering, The University of Tennessee - Knoxville***

*Prof. William J. Weber received his PhD in Nuclear Engineering from the University of Wisconsin - Madison, USA. He joined Pacific Northwest National Laboratory (PNNL) in 1977 as a research scientist and was appointed Laboratory Fellow in 1997. During 1983, he was a visiting scientist at the Institute for Transuranium Elements in Karlsruhe, Germany, He joined the faculty at the University of Tennessee in 2010 as the Governor's Chair Professor for Radiation Effects in Materials, with a joint appointment at Oak Ridge National Laboratory. His research has encompassed the fundamental aspects of radiation-solid interactions, radiation effects in materials, ion beam modification and analysis of materials, and defects and defect processes in materials. Much of his current research emphasizes the coupling of electronic and atomic energy dissipation processes and their role on radiation effects, defect evolution, formation of novel nanostructures, creation of new functionalities, and the response of materials to extreme environments. He is a member of the EU Academy of Sciences (2016), Fellow of the American Ceramic Society (2000), Fellow of the American Association for the Advancement of Science (2006), Fellow of the Materials Research Society (2008), Fellow of the American Physical Society (2010) and Fellow of the Ion Beam Society of India (2016). He is the recipient of the James I. Mueller Award from the American Ceramic Society (2020); Lee Hsun Lecture Award (2015); the Outstanding Young Alumni Award (1983) and the Distinguished Alumni Award (2009) from the University of Wisconsin - Oshkosh; the PNNL Laboratory Director's Award for Individual Lifetime Achievement in Science & Technology (2009); the PNNL Laboratory Director's Award for Scientific and Engineering Excellence (1995); the PNNL Chester L. Cooper Mentor of the Year Award (2005); and the U.S. Department of Energy's Materials Science Award for Research with Significant Implication for DOE Related Technologies (1995). He has published more than 560 journal articles, 114 peer-reviewed conference papers, and 13 book chapters. Based on the Web of Science, his publications have over 18,600 citations, with an h-index of 67; based on Goggle Scholar, his publications have been cited over 25,600 times, with an h-index of 76.*

The interaction of energetic ions with a solid is well known to result in inelastic energy loss to electrons and elastic energy loss to atomic nuclei in the solid. However, the coupled effects of these energy loss pathways and the critical role of energy dissipation processes on defect production and the evolution of defects, nanostructures and phase transformations under far from equilibrium conditions in materials are complex and not well understood. Particularly challenging are the dynamics of energy transfer processes to electrons and the exchange of energy between electrons and the atomic nuclei via electron-

phonon coupling. In general, the electrons along the ion path undergo a large degree of excitation and electron–electron scattering, and they subsequently transfer much of their energy, via electron–phonon coupling, to atoms in the same region, causing a highly-localized thermal spike. This partitioning of energy deposition and energy dissipation on the electronic and atomic structures are important to the control of ion beam modification methods to create defects and nanoscale structures that tailor materials properties or create new functionalities, as well as the development of radiation-tolerant materials and devices. Predicting and modeling such complex processes, which are temporally and spatially coupled, are grand challenges that demand fundamental understanding of materials processes at the level of electrons and atoms over several orders of magnitude in time scale, from femtoseconds to nanoseconds.

The computer code, Stopping and Range of Ions in Matter (SRIM), is widely used to describe energetic processes of ion-solid interactions; its predictive power relies on the accuracy of energy loss/transfer and collision processes being considered. While the SRIM code is commonly applied in radiation effects research to predict damage production and in the semiconductor industry to estimate ion range and dopant concentration profiles, two challenges exist that affect its use: (1) inconsistency in estimations of atomic displacements between full-cascade and quick (modified Kinchin–Pease) options and (2) overestimation of electronic stopping power for slow heavy ions in light targets (e.g., Be and Si) or in compound targets containing light elements (e.g., C, N and O in carbides, nitrides and oxides). Based on a literature review and our experimental investigations, we have identified the underlying reasons for the discrepancies, clarify the physical limitations of the SRIM predictions, and, more importantly, provide recommendations to address these challenges.

We have previously shown that above an electronic energy loss threshold of 6.5 keV/nm amorphous tracks are formed in pre-damaged $SrTiO_3$ due to melt-quenching along the ion track. In a recent study, the response of pre-damaged $SrTiO_3$ to electronic energy loss values below this threshold has been investigated using 200 keV electrons, 2 MeV He, 1.2 MeV C, 5 MeV C and 12 MeV O ions. The results indicate two distinct regimes of ionization-induced recovery with different dominant processes. While melt-quenching does not occur for C and O ions, the inelastic thermal spike causes enough local heating to induce defect recovery. With electronic energy loss values between 1.6 and 3 keV/nm, the recovery cross sections for C and O ions range from 0.27 to 0.38 $nm^2$, and molecular dynamics simulations confirm that the dominant recovery process is driven by highly-localized inelastic thermal spikes created via electron-phonon coupling. Below this electronic energy loss regime, the recovery cross section decreases by several orders magnitude to about $5.5\times10^{-4}$ $nm^2$ for 2 MeV He ions and $1.0\times10^{-5}$ $nm^2$ for 200 keV electrons, and the dominant recovery process is believed to be associated with electronic excitations that enhance defect mobility.

The origin of the blue emission in $SrTiO_3$ has been investigated as a function of irradiation fluence, electronic excitation density, and temperature using a range of ion energies and masses. The emission clearly does not show correlation with the concentration of vacancies generated by irradiation and is greatly enhanced under heavy-ion irradiation. The intensity ratio of the 2.8 and 2.5 eV bands is independent of fluence at all temperatures, but it increases with excitation rate. A key result of the present study is that, the blue (2.8 eV) and green (2.5 eV) luminescence emissions are both related to

transitions of the STE center, involving either localized states (2.5 eV), or pairs of localized and band states (2.8 eV). This represents a novel feature associated to the high electronic excitation densities achieved by both pulsed laser and ion beam irradiations. A new model for the blue emission is proposed consisting of a radiative transition from un-bound (CB) states to the ground STE level. Consequently, the two emissions (green and blue) are associated with the same localized center and imply the STE annihilation. The analysis presented here provides a unified description of the emission mechanisms and demonstrates the unique potential of ionoluminescence to unravel the rich and complex variety of effects associated with electronic carriers and oxygen vacancies in $SrTiO_3$.

Comparison between intense radiation environments present in nuclear reactors and charged particle beams is necessary for evaluating next generation fission and fusion reactor materials. However, these two irradiation environments encompass different proportions of ionizing and collisional phenomena, so exploring the different energy loss pathways is needed for appropriate analysis. Using the candidate $M_{n+1}AX_n$ phase, $Ti_3SiC_2$, as a test case, the separate and combined effects of electronic and nuclear energy loss during ion irradiation has been investigated, through a combination of 4 MeV Au, 17 MeV Pt, and 14 MeV Cl ion irradiations. Nuclear energy loss (elastic collisions) is found to be primarily responsible for the formation of a face-centered-cubic phase with anti-site defects, while intense electronic energy loss (ionization) exacerbates the effect and increases lattice strain. Further, these dissipation pathways are found to be competing or synergistic depending on their ionization and collisional ratio.

Incorporating Raman spectroscopy with transverse lift-out specimens, prepared by focused ion beam (FIB) techniques, has been demonstrated to be a robust way to accurately study irradiation damage in ion-irradiated ceramics that allows the depth variation of irradiation damage to be evaluated and avoids artefacts of signal contribution from undesired regions. In a study of SiC/SiC composites irradiated up to 1, 10 and 50 displacements per atom (dpa) at 350 ºC using 10 MeV Au ions, Raman spectroscopy on transverse lift-out specimens revealed irradiation-induced structural disorder saturation in both the SiC-fiber and SiC-matrix at doses as low as 1 dpa, despite vastly different microstructures, as inferred from similar longitudinal optical (LO) and transverse optical (TO) phonon peak shifts. Diamond (D) and graphitic (G) peaks from SiC-fibers disappear under irradiation, indicating irradiation-induced carbon packet loss, which has been confirmed by TEM characterization of the same transverse lift-out specimens used for Raman spectroscopy. The loss of the carbon packets leads to irradiation-induced SiC-fiber shrinkage.

# Innovative Energy Research at University of Stavanger

## by Mohsen Assadi, Member EUAS

Short Biography

***Present positions***

*- Professor, Gas technology, Univ. of Stavanger, Norway, since 2007.*
*- Head of energy efficiency research group at Univ. of Stavanger, Norway, since 2015.*
*- Visiting professor at Sheffield University, UK, 2016-2018.*

***Previous position***

- *Professor in Thermal Power Engineering, Dept. of Energy Sciences, Lund University, Sweden (2006-2011).*
- *Chief Scientist, Ineternational Research Institute of Stavanger, Norway, 2008-2015.*
- *Director, Center for Sustainable Energy Sloutions (cenSE), Norway, since 2009-2015.*
- *Visiting professor at Leeds University, UK, 2009-2014*

***Education***

- *PhD in Thermal Power Engineering, Dept. of Energy Sciences, Lund University, Sweden.*
- *MSc in Mechanical Engineering, Lund University, Sweden.*

***Courses and education***

*I had the main responsibility for undergraduate and master level courses as well as PhD courses at division of Thermal Power Engineering at Lund University and at University of Stavanger.*

***Course leader and curriculum design for under graduate courses at Stavanger University and Lund University***

*Theory of Turbomachinary*
*Applied Thermodynamics*
*Steam and Gas Turbine Technology*
*Project course in Energy Conversion Technology*
*Energy and environment*
*From gas to electricity*
*Drilling and well construction*

***PhD Courses***

- *Thermal Design and Optimization*
- *Theory of Turbomachinery*
- *Physical and Chemical Equilibrium*
- *Seminars in Power Plant Technology*
- *Artificial Neural Network for plant monitoring*

***Main fields of competence***

*Mohsen Assadi's research activities are focused on environmental friendly energy technologies, comprising energy system integration, carbon capture and storage (CCS), energy conversion technologies, e.g. gas turbines, fuel cells and steam cycles utilising various fossil and renewable energy sources; system modelling, integration, optimization and monitoring, data driven modeling based on Artificial Neural Networks (ANN).*

***Project leadership***
*Mohsen Assadi has been project leader for several nationally financed project in Sweden and Norway as well as several EU-projects.*
*List of selected projects:*

- *Energy system in transition (Marie Curie training program)*
- *Sustainable Energy Solutions (SIU-INCP)*
- *Roadmap for decarbonisation of Indian Energy system (SIU-INCP)*
- *Theoretical and experimental investigation of biogas fuelled technologies using advanced and intelligent modelling and monitoring tools (Bio-CHP-Monitor, NFR).*
- *Energy Efficiency Improvement via Waste Heat Recovery and Enhancement of Production Rate in Aluminum Industry (NFR).*
- *GAS-FACT, innovative carbon capture technologies for gas fueld power plants (Bilateral project).*
- *Low Emission Combustion Technology for Hydrogen-rich Syngas (H2-IGCC, EU FP7). Subproject leader for system integration.*
- *EU-GGC Clean Energy Network. EU-side working group leader for Clean Natural Gas Applications (EU, FP7).*
- *European North Sea Energy Alliance (ENSEA), holistic energy system integration for the North Sea region comprising environmental, technical, economic and political aspects (EU-FP7).*

***Scientific leadership***
*Mohsen Assadi has been supervisor of 16 PhD students, which finished their studies with PhD degree and he is supervising 4 PhD students and 3 Post-Docs. Prof Assadi has been member of PhD defense committees of 17 PhD students at different European universities. He is also member of several advisory groups, associations and networks.*

## Prof. Assadi's Energy Research at University of Stavanger

The energy industry is facing tremendous challenges due to the combination of observable impacts of the climate change, ever increasing share of the intermittent renewables in the electricity grid and the uncertainties caused by lack of international consensus concerning the way forward. The multi-dimensional nature of the energy related decisions, affected by economy, technology, policy, social acceptance and more, adds to the complexity of the case. Selection of research activities to provide knowledge and clarity in the current situation is not easy. Conflicting interests from political, economic, social and environmental point of view makes the selection of education programs and research topics difficult for the young generation.

The research activities within the energy research group at University of Stavanger (UiS) have been dealing with some aspects of the multi-facetted topic of energy system in transition and its consequences. Given the fact that distributed generation, supported by smart technologies, is foreseen to play a central role in development and transition of the energy systems globally, certain attention was given to R&D activities that can support this development at UiS. The projects listed below are providing an overview over currently ongoing and some recent projects conducted at UiS in support of transition towards carbon neutral energy systems dominated by distributed generation.

Developing validated component and system models using real plant data has enabled the research group to carry out system studies for distributed small-scale generation units as well as large scale centralized power plants, utilizing a variety of fuels. Access to

validated models provides opportunity for identification of possible system configurations and operational strategies that enable high flexibility, high efficiency and low emissions.

The current trends towards utilization of data driven modeling (also called digital twins) and artificial intelligence, covering instrumentation, data gathering/storage and data analytics have been the corner stones of the methods and tools developed by the researchers at UiS energy group for the last decade. Data from locally operated units, such as micro gas turbines, internal combustion engines, fuel cells, as well as large-scale commercial power plants have been utilized for optimization of the plant instrumentation and condition monitoring to facilitate predictive and condition based maintenance, enabling higher availability and better plant economy. Access to data driven expert systems for optimum operation and maintenance of an energy system dominated by distributed generation is essential for successful transition of the current energy systems.

Given the fact that high flexibility, both from fuel and operational point of view, is of outmost importance for security of supply in an energy system dominated by intermittent renewable energy sources, the R&D activities within our energy group have been focused on further development of the real time monitoring capabilities for techno-economic optimization of carbon free energy conversion and power generation.

Experiences from data driven modeling and research on use of artificial intelligence approaches, based on Artificial Neural Networks (ANN) for optimum operation of distributed generation based energy systems were further enriched with implementation of smart sensors and automatic data filtering. Results from these studies were presented in a conference in Tokyo and in journal papers, currently under review. Results from previous studies concerning monitoring tools for distributed and centralized energy conversion units were presented in earlier reports.

The importance of further development of fuel flexible, low emission, small-scale technologies for distributed power generation resulted in establishment of a new EU-project, supported by the Marie Curie program, financing 15 PhD students from seven partner countries. The project Next Generation Micro Gas Turbines (Next MGT) started in January 2020, aiming at further development and commercialization of the micro gas turbine technology as dispatchable generation technologies supporting the electrical grid of tomorrow dominated by intermittent renewables. All aspects of the technology development from component to system level, as well as the techno-economic aspects of manufacturing and use of this technology will be studied in this project. The project website is currently under construction and will enable access to project details in near future.

Stavanger is the petroleum capital of Norway and UiS is recognized for its strong position in petroleum related R&D. A local initiative was launched at UiS last year, aiming at supporting knowledge transfer from petroleum to renewable energy. Given the fact that geothermal energy as the renewable energy available everywhere and the strong synergies between petroleum and geothermal energy, e.g. geology, drilling, well construction, reservoir modeling, etc., the Faculty of Science and Technology at UiS established a program area on geothermal energy, led by professor Assadi, to enhance knowledge transfer between petroleum and renewable energy. The program area is a multi-disciplinary forum that engages many researchers from various fields to support commercial

development of the geothermal energy technologies.

The North Sea region has been identified as the energy hub of Europe, with both large investments in petroleum infrastructure and large potential for renewable energy generation. Within an EU-financed project, Energy System in Transition (ENSYSTRA), the potential of an integrated energy system in the North Sea region is being investigated from various points of view. The project, supported by Marie Curie training program, finances 15 PhD students from six partner countries, who are investigating the energy transition in North Sea region from different dimensions. System modeling and analysis, technology, economy and social aspects of the energy transition in the North Sea region are investigated in this project. For more information, readers are referred to http://www.ensea.eu.

The R&D activities dealing with fuel flexible and carbon neutral power generation technologies were reported in previous reports. Increased share of intermittent renewable energy, i.e. wind and solar energy, in the European energy system in combination with growth of number of electrical vehicles have increased the interest and need for distributed power generation and the impact analysis on the electrical grid. Using biogas as fuel backed up with natural gas as transfer fuel, in small-scale power conversion technologies, namely micro gas turbine, internal combustion engine and solid oxide fuel cells was investigated both experimentally and theoretically within a nationally funded project. This resulted in development of validated mathematical models as well as data driven ANN based models that can support further development of the distributed fuel flexible technologies.

$CO_2$ capture, utilization and storage have been considered as an important measure to realize carbon neutral energy systems. A research group at UiS, led by associate professor Mahmoud Khalifeh has recently patented a technology, called safe rock that is providing a carbon free replacement for cement. The preliminary tests have revealed the safe rock can also absorbed considerable amount of $CO_2$.

Utilization of low temperature heat sources and industrial waste heat for heat and power generation has been studied by the UiS energy group to provide better understanding of the economic potential of waste heat utilization. Validated models for waste heat utilization from aluminum industry were developed based on experimental data from test cell setup [36-40]. The current development in this field is focusing on utilization of geothermal energy and the knowledge transfer from the petroleum sector, especially drilling technology and well integrity, which has resulted in establishment of a multidisciplinary research group at UiS, consisting of experts from petroleum engineering, material science, energy conversion technology and socio-political science. Preliminary results of this multidisciplinary research initiative are expected in 2018.

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# Mechanistic-Empirical Analysis of Geogrid-Stabilized Layered Systems

## by Jie Han, Member EUAS

Short Biography

*Dr. Jie Han is the Glenn L. Parker professor of geotechnical engineering at Department of Civil, Environmental, and Architectural Engineering at the University of Kansas in the United States. He received his BS and MS degrees in geotechnical engineering from Tongji University in China in 1986 and 1989, respectively and then became a faculty member in Department of Geotechnical Engineering at Tongji University until 1993. He received his MS and Ph.D. degrees in Civil Engineering from the Georgia Institute of Technology in 1995 and 1997, respectively. Dr. Han worked as a design engineer, senior engineer, and then a manager of technology development at Tensar Earth Technologies, Inc. from 1997 to 2001. He has been a professional engineer in Georgia since 1998. Dr. Han became an assistant professor at Department of Civil Engineering at Widener University from 2001 to 2004 and was promoted to an associate professor in 2004. Dr. Han joined the University of Kansas as an associate professor in August 2004 and was promoted to a full professor in 2010. He has graduated 19 Ph.D. students and 19 MS students. Prof. Han's research and practical experiences have dealt with geosynthetics, ground improvement, pile foundations, buried structures, and roadways. He has conducted extensive research on geogrid, geocell, and geotextile-stabilized unpaved and paved roads more than twenty years. Prof. Han is the sole author of the book entitled "Principles and Practice of Ground Improvement" published by Wiley, has coauthored three technical books, edited or co-edited four ASCE Geotechnical Special Publications, and published more than 400 peer-reviewed journal and conference papers. Dr. Han has given more than 200 keynote or invited lectures or offered short courses in Australia, China, Colombia, Egypt, India, Israel, Japan, Kazakhstan, Korea, Malaysia, Mexico, New Zealand, Panama, Peru, Singapore, Thailand, the United Kingdom, and the USA. He, as one of two young geotechnical engineers representing China, attended the first Asian Young Geotechnical Engineers Conference held in Thailand in 1991. He was one of sixteen invited Top Name Speakers for the 1999 ASCE/Pa DOT Geotechnical Seminar. Prof. Han served as the Technical Co-chair and Proceedings Editor-in-Chief for the ASCE Geo-Institute Annual Conference – GeoFrontiers 2011 held in Dallas, Texas, USA from March 13 to 16,* 2011; *the Secretary General and Technical Committee Co-Chair for the GeoShanghai International Conference held in Shanghai, China from June 6 to 8, 2006; the co-chair of the US-China Workshop on Ground Improvement Technologies held in Orlando, the USA on March 14, 2009 and in Shanghai, China on May 27, 2018; the conference co-chair for the International Conference on Transportation Infrastructure and Materials held in Qingdao, China in 2017; and an international advisory board member, technical committee member, or session chair for a number of international conferences. He was a guest editor for the Southeast Geotechnical Engineering Journal and Geotextiles and Geomembranes and is an Associate Editor for the ASCE Journal of Geotechnical and Geoenvironmental Engineering and the ASCE Journal of Materials in Civil Engineering, a handling editor for the Transportation Research Record, and a member of the Advisory Board/Editorial Panel of the International Journal of Geomechanics, the Editorial Board of International Journal of Geomechanics and Geoengineering, Geosynthetics International, Transportation Geotechnics, and Transportation Infrastructure Geotechnology, and Ground Improvement.*

*He is the council member of the International Geosynthetics Society, the chair of the ASCE Soil Improvement Committee, the research coordinator for the Transportation Research Board (TRB) Earth Works Committee, and the member of the ASCE Geosynthetic Committee and the TRB Culverts and Hydraulic Structures Committee. He was the vice president of the International Association of Chinese Infrastructure Professionals from 2011 to 2015 and the president from 2016 to 2017. Prof. Han has received a number of research grants as a principal or co-principal investigator from the National Science Foundation, the Strategic Highway Research Program (SHRP) 2, the National Cooperative Highway Research Program (NCHRP), the Federal Highway Administration, Kansas Department of Transportation, Kansas University Transportation Research Institute, Delaware Transportation Institute, the University of Kansas, Widener University, and the geosynthetics and ground improvement industries. His total research funding as a principal or co-principal investigator has been nearly 9.0 million U.S. dollars. Prof. Han received the Short-Term Invitation Fellowship for Research in Japan from the Japan Society for the Promotion of Science (JSPS) in 2002. He was the recipient of the 2006, 2009, 2015, and 2018 Bellows Scholar Awards, the 2008, 2011, 2012 and 2014 Miller Scholar Awards, the 2007 Miller Professional Development Award for Distinguished Service to the Engineering Profession, and the 2019 Henty E. Gould Award for Distinguished Service in Academic Advising from School of Engineering at the University of Kansas. Prof. Han received the Best Paper Award in Soil Mechanics from the U.S. Transportation Research Board in 2008, the 2011 Shamsher Prakash Prize for Excellence in Practice of Geotechnical Engineering (cited for advancements in geosynthetic–reinforced earth structures and ground improvement), the International Geosynthetics Society (IGS) Award in 2014 for the contribution toward the development of design procedures for geosynthetics-reinforced paved and unpaved roads and for the expansion of road design procedures to include geocells, the 2014 Associate Editor of the Year Award from the ASCE Journal of Geotechnical and Geoenvironmental Engineering, the 2014 Fumio Tatsuoka Best Paper Award by the Transportation Infrastructure Geotechnology journal, the Best of the Best Presentation Award at the ASCE GeoStructures Congress in Phoenix, Arizona in 2016, the 2016 Design and Construction Group Practice Ready Paper Award from the U.S. Transportation Research Board, the 2017 ASCE Martin S. Kapp Foundation Engineering Award, and the ASCE Kansas City Section 2018 Civil Engineer of the Year Award. He was the Sun Jun Lecturer at Tongji University in China in 2012, the State of the Practice Lecturer at the 21st Annual George F. Sowers Symposium in Atlanta, USA in 2018, and the 18$^{th}$ IGS UK Invitation Lecturer at the Institution of Civil Engineers, London, UK in 2018. Prof. Han was elected to the ASCE Fellow in 2014.*

## Mechanistic-Empirical Analysis of Geogrid-Stabilized Layered Systems: Part I. Solutions

Xiaohui Sun and Jie Han

### Abstract

It is well known that the mechanisms of geogrid in stabilizing base courses over subgrade include lateral restraint and tensioned membrane effects. However, no elastic solutions are available to quantify the responses of base and subgrade due to the effect of a geogrid. This study aimed to develop elastic solutions for geogrid-stabilized base courses over subgrade by considering lateral restraint and tensioned membrane effects. For the analysis of the geogrid-stabilized layered elastic system, lateral resistance and vertical support of

the geogrid were expressed as two external stresses determined by the vertical and lateral deformations. The external stresses were then applied at the interface of the two-layer elastic system as continuity conditions and the elastic solutions under a circular load in a cylindrical coordinate were developed according to the elastic theory. The solutions are able to simulate the elastic responses of the soil layers due to the effect of the geogrid, e.g., elastic strains, vertical stresses, and radial stresses. In addition, the lateral restraint and tensioned membrane effects can be separated by only applying the corresponding external stress at the interface. In the companion paper, the solutions are verified by test data and then discussed.

**Mechanistic-Empirical Analysis of Geogrid-Stabilized Layered Systems: Part II. Analysis**

Xiaohui Sun and Jie Han

**Abstract**

In recent years the mechanistic-empirical design method has become popular for pavement design. In the mechanistic-empirical design of geogrid-stabilized roads, the elastic solutions for the geogrid-stabilized layered system are necessary but not available yet. In the companion paper, the analytical solutions for the geogrid-stabilized layered system were derived according to the layered elastic theory and the mechanistic-empirical approach. In this study, the elastic responses (i.e., vertical stresses, radial stresses, and elastic strains) due to the effect of the geogrid were investigated based on these solutions. The analytical solutions were then employed to estimate the reduction of vertical stresses underneath the geogrid as compared with the measured results, which showed reasonable agreement. A parametric study was conducted to investigate the effect of lateral restraint and tensioned membrane on the elastic responses with the surface deformation under base thickness and base-to-subgrade modulus ratios. The results clearly show that the lateral restraint effect is more significant as compared with the tensioned membrane effect when a surface displacement is less than 75 mm, especially in a section with a relatively thick base course. The analytical solutions may be implemented in the mechanistic-empirical design of the geogrid-stabilized unpaved roads.

**Time-Dependent Field Performance of Steel-Reinforced High-Density Polyethylene Pipes in Soil**

Fei Wang, Jie Han, Deep K. Khatri, Robert L. Parsons and Ryan Corey

**Abstract**

Steel-Reinforced High-Density Polyethylene (SRHDPE) pipe was developed to overcome the disadvantages of steel and HDPE pipes. Considering long-term serviceability of buried pipes, time-dependent performance of SRHDPE pipes deserves investigation. In this study, three 8-m (26.2 ft) long SRHDPE pipes were installed in a trench in the field with a soil cover thickness of 0.9 m (3 ft). The backfill materials were well-graded Aggregate Base 3 (AB3) aggregate and poorly-graded crushed stone. A new concept of equivalent pipe stiffness factor was proposed to consider the large stiffness difference between pipe and soil for calculating the pipe deflection under the long-term condition. The test sections were instrumented with earth pressure cells, displacement transducers, and strain gauges

and monitored continuously for 680 days. Measured data indicated that earth pressures increased with time in both AB3 aggregate and crushed stone sections. Vertical Arching Factor (*VAF*) increased faster in the crushed stone section than that in the AB3 aggregate section. Pipe deflections in both sections increased with time. The maximum pipe deflections in the AB3 aggregate and the crushed stone sections were 0.3% and 0.4% of the pipe diameter at 680 days after installation, respectively. Strains of plastic valley, plastic cover, and steel ribs in both sections were all smaller than the AASHTO limit within 680 days. Finally, empirical relationships were developed for the *VAF* and the equivalent pipe stiffness factor to predict the performance of SRHDPE pipes at a given time.

**General Analytical Framework for Design of Flexible Reinforced Earth Structures**
Jie Han and Dov Leshchinsky

**Abstract**

Current design methods divide reinforced earth structures into walls and slopes by using an arbitrary face inclination of $70^o$ as the boundary. The required maximum strength of reinforcement computed for reinforced walls are significantly higher than that computed for reinforced slopes even if the inclination is practically the same. Presented is a general analytical framework for design of flexible reinforced earth structures regardless of the slope face inclination. In fact, the framework is consistent for any structural geometry and any applicable slope stability analysis although, for demonstration purposes, the simple Culmann formulation is utilized for simple geometry with zero batter. Using an adequate slope stability formulation, the required tensile resistance of reinforcement for a given layout is calculated so as to produce the same prescribed factor of safety anywhere within the reinforced zone. That is, using the design shear strength of the soil, the required reinforcement resistance along each layer is computed to fully mobilize this shear strength for all possible slip surfaces. That is, a baseline solution is produced for an ideal long-term strength of reinforcement at any location. Consequently, the required strength of the connection between each reinforcement layer and the facing unit can also be determined. This connection strength, however, assumes small facing units with negligibly small shear and moment resistance. Parametric study is conducted to demonstrate the reasonableness of the presented framework. It is shown that the required tensile resistance and connection strength depend on factors such as: reinforcement length, intermediate reinforcement, percent coverage, and quality of fill. When compared with the current AASHTO design for walls, the required maximum long-term strength of the reinforcement as well as the required connection strength in the proposed approach are substantially smaller.

**Analysis of Laterally Loaded Piles in Sand Considering Scour Hole Dimensions**
Cheng Lin, Jie Han, Caroline Bennett and Robert L. Parsons

**Abstract**

Scour is a process of soil erosion which can occur around foundations of bridges or offshore structures by the action of flowing water, thus reducing the capacity of the foundations and sometimes leading to the failure of the structures. During an analysis of

scour effects on laterally-loaded piles, the scour hole geometry is often ignored. Instead, scour effects are considered by simply removing the whole soil layer to the scour depth. However, a scour hole has not only depth, but also width and a slope. At present the widely-used *p-y* method for analyzing laterally-loaded piles cannot consider three-dimensional scour hole dimensions. For this reason, a simplified method was developed herein for the analysis of laterally-loaded piles in sand under a scour condition. The *p-y* curves in this method were based on a wedge type of failure. The effects of the scour hole dimensions on the response of laterally loaded piles in sand were evaluated using this simplified method. The computed results from the simplified method compared well with those from the three-dimensional finite difference method. Scour depth was identified as the most influential factor on the pile response when compared with scour width and scour hole angle. Based on the parameters investigated in this study, a model that removes the entire soil layer to the scour depth resulted in 49% to 68% higher ground line lateral displacements of the pile than a model that incorporates the three-dimensional scour hole dimensions.

**Numerical Analysis of Geosynthetic-Reinforced and Pile-Supported Earth Platforms over Soft Soil**

J. Han and M.A. Gabr

**Abstract**

Geotechnical engineers face several challenges when designing structures over soft soils. These include potential bearing failure, intolerable settlement, large lateral pressures and movement, and global or local instability. Geosynthetic-reinforced and pile-supported earth platforms provide an economic and effective solution for embankments, retaining walls, and storage tanks constructed on soft soils; especially when rapid construction and/or strict deformation of the structure are required. The inclusion of geosynthetic(s) in the fill enhances the efficiency of load transfer, minimizes yielding of the soil above the pile head, and potentially reduces total and differential settlements. A numerical study has been conducted to investigate pile-soil-geosynthetic(s) interactions by considering three major influence factors, such as the height of the fill, the tensile stiffness of geosynthetic, and the elastic modulus of pile material. While current methods have ignored important effects of the geosynthetic stiffness and pile modulus on the soil arching ratio, numerical results suggested that the stress concentration ratio and the maximum tension in geosynthetic increase with the height of embankment fill, the tensile stiffness of geosynthetic, and the elastic modulus of the pile material. The distribution of tension in geosynthetic indicated that the maximum tension occurs near the edge of the pile.

# Data Science with Integration of Methodology and Application Domain

## by Fionn Murtagh, Member EUAS

Short Biography

*1993, HDR (Habilitation à diriger des recherches), "Méthodes de reconnaissance des formes en astronomie" ("Pattern Recognition Methods in Astronomy"), Université de Strasbourg.*
*1981, PhD – Doctorat de 3ème cycle (Mathematical Statistics), "Classification et discrimination sous contrainte de contiguîté continue" ("Classification and discrimination subject to a continuous contiguity constraint"), Université P&M Curie, Paris 6, in collaboration with BRGM, Bureau de Recherches Géologiques et Minières, Orléans.*
*1979, MSc (Computer Science – Information Retrieval), Trinity College Dublin.*
*1976, BA (Mathematics), BAI (Engineering Science), Trinity College Dublin.*
*1972, Leaving Certificate (O'Connell's Schools, Dublin). Institute of Physics medal for First place in Ireland in Physics.*
*In secondary school, this included some months each summer in the national train engineering and production centre in Dublin, including a wide range of production and maintenance; in the Guinness brewery, in the Cadbury chocolate and food factory, in Dublin, and in Brown Boveri & Cie., in Baden, Switzerland, which later merged with Asea to become ABB, Asea Brown Boveri.*

**Biography with Career details**

**June 2017 to date: Professor of Data Science, University of Huddersfield, Director, Centre of Mathematics and Data Science.**

Director of a Centre that is to become an Institute of Mathematics and Data Science, and this can be based on the model of a Fraunhofer Institute. Courses include new BSc in Mathematics, MSc in Data Analytics, and soon an MSc in Industrial Mathematics.

I have been External Examiner in the University of Ulster, Northern Ireland, for the past few years, and I am External Examiner for Mathematics, Master and undergraduate degrees in University of Essex. BICDaS (Bielefeld Center for Data Science) Advisory Board Member, Bielefeld, Germany.

**May 2015 to 2017: Professor of Data Science, University of Derby, Derby** (0.8 FTE)**. Professor of Data Science, Goldsmiths, University of London** (0.2 FTE).

University of Derby: courses taught, for undergraduates, were Statistical Methods, and Advanced Analytics. Module lead on Advanced Analytics delivered at BAC International,

Dhaka, Bangladesh.
There have been company partners, a link with CERN, Rolls-Royce, Transport for London, and many more. In a metro station in London, a company that redeveloped the station used Vodafone mobile phone connectivity to have analysis of all people's travel. A KTP (Knowedge Transfer Partnership was started with SR4B, a retail and supply logistics data analytics firm, based Nottingham, and carrying out work for many retail companies, including Walmart in the US. For Goldsmiths, I continue to be a Visiting Professor. My MSc course was Geometric Data Analysis.

**Juiy 2013 to end 2014: Professor and Head of School, School of Computer Science and Informatics, De Montfort University, Leicester. 2015- Honorary Professor.**

The School of Computer Science and Informatics comprised 106 Professors, Lecturers, part-time lecturers, Research Fellows (all with teaching roles included). Research and commercialization income: £1.2 million per annum. Number of taught students in the School: 1151. For some MSc courses, Distance Learners were in the majority, relative to locally based students. The School also covered Mathematics, with a new undergraduate degree starting in Sept. 2014. The School had formal teaching course agreements with Hewlett-Packard (H-P), Deloitte, SAS, and also had a formal agreement with Airbus Group (formerly EADS) in the SCADA (supervisory control and data acquisition) security area. I had oversight of renewal of the H-P agreement, and I also had th Head of School post when the Airbus Group agreement was made. With the start of Horizon 2020 in 2014, about £9 million in grant proposals was submitted by my School. For MSc in Business Computing,
I was teaching SAS Analytics Programming, and in the 2nd semester 2013-2014, I did a short course on research methods, "Analysis of Questionnaires: Geometric Data Analysis for Interpretation and Communication of Results".

In my listing of many conferences attended each year, and additional conferences where I am am a Programme Committee member, this has included summer schools in Estonia, in Romania, and short courses at conferences in Toyko, Japan, and in Marrakech, Morocco, and in Bologna, Italy,and in London, England. My listing of conferences is here:
www.multiresolutions.com/home/conf-socs-2015-2021.html

**2004 to June 2013, Professor of Computer Science, Royal Holloway, University of London (RHUL), 2005-2007, Head of Department, Department of Computer Science, RHUL** (Secondment at SFI, see below, 2007-2012.) **July 2013 onwards: Honorary Professor in Computer Science, RHUL, and Fellow CLRC, Computer Learning Research Centre.**

**Oct. 2007 – Oct. 2012, Director, Information Communications & Emergent Technologies Directorate, Science Foundation Ireland (SFI), Dublin.**

SFI is an autonomous agency within the Department of Jobs, Enterprise and Innovation, supporting research in universities and similar institutes in Ireland. I was directly responsible for the areas of ICT (Information & Communications Technologies), Mathematics, Energy, Materials Science and Nanotechnology, covering over half of SFI's multi-annual budget of about €1.5 billion. I wrote briefing notes to government Ministers on Cybersecurity, and in 2011 I contributed to the National Research Prioritisation Exercise, now implemented by government. I was a member of the (Government departments and agencies) Cloud

Computing Implementation Group. When SFI obtained its mandate for supporting Renewable Energies and Energy Efficient Technologies in May 2008, I built SFI work in this area from scratch, including running a SRC (Strategic Research Cluster) Progamme in energy in 2010.

I was, for a number of years, a member of: Industrial Research Commercialization Committee (Enterprise Ireland); Board of HEANet Ltd. (providing network infrastructure for schools and universities in Ireland); Finance Sub-Committee of HEANet Board; Climate Change Research Committee of Environmental Protection Agency; Scientific Advisor to the Irish European Space Agency Delegation. I represented SFI on: Smart Ocean Strategy Group; Ocean Energy Development Unit; Agency Steering Group on Silver Technologies. I provided expert advice to the Department of Enterprise on (European Union and other) Military Dual Control Regulation and Export Controls (in particular relating to encryption), and to the Interdepartmental Committee on Non-Profileration of Weapons of Mass Destruction. I was a member of the European Commission's National ICT Research Directors Forum. I was a member of the Governing Board of the JPI (Joint Programming Initiative) Urban Europe.

For the National Science Foundation (US): I was evaluation panelist for NSF's STC, Science & Technology Centers program (June 2012, December 2012). Now, 2020, I am a long time member of Research Councils in the UK, and I have been a member with a lot of work in Portugal and also for Research Council in Russia, in some other countries sometimes such as in Greece, Germany, Austria, The Netherlands, Canada, Chile, and so on. International Review of Computer Science in Finland, panel member, carried out for Academy of Finland, July 2007 (review of research of all university departments and labs in computer science and engineering in Finland). EU Framework Programme evaluator and evaluation panelist (few occasions in the past). Member of validation panel for Arab Open University Information Technology Program, held in Kuwait City, March 2007.

**1988-2007, Professeur Associé Sciences & Techniques (PAST – Adjunct Prof.), Astronomical Observatory, University of Strasbourg, France.**

Course taught each year in the DEA (1st year of PhD programme) now the second year of a Masters Degree, on Astrostatistics and related work, a few times also on wavelet transform in image and signal processing.

**1999-2004, Professor of Computer Science, Queen's University Belfast.**

In addition to my work in teaching and research, I developed networks in medical devices and Bioengineering: Executive Member of the Medical Imaging Forum of Northern Ireland (NI) Regional Medical Physics Agency; Council member of NI Biomedical Engineering Society. Founder of the Irish Machine Vision and Image Processing Conference series. Session organizer and proceedings editor of SPIE Opto-Ireland conferences in Galway, 2002; and Dublin, 2005.) Outcomes of my industry/government/finance/clinician work: 2 industry-funded research projects, at least 2 Framework Programme projects at any given time, and some national projects, including being a founder-member of the £9M Astrogrid.
I was one of the principals involved in the establishment of the successful: (i) Sonic Arts Research Centre, funded at £5M through SPUR, Support Programme for University Research; and (ii) ECIT, Institute of Electronics, Communications and Information

Technology, initially with £40M funding.

**1996-1999, Professor of Computing, Magee College, Derry, University of Ulster.**

Research and teaching visitor, University of Washington, each year for about 10 years in all, availing of US corporate and other (Office of Naval Research, ONR) funding for this. Active in various cross-border initiatives (e.g. Board member of ERNACT, a cross-border – Ireland and Northern Ireland – ICT industry/public sector consortium). I set up digital signal processing software and consultancy company, Multi Resolutions Ltd.

**1984-1996, Senior Scientist, Space Science Department, European Space Agency.**

Based at the European Southern Observatory (ESO), Garching/Munich, on the Hubble Space Telescope (HST) project. I participated in the origins and early development of many modern developments. This includes the growing domains of Astrostatistics, and Astroinformatics. I developed innovative image and signal deconvolution algorithms to cater for the spherically aberrated primary mirror on HST following the delayed (due to the Challenger space shuttle 1986 disaster) 1990 launch. By the summer of 1993, I set up and managed ESO's web site on two continents, Europe and South America. (The web as we know it effectively started in 1993.)

**1984, Scientist, Joint Research Centre, Ispra, Italy.**

I was working in the nuclear reactor safety division, on data analytics. (Event, Incident and Abnormal Occurrence data analysis.)

**1980-1984, Lecturer, Computer Science, University College Dublin.**

Teaching included: Algorithms and Data Structures. Mathematics for Computer Science. Introductory Computer Science for Engineering.

**1976-1978 (one year full-time, and then one year half time, because I was doing my MSc), Statistician-Programmer, Educational Research Centre, St Patrick's College, Dublin. (Now in DCU, Dublin City University).**

National level, norm-referenced and criterion-reference educational testing and analysis. Coverage: primary and secondary school system.

**Profile Summary**

Research in Data Science, Web Science, Open Linked Data, *Digital Content Analytics, Big Data*, *Computational Science*, including innovative models and paradigms from digital humanities and quantitative social sciences. I have been Head of School and Head of Department in UK universities, at important times relating to the national Research Evaluation Framework. When Director at Science Foundation Ireland, I advised Irish Government Ministers in various domains, and was responsible for the awarding of approximately 1 billion Euro in research funding. I have a strong track record in research with industrially-relevant consequences, and in teaching and learning. I am a global leader in research, and applications, of clustering and data analysis, computational statistics, and

modelling and statistical analysis in image and signal processing. For more than a decade, I have been Editor-in-Chief of the Computer Journal, the British Computer Society's flagship journal. Now I am section editor for Section C: Computational Intelligence, Machine Learning and Data Analytics. I am an Editorial Board member of many other journals. I have a leading role in classification societies: I am ex-President of the Classification Society of North America, now titled Classification Society, and a Board Member for many decades, and again now President of the British Classification Society, former council member of the International Association for Statistical Computing (IASC) and now a Council Member of International Statistical Institute, and of IFCS, International Federation of Classification Societies, as well as long term member, and Fellow of the British Computer Society, and a Fellow of many other organisations. I am a Board Member of EuADS, European Association of Data Science. I am an elected member of the scholarly academies, the Royal Irish Academy and Academia Europaea, and, here, EUAS, EU Academy of Sciences. I have been awarded Fellowships in many organisations, including: Institute of Mathematics and Its Applications, International Association for Pattern Recognition, Royal Statistical Society. I have approximately 300 published papers, and 30 books, and have been a lead investigator in winning about £60 million in research funding.

**Recent Award, Medal and Certificate**

Outstanding Contributions to Astrostatistics Award 2016. Awarded, May 2016, by: IAA Awards, International Astrostatistics Association. See:
http://www.cambridge.org/us/academic/international-astrostatistics-association-award-winners. Commendation: "For his long time contributions to astroinformatics and relatedareas in the computational sciences; advancing scientific knowledge in classification theory and image analysis; for his contributions to the success of the Hubble Space Telescope; for his role on the organizing committee of the IAU Commission B3 on Astroinformatics Astrostatistics; and for his long time efforts in dealing with the statistical analysis of "Big Data".
My publications can be seen here: http://www.multiresolutions.com/home/pubs.html
This is a very relevant book for my project planning and collaborations:
F. Murtagh, **Data Science Foundations: Geometry and Topology of Complex Hierarchic Systems and Big Data Analytics**, Chapman and Hall, CRC Press, 2017.

**A few recent articles include**

(1) F. Murtagh, "Health and Medical Analytics, through Analytical Focus and Contextualization, with new Challenges and Opportunities in the Context of Big Data", **EC Pharmacology and Toxicology**, 7(6), 488-493, 2019.
(2) F. Murtagh and G. Iurato, "Core Conflictual Relationship: Text Mining to Discover What and When", **Language and Psychoanalysis**, 7 (2), 1-26, 2018.
(3) F. Murtagh and K. Devlin, "The Development of Data Science: Implications for Education, Employment, Research, and the Data Revolution for Sustainable Development", **Big Data and Cognitive Computing**, 2(2), 14, 2018.
**(4)** F. Murtagh, "Data Mining and Big Data Analytics: Exploiting Resolution Scale, Addressing Bias, Having Analytical Focus", **International Journal of Computer and Software Engineering**, 3: 127, 2018.
**(5)** F. Murtagh, M. Orlov and B. Mirkin, "Qualitative Judgement of Research Impact: Domain Taxonomy as a Fundamental Framework for Judgement of the Quality of Research", **Journal of Classification**, 35(1), 5-28, 2018**.**

# Photon Generation by Electron Transfer Reactions at Electrodes and Development of Sensors

## by Kalathur Santhanam, Member EUAS

Short Biography

***Positions Present and Past***

| | |
|---|---|
| *2012-Present* | *Professor of Chemistry , Rochester Institute of Technology, Rochester, NY* |
| *2002-2012* | *Director of Materials Science and Engineering, and Professor of Chemistry, Rochester Institute of Technology, Rochester, NY, USA* |
| *2000-2002* | *Visiting Professor of Chemistry, Rochester Institute of Technology, Rochester, NY, USA* |
| *1998-2000* | *Consultant, Pactiv Corporation and adjunct professor at Rochester Institute of Technology, Rochester, NY, USA* |
| *1993-1998* | *Senior Professor, Tata Institute of Fundamental Research (TIFR), India* |
| *1990-1993* | *Professor, Tata Institute of Fundamental Research (TIFR), India* |
| *1982-1990* | *Associate Professor, Tata Institute of Fundamental Research (TIFR), Mumbai, India* |
| *1976-1982* | *Reader, Tata Institute of Fundamental Research (TIFR), Mumbai, India* |
| *1969-1976* | *Fellow, Tata Institute of Fundamental Research (TIFR), Mumbai, India* |
| *1968-1969* | *Visiting Fellow, Tata Institute of Fundamental Research (TIFR), Mumbai, India* |
| *1967-1968* | *University of Victoria, B.C., Canada* |
| *1964-1967* | *Welch Post-doctoral Fellow, University of Texas, Austin, Tx, USA* |
| *1963-1964* | *National Institute of Sciences of India (currently called Indian National Science Academy) Fellow, Sri Venkateswara University, Tirupati, India* |
| *1960-1963* | *University Grants Commission Scholar (UGC, New Delhi), Sri Venkateswara University, Tirupati, India* |
| *1958-1960* | *Demonstrator, Department of Technology, University of Madras, Madras, India* |

***Education***

| | |
|---|---|
| *B.Sc (Hons)* | *Major: Chemistry (First Class), Subsidiaries: Physics (First Class), Mathematics (First class)*<br>*Sri Venkateswara University, Tirupati, India* |
| *Ph.D.* | *Thesis: Controlled Potential Coulometric Oxidation of Organic Compounds, Sri. Venkateswara University, Tirupati, India*<br>*Work done under University Grants Commission Scholarship and National Institute of Sciences of India Fellowship.*<br>*Awarded the Best thesis of the Year.* |

***Visiting Positions***

| | |
|---|---|
| *1971-1973* | *Visiting Scientist, University of Michigan, Ann Arbor, MI, USA* |
| *1976* | *Research Associate, University of Texas, Austin, TX, USA* |
| *1979-1980* | *Visiting Professor, University of Guelph, Ontario, Canada* |
| *1980-1981* | *University of Texas, Austin, TX, USA* |
| *1982-1989* | *Visiting Scientist, University of Victoria, B.C., Canada* |
| *1986* | *Visiting Scientist, Brookhaven National Laboratory, USA* |
| *1989* | *Visiting Scientist, CNRS, Meudon, France* |
| *1989* | *Visiting Fellowship, British Council, Mumbai, India* |
| *1991-1992* | *Visiting Scientist, Paul Scherrer Institute, Switzerland* |
| *1998* | *Visiting Scholar, Rensselaer Polytechnic Institute, Troy, USA* |

***Professional and Academic Honors***

*Chairman, Bombay Association for Science Education (1981-'84)*
*Chairman, Society for Advancement of Electrochemical Science & Technology SAEST (Bombay) (1985-'92)*
*Member, Scientific Advisory Committee of Central Electrochemical Research Institute (1975-'76)*
*Member, Scientific Committee of Nehru Science Center (1983-'86)*
*Member, Asian Coordinating Group of Chemistry X, UNESCO, New Delhi (15-16 February, 1993)*
*Chairman, Bioelectrochemical Society of India (1990-1998)*
*Elected Full Member Sigma XI - The Scientific Honor Society of North America (1964)*
*Merit Certificate - Chemical Abstracts (1971)*
*Member Editorial board - Trans. SAEST, India (1973 -1984)*
*Recognized guide for Ph.D. degree- Bombay University, India (1984)*
*Member Editorial Board - Journal of Electro-Analytical Chemistry Bioelectrochemistry-Bioenergetics (1990 - 2002)*
*Invited speaker for Conducting polymer Energy Storage Systems-American Chemical Society Meeting, Washington D.C. (1992)*
*Prof. T.L. Rama Char Endowment Lecture - Electrochemical Society of India (1993)*
*Elected Corresponding Member of German Academy of Sciences - Sachsische Akademie der Wissenchaften (1995)*
*Golden Jubilee Fellow - UDCT, Bombay University (1995)*
*ABI Recognition Honorary Research Board of Advisors (2002)*
*Invitation to attend NSF-3-D Nanomanufacturing Workshop (2002)*
*Session Chairman-International workshop on Fuel Cell Technology for Advanced Vehicles, RIT (2002)*
*Chair the Carbon nanotubes session at the 203rd Electrochemical Society Meeting in Paris (2003)*
*Invited speaker in International Conference on Electroactive polymers (2007)*
*Certificate of Accomplishment by Commission for promoting pluralism (2007)*
*Honorable mention of Who is Who in USA (2008)*
*Invited speaker at Nanotube session of Electrochemical Society, Vancouver (2009)*
*Honorary member, Institute of Integrative Omics and Applied Biotechnology (IIOAB) (2009)*
*Certificate of appreciation for valuable contribution and dedicated service by American Chemical Society (2011)*
*Editor, Special issue, MDPI Journal Chemical Engineering (2018-2020)*
*Elected Member European Union Academy of Sciences (2020)*

***PUBLICATIONS***

*More than 200 papers in international journals*

***BOOKS PUBLISHED***

*Workshop on Electrochemical Instrumentation, SAEST(Bombay), 1985*
*(Co-authors: R. Sundaresan, M.K. Totlani)*
*Photoelectrochemical Solar Cells, Elsevier Science Publishers, Amsterdam, 1988 (co-, author: M. Sharon)*
*Ion-sensing Electrodes and Electrochemical Instrumentation, World*
*Scientific Publishers, Singapore-New Jersey- London, 1990 (Dedicated to my mentor Prof. A.J. Bard)*
*Metallic Corrosion (Co-editors: A.S. Khanna, S.N. Malhotra and M.K. Totlani); Wiley-Eastern, New Delhi, 1994*
*Introduction to Hydrogen Technology (co-authored: R. Press, A. Bailey,M.Miri and J. Takacs)*
*Wiley, NJ, 2009*
*Clean Energy: Hydrogen/Fuel cells Laboratory Manual, (co-authored: R. Press, A. Bailey, M.Miri and J. Takacs), World Scientific, Singapore, New Jersey, 2016*
*Introduction to Hydrogen Technology (co-authored: R. Press, A. Bailey, M.Miri and J. Takacs)*
*Wiley, NJ, 2017 (second edition)*

## Research

I started my research career at the University of Madras (now called Chennai) in Controlled potential electrolysis but had to move to Sri Venkateswara University when I was awarded the University Grants Commission Scholarship (UGC, New Delhi) to pursue this research under Dr. V.R. Krishnan, Ph.D. (Kansas). My interest grew in electrochemistry due to two distinguished scientists, Prof. A.N. Frumkin (Russian electrochemist, a nominee for Nobel Prize) and Prof. A.J. Bard (University Texas). When I presented my first paper on controlled potential oxidation of thiourea under the Chairmanship of Prof. Frumkin at Central Electrochemical Research Institute, he commented that it was a nice work. Later, this paper was published in Zeichrift fur physicalishe chemie [Zeitschrift fur Physikalische. Chemie (NF), 34, 312 (1962)] followed by another publication in American Chemical Society Journal [Anal. Chem., 33, 1493 (1961)]. Prof. Bard inspired me by his Analytical Chemistry Annual Reviews on Coulometry which led me to have an ambition to do post-doctoral research with

him. I succeeded in getting an opportunity when I completed my Ph.D. degree. At that time, organic electrochemistry was a hot area as techniques like electron spin resonance (ESR) were used to trap the intermediates in the mechanism of the ultimate formation of the products. We were interested in the generation of free radicals of aromatic hydrocarbons like diphenyl anthracenes and examining the possibility of the free radical anion and free radical cation to react to produce the excited state of the molecule that would result in the emission of photons. We succeeded electrochemically by pulsing experiments and ESR identifications in evolving a mechanism for the emission [J. Am. Chem. Soc., 87, 139 (1965), J. Am.Chem. Soc., 88, 2669 (1966); J. Phys. Chem.,70, 404 (1966); J. Phys. Chem., 71, 2223 (1967)]. While the general mechanism envisages that the free radical anion and free radical cation of the same hydrocarbon will have enough energy to produce the first excited singlet state of the molecule, energetically deficient reactions were also identified to produce the excited state through the triplet state of the molecule. To distinguish the two routes of formation of the excited state, efficiency measurements and magnetic field effects were explored [J. Chem. Phys., 58, 821 (1973); Proc.Ind. Acad., 80A, 194 (1974); Can. J. Chem., 53, 76 (1975); Pramana, 5, 339 (1975); Chem. Phys. Lett., 51, 442 (1977); J. Chem. Soc. Chem. Commun., 2409 (1994); Chem. Phys., 185, 113 (1994)]. A direct generation of emission of photons was discovered during electrolysis of a heterocycle, carbazole; this does not require a pulsing technique to be used [Fluorescence, Ed. G.G.Guilabault, Chapter 14, MarcelDekker, New York, 1967; Canadian Journal of Chemistry, 47(8),1355-1359, 1969; Can. J. Chem., 49, 3577 (1971)]

From the above studies involving artificial systems, I turned to examine the processes that result in the emission of photons in real systems such as earthworms and fireflies. There are several genera of earthworms but out of which only a few of them produce photons. Lampito Maurutii is a species that produce photons upon excitation. I had the opportunity to do initial work on the electrochemistry of biological molecules at the University of Michigan, Ann Arbor [, J. Am. Chem. Soc., 95, 5482 (1973); Bio electro chem. Bioenergetics, J. Electroanal., (2), 147 (1974); J. Electrochem. Soc., 121, 345 (1974); J. Am. Chem. Soc., 96, 1653 (1974); J. Electrochem. Soc., 121,1032 (1974); J. Am. Chem. Soc., 97, 5083 (1975); J. Am. Chem. Soc., 97, 2591 (1975)]. To understand the mechanism of living systems producing photons, electrochemical techniques, electroporation and incorporation of the isolated active center into a nonbioluminescent earthworm have been examined and accomplished [J. Electroanal. Bioelectrochem. Bioenergetics, 192(14), 405 (1985); J. Electroanal. Chem. Bioelectrochem. Bioenergetics, 211 (15), 341 (1986); Proc. Ind. Acad. Sci., 97, 479 (1986); J. Electroanal. Chem. Biolectrochem. Bioenergetics, 213(17), 105 (1987); J. Electroanal. Chem. Bioelectrochem. Bioenergetics, 253(19), 9 (1988); J. Electroanl. Chem. Biolectrochem. Bioenergetics, 253(19), 21 (1988); J. Biolectrochem., 32, 211 (1993); Charge transfer effect on coelomic cells in exalted bioluminescence of Lampito mauritii in "Charge and Field effects in Bio-system-3, Eds. M.J. Allen et al, Birkhauser Pub., Boston, p.169 (1992); Bioelectrochemistry and Bioenergetics; 43, 197 (1997)]. We introduced electrochemiluminescence and electrobioluminescence as a tool for analytical determinations [Ind. J. Phys., 51B, 446 (1977); J. Electroanl. Chem. Biolectrochem. Bioenergetics, 276(22),219 (1989); J. Electroanal. Chem. Bioelectrochem. Bioenergetics, 276(22),231 (1989); J. Biolectrochem. Bioenergetics,

40,59 (1996)].

**Organic Conducting Polymers**

Discovery of polycarbazole which is formed during electrochemiluminescence on the anode led to investigation of its properties [J. Power sources, 32, 1 (1990); J. Mater. Chem. (Royal Society of Chemistry, London), 2(9), 965 (1992); Synthetic metals, 28, 27 (1989); Mol Crystals & Liquid Crystals, 160, 103 (1988); J. Solid state Electrochem., 2, 123 (1998); J. Solid state Electrochem., 2, 99 (1998); J. Pure and Applied Chemistry (IUPAC), 70, 1260 (1998); Macro '98, 395 (1998); Advanced Mater., 11, 1028 (1999) ]. The developments in this area of activity led to construction of cotton fiber batteries and polycarbazole battery [Trends in Polymer Sci., 1, 284 (1993); Chem. Rev., 97, 207 (1997)].

**Carbon Nanotubes and Graphene**

The discovery of carbon nanotube opened up the possibility of its practical applications. We developed carbon nanotube electrode and demonstrated its potentiality for fast electron transfer reactions [J. Bioelectrochem. Bioenergetics, 41, 121 (1996); Advanced Mater., 11, 154 (1999); Nano Letters, 1, 77 (2001)]. Introduced nanodimensional reactions using carbon nanotubes [Int. J. Nanoscience, 1, 285, (2002); Int. J. Nanoscience, 1. 277, (2002); Fullerenes--Volume 13: Fullerenes and Nanotubes, 285-288 (2003); J. Nanosci. Nanotechnol. 14, 2679-2682 (2014); J. Nanosci. Nanotechnol. 14, 2842-2851 (2014) ] and sensors [Sensors and Actuators, B: Chemical B106(2), 766-771 (2005), J. Nanoscience and nanotechnology**,** 8, 1 (2008); Sensors and Actuators B 142, 147–151 (2009); Encyclopedia of Nanoscience and Nanotechnology, Vo. 24, p.249, (2011); J. Nanoscience and nanotechnology, 10,3799 (2010); J. Nanoscience and nanotechnology, 10,3799 (2010); Sensors and Actuators B 191, 545– 552 (2014)]. Graphene as a 2D material provided an opportunity for its usage as an electrode for sensor and thermal applications. We developed a new electrochemical method of making graphene and graphene quantum dots that could be used without the need for purification and applied it to sensors and thermal applications [Patent No. US 9,840,782 B2, December 12, 2017; MRS Volume 3, Issue 22 (Energy and Sustainability), pp. 1221-1228 (2018); MRS Advances 3,15-16 (2018): 825-830; Journal of The Electrochemical Society, 165, 5, B232-B239 (2018):. Journal of The Electrochemical Society, 163, 166 (2016); Journal of Power Sources, 332, 337-344 (2016); Journal of The Electrochemical Society, 163 (6),E166-E172 (2016); MDPI *Chemical Engineering* 3. 80 (2019)]. Currently, efforts are being made to develop greenhouse gas sensors and nanopipette electrodes with graphene to achieve higher resolutions.

# Global Potential Energy Surface for HO2+ Using the CHIPR Method

## by António Varandas, Member EUAS

Short Biography

*António J. C. Varandas obtained a degree in Chemical Engineering from University of Porto (1971), and a Ph.D. in Theoretical Chemistry from University of Sussex(1976) under the supervision of Professor John N. Murrell. After graduation, he joined the Department of Chemistry of Universidade de Coimbra, where he is Full Professor since 1988. He has recently been appointed Distinguished Professor at Qufu Normal University (China). With an impact factor of h=54 (by Google Scholar),he has published 430 papers, co-authored the first monograph in Molecular Potential Energy Functions (Wiley 1984), and 2 others in portuguese. He has received awards:Prize Artur Malheiros for Physics and Chemistry of Lisbon Academy of Sciences (1985), Prize Ferreira da Silva of Portuguese Chemical Society (2001), and Prize Stimulus to Excellence of Portuguese Ministry of Science, Innovation and High Studies (2004). He serves amongst others the editorial board of Journal of Theoretical and Computational Chemistry where he recurrently also acts as Editor. He has received honorific recognitions abroad, the most recent one in China where he was awarded in 2018 the Title of Shandong Provincial Distinguished Foreign Expert. In 2006, he was elected corresponding member of the Academia de Ciências de Lisboa and, in 2014, of the EU Academy of Sciences.*

1**. Gonzalez, M. Martinez, Varandas, A. J. C., Xavier, F. George D., Global Potential Energy Surface for HO2+ Using the CHIPR Method, J. Phys. Chem. A, 123, pp 1613-1621, 2019.**

**DOI: 10.1021/acs.jpca.8b12005**

**Abstract**

An analytical potential energy function for the title ion based on the combined hyperbolic inverse power representation (CHIPR) method and its characteristics are discussed at length in the present work. The curves of two diatomic ions, O2+ and OH+, are also obtained within the same approach. The model PES so obtained exhibits extraordinary flexibility in describing with subchemical accuracy even the weak topological features near the higher energy regions. Thus, structural properties predicted by the model may help spectroscopists who want to compare their experimental values with the ones from theory.

The relaxed PESs in various coordinates have been calculated by relaxing the O2 bond distance using the present model, thus throwing light on all the possible isomers and their interconversions. The latest estimates of IR frequencies for three vibrational modes have been compared with the computed frequencies using the present model, and the agreement seems encouraging.

**2. Rocha, C. M. R., Li, Jing, Varandas, A. J. C., Difficulties and Virtues in Assessing the Potential Energy Surfaces of Carbon Clusters via DMBE Theory: Stationary Points of C-kappa (kappa=2-10) at the Focal Point, J. Phys. Chem. A, 123, pp 3121-2130, 2019.**

**DOI: 10.1021/acs.jpca.8b11632**

**Abstract**

The previously reported potential energy surfaces (PESs) of ground-state singlet C3 and triplet C4 are here utilized as input for the construction of approximate cluster expansions for larger Cκ (κ = 5–10) species. Relying primarily on the double many-body expansion (DMBE) approach, global potentials are obtained by summing the total interaction energies of all atomic subclusters up to four-body terms. The notable capability of the final forms in predicting good estimates of the linear global minima and their thermochemical/structural properties may provide important insights into the structure-determining nature of the (2 + 3 + 4) terms. The main difficulties and virtues in assessing Cκ's via DMBE theory are analyzed and new prospects given for the construction of global reliable PESs for the target species.

**3. Varandas, A. J. C., CBS extrapolation of Hartree-Fock energy: Pople and Dunning basis sets hand-to-hand on the endeavour, Phys. Chem. Chem. Phys., 21, pp 8022-8034, 2019.**

**DOI: 10.1039/c8cp07847e**

**Abstract**

The Hartree–Fock (HF) energy is shown to be extrapolatable from subminimal, minimal, and extended basis sets. Unprecedentedly, it can be reliably extrapolated to the complete basis set limit (CBS) from as small as Pople's STO-2G up to the largest aug-cc-pVXZ basis sets of Dunning's correlation-consistent type and even more complete variants of such ansatzes. The approach is tested on a panoply of small, medium and large molecular systems. As a case study, extrapolation is shown to be particularly reliable and cost-effective (typically an order of magnitude more economical for similar accuracy) when employing a hybrid (STO-2G,extended) basis set pair. The additional cost relative to a single-point calculation with the extended basis set is of no significance. After training the novel scheme with a meager set of 18 systems (TS-18), four test sets covering from neutrals (TS-105) to neutrals plus cations (TS-26) and anions (TS-17), these involving up to third-row elements, as well as tetrapeptide conformers (TS-10) were utilized for its validation. Although the answer to the question of whether all basis sets converge to the same HF/CBS limit is a clear yes, that of whether they show the same convergence rate is open, an issue also examined in the present work. For systems involving atoms up to the

second-row of the periodic table the answer seems to be a clear yes, at least when using correlation-consistent basis sets, but it is shown to be a no when the study is extended to anionic systems containing third-row elements. For the latter, augmented correlation consistent basis sets display a faster, perhaps optimal, convergence rate. The implications of this in practice can hardly be anticipated. For example, it cannot be predicted a priori which of such basis sets will yield the best relative energies for those anions, although a logical expectation suggests it to be the augmented ones which turn out to display the fastest convergence. As a blind-test type illustration, the novel scheme is applied to the conformational analysis of 2 tetrapeptides with 5 conformers each, using from subminimal up to extended basis sets as large as cc-pV5Z and aug-cc-pVQZ. The (STO-2G,extended) results so obtained are predicted to be in very good agreement with the best data reported thus far

**4. Borges, Y. G., Galvao, B. R. L., Mota, V. C., Varandas, A. J. C., A trajectory surface hopping study of N-2(A(3)Sigma(+)(u)) quenching by H atoms, Chem. Phys. Lett., 764, pp 61-64, 2019.**

**DOI: 10.1016/j.cplett.2019.05.016**

**Abstract**

Quasiclassical trajectories have been run for N2A3Σu++H2S collisions allowing for electronic transitions through surface hopping. An accurate multi-sheeted representation of the $HN_2$ potential energy surface has been employed. For the rate constant at room temperature, we obtain 9.85±0.16×10-10cm3s-1, a value fivefold larger than the recommended experimental one. Unprecedently, we investigate the temperature dependence of the rate constant, and obtained an essentially flat Arrehenius plot. We estimate that the NH yield is at least one order of magnitude lower than the experimental upper limit.

**5. Alves, M., V., Goncalves, C. E. M., Braga, J. P., Mota, V. C., Varandas, A. J. C., Galvao, B. R. L., Quasiclassical Study of the C(P-3) + NO(X-2 Pi) and O(P-3) + CN(X-2 Sigma(+)) Collisional Processes on an Accurate DMBE Potential Energy Surface, J. Phys. Chem. A, 123, pp 7195-7200, 2019.**

**DOI: 10.1021/acs.jpca.9b03860**
Abstract

The predicted rate constants for C + NO and O + CN collisions in three potential energy surfaces (PESs) for the 2A′ state of the CNO molecule are compared using quasiclassical trajectories. Different temperature dependencies are obtained for the C + NO reaction, which are explained in terms of the long-range properties of the PESs. Recommended values and mechanistic details are also reported. For O + CN collisions, a better agreement between the theoretical results is found, except for temperatures below 100 K

**6. Rocha, C. M. R., Varandas, A. J. C., Accurate CHIPR Potential Energy Surface for the Lowest Triplet State of C-3, J. Phys. Chem. A, 123, pp 8154-8169, 2019.**

**DOI: 10.1021/acs.jpca.9b03194**

**Abstract**

We report the first global ab initio-based potential energy surface (PES) for ground-state triplet C3(3A′) based on accurate energies extrapolated to the complete basis set (CBS) limit, and using the combined-hyperbolic-inverse-power-representation method for the analytical modeling. By relying on a cost-effective CBS(D,T) protocol, we ensure that the final form reproduces all topographical features of the PES, including its cyclic-linear isomerization barrier, with CBS(5,6)-quality. To partially account for the incompleteness of the N-electron basis and other minor effects, the available accurate experimental data on the relevant diatomics were used to obtain direct-fit curves that replace the theoretical ones in the many-body expansion. Besides describing properly long-range interactions at all asymptotic channels and permutational symmetry by built-in construction, the PES reported here reproduces the proper exothermicities at dissociation regions as well as the spectroscopy of the diatomic fragments. Bound vibrational state calculations in both linear and cyclic isomers have also been carried out, unveiling a good match of the available data on C3(ã 3Πu), while assisting with IR band positions for C3(3A2′) that may serve as a guide for its laboratory and astronomical detection.

**7. Ghosh, S., Sharma, R,. Adhikari, S., Varandas, A. J. C., Fully coupled (J > 0) time-dependent wave-packet calculations using hyperspherical coordinates for the H + O-2 reaction on the CHIPR potential energy surface, Phys. Chem. Chem Phys., 21, pp 20166-20176, 2019.**

**DOI: 10.1039/c9cp03171e**

**Abstract**

Quantum dynamics of the H + O2→ O + OH reaction has been extensively studied on the adiabatic ground state of CHIPR [A. J. C. Varandas, J. Chem. Phys., 2013, 138, 134117] potential energy surfaces by employing a coupled 3D time-dependent wavepacket approach in hyperspherical coordinates. Calculations have been performed for all non-zero J values for various initial rotational states of the diatom [O2(v = 0, j = 1–5)]. State-to-state and total integral cross sections are calculated using fully converged reaction probabilities, where initial state selected and Boltzmann averaged thermal rate constants are also subsequently calculated. Moreover, a comparison of various reaction attributes obtained by using the fully close coupled approach with the ones obtained from the J-shifting approximation and extrapolation scheme is presented along with other theoretical results and experimental observations.

**8. Rocha, C. M. R., Varandas, A. J. C., A global CHIPR potential energy surface for ground-state C3H and exploratory dynamics studies of reaction C-2 + CH -> C-3 + H, Phys. Chem. Chem Phys., 21, pp 24406-24418, 2019.**

**DOI: 10.1039/c9cp04890a Abstract**

**Abstract**

A full-dimensional global potential-energy surface (PES) is first reported for ground-state doublet C3H using the combined-hyperbolic-inverse-power-representation (CHIPR)

method and accurate ab initio energies extrapolated to the complete basis set limit. The PES is based on a many-body expansion-type development where the two-body and three-body energy terms are from our previously reported analytic potentials for C2H(2A′) and C3(1A′,3A′), while the effective four-body one is calibrated using an extension of the CHIPR formalism for tetratomics. The final form is shown to accurately reproduce all known stationary structures of the PES, some of which are unreported thus far, and their interconversion pathways. Moreover, it warrants by built-in construction the appropriate permutational symmetry and describes in a physically reasonable manner all long-range features and the correct asymptotic behavior at dissociation. Exploratory quasi-classical trajectory calculations for the reaction C2 + CH → C3 + H are also performed, yielding thermalized rate coefficients for temperatures up to 4000 K.

**9. Varandas, A. J. C., Pansini, F. N. N., Optimal diffuse augmented atomic basis sets for extrapolation of the correlation energy, Int. J. Quantum Chem., article number e26135, 2019.**

**DOI: 10.1002/qua.26135**

**Abstract**

We seek correlation-consistent diffuse-augmented double-zeta and triple-zeta basis sets that perform optimally in extrapolating the correlation energy to the one-electron complete basis set limit, denoted oAVXZ and oAV(X + d)Z. The novel basis sets are method-dependent in that they are trained to perform optimally for the correlation energy at each specific level of theory. They are shown to yield accurate results in calculating both the energy and tensorial properties such as polarizabilities while not significantly altering the Hartree-Fock energy. Quantitatively, complete basis set limit (CBS)-/(oAVdZ,oAVtZ)-extrapolated correlation energies typically outperform, by 3- to 5-fold, the ones calculated with traditional ansatzes of similar flexibility. Attaining energies of CBS/(AVtZ,AVqZ) type or better accuracy, they frequently outperform expensive raw explicitly correlated ones. Promisingly, a limited test on CBS-extrapolated energies based on conventional basis sets has shown that they compare well even with extrapolated explicitly correlated ones. Calculated atomization and dissociation energies, molecular geometries, ionization potentials, and electron affinities also tend to outperform the ones obtained with traditional Dunning's ansatzes from which the new basis sets have been determined. The method for basis set generation is simple, and there is no reason of principle why the approach could not be adapted for handling other bases in the literature.

**10. A.J.C. Varandas, J. da Providência, and J.P. da Providência, Binding of muonated hydrogen molecules and Born–Oppenheimer approximation revisited,** Canadian J. Physics, Art: cjp-2019-0061

**Abstract**

The stability of four fermionic particles with unit charge, of which two are positively and two negatively charged, is discussed. Except for using the simplest approximation of a single Gaussian orbital per particle, the problem is exactly solved variationally by varying the masses to simulate molecular di-hydrogen, mono-muonated di-hydrogen, and di-muonated dihydrogen. We illustrate the celebrated Born–Oppenheimer approximation 2

years after the occasion of its 90th anniversary. It is suggested that this method is valid only for di-hydrogen.

**11.** C.M.R. Rocha and A.J.C. Varandas, **A general code for fitting global potential energy surfaces via CHIPR method: Triatomic molecules,** Computer Physics Communications,

**Abstract**

A general program to fit global potential energy surfaces of ABC, AB2, and A3 triatomic molecules to ab initio points is reported. It is based on the Combined-Hyperbolic-Inverse-Power-Representation (CHIPR) method. The final form describes all dissociating fragments, long-range and valence interactions, while warranting the system permutational symmetry. The code yields as output a Fortran 90 subroutine that readily evaluates the potential and gradient at any arbitrary geometry.

**12. V. C. Mota, B. R. L. Galvao, D. V. B. Coura, and A. J. C. Varandas, Accurate Potential Energy Surface for Quartet State HN2 and Interplay of N(4S) + NH(X̃3Σ−) versus H + N2(A3Σu +), Reactions**

**Abstract**

A global potential energy surface for the lowest quartet state of HN2 is reported for the first time from accurate multireference ab initio calculations extrapolated to the complete basis set limit using the double many-body expansion method. All its stationary points are characterized, with the lowest quartet of HN2 predicted to have a bent global minimum 36 kcalmol−1 below the N(4S) + NH(X̃3Σ−) asymptote, from which it is barrierlessly achievable. The entire set of calculated ab initio points has been fitted for energies up to 1000 kcal mol−1 above the global minimum with an RMSD of 0.89 kcal mol−1, a gap comprising all identified stationary points. Special care is taken in modeling the involved long-range forces and cusps caused by crossing seams. The novel PES prompts for the calculation of rate constants for several unexplored reactions that are relevant for combustion, plasma, and atmospheric chemistry

# New Contributions of Robotics for Societal Services

## by Aarne Halme, Member EUAS

Short Biography

*Aarne Halme is emeritus professor of Aalto University (before Helsinki University of Technology), Finland, and Chairman of the Board of GIM Ltd. His background is in control and systems engineering. He started academic carrier in 1972 as an associate professor of control engineering at Tampere University of Technology. In 1977 he moved to Oulu University, where he was professor of control and systems engineering. From 1986 until retirement he has been professor of automation technology at Helsinki University of Technology, where the period 2008-2013 he was the head of the Academy of Finland Centre of Excellence in Generic Intelligent Machines. After retirement 2014 he established with his colleagues GIM Robotics company (www.gimltd.fi), which continues the activities of the Excellence Centre on commercial bases. He has made both theoretical and practical research in many fields of systems science and automation. Since mid 80's he has worked actively with intelligent field and service robotics research including development of mobility means, like walking and hybrid mechanisms, navigation and perception systems, and interactive human robot interfaces. His scientific interest includes also new energy technologies especially fuel cell systems intended to use in mobile devices. Publishing includes more than 200 articles in scientific journals, conference and books*

My interest in robotics is in the field and service robotics. This genre of robots comprises robotic machines that work outside factories replacing people in tasks, which are monotonous, dangerous or do not any more fulfill the minimum requirements for human work. The robots operate often in an environment unfriendly for humans or offer help or entertainment services to people in their homes and public places. Task scenario usually includes an environment, which is not well structured, not a priori known in details and may be changing with time. Often high autonomy is needed. Such environments are typical also for biological species that often act as models for engineering designing. In most cases robots must be mobile, because tasks cannot be moved to the robots (like in factories), but robots must move to the tasks. Research and development of field and service robots has been active since mid 80s and we have seen many interesting robots in media.. It is important to note that appearance of those robots may vary a lot depending on their application field, size and tasks they are intended. Human like robots are rather exceptions than the rule. Many field robots are designed by automating existing work machines. In the figure below some of those robots are visualized.

**In field robotics** applications vary from farming, construction and utilization of natural resources like mining, to exploration of planetary system (moon, planets, asteroids). Important application area is also undersea operations, where robots replace people in deep waters. **In service robotics** home services, entertainment, disabled support, replacing manpower in human-intensive non-industrial work in offices, hospitals, public places, hostile urban environment (cleaning streets, sewers etc) are the main application areas. Outside normal civil tasks military technology, rescue operations and catastrophe aftercare use increasingly robots today.

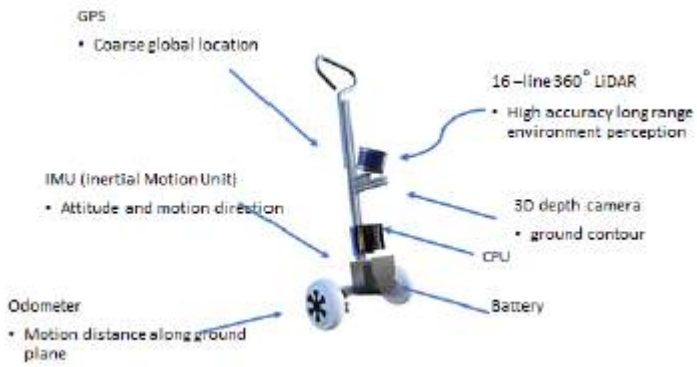
There are two main challenging technological steps in modern robotics in its way from factories to among people. The first to be taken is to obtain fluent mobility in unstructured, changing environment, and the second is to obtain the capability for intelligent communication with humans together with a fast, effective learning/adaptation to new work tasks. The first step has almost been taken today. The rapid development of sensor technology – especially inertial sensors and laser scanners or LiDARs (Light Detection and Ranging) – with constantly increasing computer processing power allowing heavy image processing, and techniques for simultaneous localization and mapping (SLAM), have made it possible for robot technology to enter in the same areas with humans. However, if we compare the present capability of robots to animals, like our pets in homes, it can be said without no doubt that improvements are still possible and desirable. The second step is still far away. The bottlenecks are the human – robot interface (HRI) and the robot intelligence, which are strongly limiting both the information transfer from the user to the robot as well as the learning of new tasks.

Despite huge efforts in Artificial Intelligence (AI) and robotics research, the word “intelligence” has to be written today in quotes. Researchers have not been able to either model or imitate the complex functions of human brains or the human communication, thus today’s robots hardly have either the creativity or the capacity to think. The main requirement for a service robot HRI is to provide easy humanlike interaction, which on the one hand does not load the user too much and on the other hand is effective in the sense that the robot can be kept in useful work as much as possible. Note that learning of service robots new tasks is not counted as useful work! The interface should be natural for human cognition and based on speech and gestures in communication. Because the robot cognition and learning capabilities are still very limited the interface should be optimized between these limits by dividing the cognitive tasks between the human brains and robot “intelligence” in an appropriate way. The answer is to use multi-modalities i.e use all communication means natural to human to communicate the task to the robot. This means using audio-visual means together with traditional IT-communication means. The picture below illustrates a robot, called WorkPartner- a test bead in our lab, and a task (cleaning

snow from yard) we have used to research different means to communicate the task effectively on-line to the robot. In this case we utilize human cognition and common spatial awareness of the robot and the human. The key component in communication is a sign showing position and direction which the robot can read by camera vision. The software recognize the task details and control the robot after the human has marked off the area to be cleaned and gives voice commands define the details of the work (like where to heap the snow). By this way we avoid the time consuming use of map based configuring of the task which is be the traditional way doing it.

During last ten- fifteen years there has been growing interest to use robotics in **societal services** to support activities like senior citizens living in their homes, disabled persons mobility, guarding and security in public places, only to mention a few. Basically the tendency is to increase the level of automation but in a way that fits to peoples living environment. In all these applications the human user is very close to the robot and the meaning of the interface is crucial in successful cooperation. In many cases it is useful to use multi-modalities in communication, i.e. speech, haptics and gestures in addition to traditional keyboard type of interfaces. It is also important to balance the human decisive actions with the robot own "intelligence". In addition to avoid unwelcome development in artificial intelligence we can often reduce significantly size of the robot software. This in turn means usually increasing reliability and decreasing price of the robot as a product.

Currently my interest in this genre of robots is focused to developing a guide robot for visually impaired people. It is a robot that functions like today's trained guide dogs providing the guiding services when blind people move outdoors on their practiced routes. Why a guide robot? Based on WHO statistics in EU alone there are 2,55 Million fully blind people who need assistive seeing guide to move in their everyday life. Unfortunately there exist today only two possibilities for such a guide: another person or a trained guide dog. Those both are of extremely shortage, which means serious limitation to activities of visually impaired people. The guide robot we are currently developing in GIM Robotics will remove this shortage. It performs about the same functions than a guide dog, but as a technical device it can be produced according to the need and it fits also to those people who cannot keep an animal. The robot prototype, called RoboGuide, is illustrated in the picture below with its main components.



The RoboGuide helps the visually impaired user to find a passable path by pulling with a slight force like a guide dog. LiDAR sensor and camera replace the dog's eyes. The picture on the right illustrates LiDAR temporal scanning information. The user is in the middle and talking with another person while a bicycle is passing.

Guide dogs are specially trained, selected dogs and their training and administration is expensive.. A dog is also a pet, the robot can't and should not compete in this role. On the other hand, a robot as a technical device does not commit the user in the same way as a dog. The benefits of robot technology are economy, easy duplicating, precision with modern sensor technology and many additional services that can be built into the system.

**Related Publications**

Harmo P., Taipalus T., Knuuttila J., Vallet J., Halme A., Needs and Solutions - Home Automation and Service Robots for the Elderly and Disabled , 2005 IEEE/RSJ International Conference on Intelligent Robots and Systems, 2005

Halme A., Leppänen I., Suomela J., Ylönen S., Kettunen I., WorkPartner: Interactive human-like service robot for outdoor applications, International Journal of Robotics Research ,22, 7-8 SPECIAL ISSUE, 2003

Halme A., Common Situation Awareness as Basis for Human-Robot Interface, Climbing and Walking Robots pp 3-18, Springer,2006

Heikkilä M., Terho S., Hirsi M., Halme A., Forsman P., Using signs for configuring work tasks of service robots, Industrial Robot ,33, 4, 2006

Halme A., Luksch T., Ylönen S. Biomimicing motion control of the WorkPartner robot, Industrial Robot , 31,2, 2004

Ylönen S.J., Halme A.J.,WorkPartner - Centaur like service robot, IEEE International Conference on Intelligent Robots and Systems , 2002

Suomela J., Halme A., Novel interactive control interface for centaur-like service robot, IFAC Proceedings Volumes (IFAC-PapersOnline), 15,1, 2002

Heikkilä, S., Halme A., Affordance-Based Indirect Task Communication for Astronaut-Robot Cooperation, Schiele, A., Journal of Field Robotics 29(4), 2011

# Electrochemical Surface and Interface Science of Applied Electrochemical Systems

## by Roland De Marco, Member EUAS

Short Biography

***Present Position(s):*** *Deputy Vice-Chancellor (Research and Innovation) at the University of the Sunshine Coast in the Office of Research and Professor of Chemistry in the Faculty of Science at the University of the Sunshine Coast since 2016 [preceded by Pro Vice-Chancellor (Research) from 2011 and 2015].*

***Role Strengths:*** *From July 2001 to December 2010, Roland De Marco contributed significantly to leadership and management at Curtin University progressing from Head of Chemistry to Dean of Research in Science and Engineering culminating with his past position of Associate Deputy Vice-Chancellor (Research Strategy). He is presently the Deputy Vice-Chancellor (Research and Innovation) at the University of the Sunshine Coast (from January 2016) after serving as the inaugural Pro Vice-Chancellor (Research) from 2011 and 2015.*

*Roland De Marco is an internationally recognized leader in the field of electrochemical sensors. His major strength is in the field of electrochemical surface and interface analysis, and he has a strong track record in the use of state-of-the-art electrochemical and surface analytical techniques in the micro- and nano-characterization of electrochemical devices.*

***Experience:***

***January 2011-December 2020:*** *Adjunct Professor in the Fuels and Energy Technology Institute at Curtin University*

***June 2015-June 2018:*** *Honorary Professor of Chemistry in School of Chemistry and Molecular Biosciences at The University of Queensland.*

***January-December 2010:*** *Associate Deputy Vice-Chancellor (Research Strategy) in the Office of Research and Development, Curtin University and Professor of Chemistry in the Department of Chemistry, Curtin University.*

***July 2007-December 2009:*** *Dean of Research, Faculty of Science and Engineering, Curtin University and Professor of Chemistry, Department of Chemistry, Curtin University.*

***July 2001-July 2007:*** *Professor of Chemistry and Head of Department in Chemistry at Curtin University.*

***February 1995-January 2011:*** *Lecturer, Senior Lecturer, Associate Professor, Professor in Chemistry at Curtin University.*

***March 1992-February 1995:*** *Lecturer in Chemistry at The University of Tasmania.*

***October 1990-March 1992:*** *Research Scientist at CSIRO Minerals.*

***Research Focus:*** *Major interest in the application of electrochemical sensors to environmental and clinical analysis. I am particularly interested in research leading to publications in high impact international journals, and knowledge transfer to industry and/or the government sector.*

***Leadership Focus:****The pursuit of academic excellence, so as to build internationally significant and competitive research capacity across the University. My modus operandi comprises leadership by example, "hands on" assistance to the research community, facilitation of scholarly excellence through high impact grants and publications, as well as the recruitment and retention of excellent research staff.*

***Major Awards and Prizes:***

*2008 RACI Analytical Chemistry Lloyd Smythe Medal for excellence in research, teaching and service to the chemical profession in Australia*

*1999 Curtin University, Centre for Educational Advancement Innovative Teaching Award*

*1989 Bloom-Guttmann Prize for the best presentation by a young electrochemist at the 10$^{th}$ Australian Symposium on Analytical Chemistry*

***Publication Summary:***

*142 Papers in International Journals and 2 Book Chapters at H-Index of 30 and field weighted citation impact (FWCI) of 2.03 (sourced from Scopus/SciVal on 6 March 2020)*

**Career Overview**

CI De Marco is an international leader in electrochemical surface and interface science of applied electrochemical systems, especially using cutting-edge ex-situ and in-situ synchrotron radiation, neutron and other materials characterisation techniques. Evidence of his standing in the field is that he is often invited to lead the electrochemical surface and interface science components of major national and international research programs with world leading international scientists, e.g., Swedish Research Council supported research on electrochemical sensors with A/Prof Gaston Crespo at KTH University, ARC Discovery Project grants on fuel cells and electrocatalysts with Prof San Ping Jiang at Curtin University, National Science Foundation China funded projects on corrosion with Prof Huang Yanliang at the Institute of Oceanology, Chinese Academy of Science, ARC funded research on novel organometallics with Prof Alan Bond at Monash University, European Commission FP7 International Research Staff Exchange Scheme (IRSES) supported project with Prof Eric Bakker at The University of Geneva and Prof Johan Bobacka at Abo Akademi University, and US NSF supported research on chemical sensors with Prof Ernö Lindner at The University of Memphis and Profs Martz and Barbeau at the University of California, San Diego.

**Honours and Awards**

CI De Marco won the 1989 Royal Australian Chemical Institute Bloom-Gutmann Prize for the best presentation by a young Australian electrochemist, and the prestigious 2008 Royal Australian Chemical Institute Analytical Chemistry Division Lloyd Smythe Medal for excellence in research in Analytical Chemistry. These are major national research prizes, and are a testimony of the high national and international standing of CI De Marco. Significantly, CI De Marco has won a career total in ARC and other grants to a value of over $15,000,000 in the general field of the surface and interface science of electrochemical systems, with a particular emphasis on the use of cutting edge materials characterisation methods.

**Research End User and Societal Impacts**

CI De Marco's research has achieved impacts beyond the realms of academia, as outlined below:

1) his CSIRO-based research into the role of minor elements in lead on the performance of lead/acid batteries has demonstrated that bismuth exerts a beneficial effect, and this positive outcome has enabled Pasminco Metals to refine its lead smelting process, eliminating the need for the costly de-bismuthization step;
2) the major outcomes of his research into the development of a copper electrochemical sensor for the analysis of seawater have been implemented by the US Office of Naval Research;
3) his Ondeo-Nalco sponsored ARC SPIRT Project led to a reliable quantitative structure activity relationship (QSAR) for oil field corrosion inhibitors, and has become a "gold standard" in the selection of active commercial corrosion inhibitors.

**Collaboration**

CI De Marco has a deep working knowledge together with excellent skills in the management of Industry/University partnerships as well as the pathways for adoption of technology that has been developed through research and development. Notable examples are CI De Marco's leadership on productive research partnerships with Woodside/Chevron, Water Corporation of Western Australia and the Alumina Technical Panel in the establishment of industry-engaged research centres at Curtin University, his work in establishing an industry-engaged National Centre of Timber Durability between USC, Forest Wood Products Australia, University of Queensland and DAF Queensland, and his work in establishing productive research partnerships between USC, Terragen Pty Ltd, Servatus Pty Ltd, Capilano Honey Pty Ltd and the Queensland Motor Accident Insurance Commission (MAIC) in delivering strategic basic research for these end user organisations.

**Publications – Summary data**

CI De Marco has 2 Book Chapters, 142 journal papers, his H-index is 30, and his field weighted citation impact or FWCI (2016-2019) is 2.03 (SciVal – 6 March 2020). On 6 March 2020, the Scopus database revealed that his papers had attracted 3,395 citations (i.e., average of 23.6 citations per article).

**Selected Key Publications**

1. Y. Cheng, S. Zhao, B. Johannessen, J.P. Veder, M. Saunders, M.R. Rowles, M. Cheng, C. Liu, R. De Marco, H.M. Cheng, S.Z. Yang and S.P. Jiang. Atomically Dispersed Transition Metals on Carbon Nanotubes with Ultra-High Loading for Selective Electrochemical Carbon Dioxide Reduction. Adv. Mater., 2018, 30, 1706287 (Cover
Page) [Impact Factor (IF)=25.809 and 120 citations].
2. L. Ge, Y. Yang, L. Wang, W. Zhou, R. De Marco, Z. Chen, J. Zou and Z. Zhu. High Activity Electrocatalysts from Metal-Organic Framework-Carbon Nanotube Templates for the Oxygen Reduction Reaction. Carbon, 2015, 82, 417 424 (IF=7.466 and 96 citations].
3. X. Li, Z.H. Zhu, R. De Marco, J. Bradley and A. Dicks. Evaluation of Raw Coals as Fuels for Direct Carbon Fuel Cells. J. Power Sources, 2010, 195, 4051-4058 (IF=7.467 and 109 citations).
4. X. Li, Z.H. Zhu, R. De Marco, A. Dicks, J. Bradley and G.Q. Lu. Surface Modification of Carbon Fuel Cells for Direct Carbon Fuel Cells, J. Power Sources, 2009, 186, 1 (IF=7.467 and 123 citations).
5. R. De Marco, J.P. Veder, G. Clarke, R. Chester, A. Nelson, K. Prince, E. Pretsch and E. Bakker. Elimination of Undesirable Water Layers in Solid Contact Polymeric Ion-Selective Electrodes, Anal. Chem., 2008, 80, 6731-6740 (IF=6.350 and 90 citations).
6. W. Durnie, R. De Marco, A. Jefferson and B. Kinsella, Structure Activity of Oil Field Corrosion Inhibitors, J. Electrochem. Soc., 1999, 146, 1751-1756 (IF=3.120 and 288 citations).

**Plenary, Keynote and Invited Talks**

CI De Marco has presented multiple invited papers at national and international conferences such as the ONR Workshop on Copper in Seawater at the US Naval Academy in Annapolis Maryland, Electrochemical Sensor conferences held in Matrafured Hungary, Pittcon conventions in the USA, EDRACI Electrochemistry Conferences in Australia, etc.

**Service and Discipline Involvement**

CI De Marco is a Fellow of the Royal Australian Chemical Institute (RACI), an elected

member of the EU Academy of Science (EUAS) and elected member of the American Chemical Society (ACS).
Notably, CI De Marco's high standing in the Australian Synchrotron scientific community is confirmed by his appointment as the Chairperson of the WA Synchrotron Users Committee (2008 to 2010), his selection as the inaugural Chairperson of the National Users Advisory Committee of the Australian Synchrotron (2009) and his Chairmanship of the Proposal Assessment Committee (PAC) for the soft X-ray beamline at The Australian Synchrotron (2015-2017). Similarly, he has been recognised for his high standing in the Australian neutron science community through his appointment to the AINSE Materials, Structures and Dynamics Specialist Committee (since 2010-2016). Since December 2007, he has also served on the Editorial Board of the Elsevier journal, Sensors and Actuators B: Chemical, and he presently serves as a handling Editor for the Elsevier journal, Sensing and Biosensing Research (2014-present). Furthermore, in 2018, CI De Marco was appointed as a non-Executive Director of the Board of AINSE Ltd, and was elected member of the Australian Synchrotron Stakeholders Committee presiding over the build of the next suite of beamlines associated with the BR-IGHT initiative.

**Mentoring and Research Training**

CI De Marco has supervised a number of PhD (17), Masters (2) and Honours (23) research students to completion, as well as 6 Research Associates. Many of his graduates/staff have built successful research careers. Here, CI De Marco has a strong record of producing graduates/mentees who have secured applied research jobs at CSIRO (e.g., Drs Pejcic and Veder from CU and Dr Lamb from USC), industry [e.g., Dr Durnie (Nalco, BP and Woodside), Drs Chan, John and Chuan (Woodside) and Dr Sohail (King Fahd University of Petroleum and Minerals)] as well as academia (e.g., Dr Veder at CU, Dr Alam at Oxford University, Dr Martin at UNSW, and Dr Lamb at Griffith University).

**Relative to Opportunity (where relevant)**

CI De Marco received his Doctor of Philosophy (PhD) in Chemistry/Physics from La Trobe University in 1992, and has been in full-time employment as a Researcher for 28 years since his PhD graduation. He has had no periods of career interruption.
From 2001 to 2007, CI De Marco worked as Head of Chemistry at Curtin University (50% leadership/management/administration, 25% teaching and 25% research). Despite this load, he built a productive research career and was promoted to full Professor in 2006.
From 2007 to 2010, he was Dean of Research (50% leadership and management as well as 25% for teaching and 25% for research) in Science and Engineering at Curtin University providing research leadership to over 300 staff across diverse disciplines.
CI De Marco was promoted to full-time Associate Deputy Vice-Chancellor (Research Strategy and Development) in 2010. This role elevated CI De Marco's research leadership to a University-wide level comprising 75% leadership/management as well as 25% research.

In 2011, he was appointed as Deputy Vice-Chancellor (Research and Innovation) at University of the Sunshine Coast, and his present role embodies 75% leadership and 25% research.

# Constitutive Model of Material Behavior

## by Viktor P. Astakhov, Member EUAS

Short Biography

*Viktor P. Astakhov, PhD, Dr. Sci. FSME*
*Tool Research and Application Manager – Research Professor*
*Production Service Management Inc – EWIE Group of Companies*
*Professor, St. Petersburg State Polytechnic University, St. Petersburg, Russia*

*Viktor P. Astakhov earned his PhD in mechanical engineering from Tula State Polytechnic University, Tula-Moscow, USSR-Russia, in 1983. He was awarded a DSci designation (Dr. habil., Docteur d'État) in 1991 and the title "State Professor of Ukraine" in 1991 for the outstanding service rendered during his teaching career and for the profound impact his work had on science and technology. An internationally recognized educator, researcher, and mechanical engineer, he has won a number of national and international awards for his teaching and research. In 2011, he was elected to the SME College of Fellows.*

*Dr. Astakhov currently serves as the Tool Research and Application Manager – Research Professor at Production Service Management Inc – EWIE Group of Companies and Professor, St. Petersburg State Polytechnic University, St. Petersburg, Russia. He has published monographs and textbooks, book chapters, and many papers in professional journals as well as in trade periodicals. He has authored the following books: Geometry of Single-Point Turning Tools and Drills: Fundamentals and Practical Applications, Tribology of Metal Cutting, Physics of Strength and Fracture Control, and Mechanics of Metal Cutting. He serves as associate editor of International Journal of Manufacturing, Materials and Mechanical Engineering (IJMMM) and International Journal of Machining and Machinability of Materials (IJMMM), board member, reviewer, and advisor for more than 20 international journals and professional societies.*

***Professional service***

- *Associated Editor, International Journal of Manufacturing, Materials and Mechanical Engineering – IJMMME*
- *Associated Editor, the International Journal of Machining and Machinability of Materials (IJMMM)*
- *Board Member, International Journal of Machine Tools and Manufacture*
- *International Editorial Advisory Board member, Machining Science and Technology, An International Journal*
- *Board Member, World Science Journal*
- *Advisory Board Member of the Open Mechanical Engineering Journal, Open Mechanical Engineering Reviews, and Open Mechanical Engineering Letters*
- *Board Member, Journal of Manufacturing Technology Research*
- *Honorary Board Member, International Journal of Automotive & Mechanical Engineering (IJAME)*
- *Board Member, ISRN Mechanical Engineering.*

***Major honors***

- *2018 Elected as a member of European Union Academy of Science*
- *2011 Elected to the Collage of Fellows of Society of Manufacturing Engineers*
- *2009 SME Certificate of Appreciation – Service Award*
- *2008 SME Certificate of Appreciation - Service Award*
- *2008 SAE Certificate of Appreciation - Award for substantial contribution to the SAE 2008 World Congress program*
- *2007 SME Certificate of Appreciation - Award for a substantial contribution to SME*
- *2006 SME James Beabers Lifetime Achievement Award, - In recognition for significant long term contributions to education, management and mentorship activities in SME.*
- *2006 SME Certificate of Appreciation - Award for a substantial contribution to SME*
- *2005 SME Certificate of Appreciation - Award for a substantial contribution to SME*
- *2004 SME Best Paper Award – The most valuable paper to the Manufacturing community*
- *2004 SME Certificate of Appreciation – Award for a substantial contribution to SME*
- *2003 SME Certificate of Appreciation – Award for service (training) to Manufacturing Community*
- *2000 SME Senior Member Certificate for Achievements in Advanced Manufacturing*
- *1999 ASME Certificate of Appreciation*
- *1998 Canada China Faculty Exchange Award.*
- *1997 ASME "Boss Award" – ASME Manufacturing Division leadership award*
- *1997 ASME Certificate of Appreciation.*
- *1994 "State Professor of Manufacturing Engineering" (The Education Ministry of Ukraine) for outstanding achievements in teaching and supervising of graduate students.*
- *1986 "State Researcher" (The National Research and Education Committee of U.S.S.R.) for excellence in university-based research.*
- *1986 Medal "Inventor of the USSR."*
- *1985 Bronze Medal for Achievements in Development of Industry of the Ukraine.*
- *1984 Bronze Medal for Achievements in Development of Industry of the USSR.*

**Current Research**

Structures in engineering applications are generally operated under complex loading conditions. An accurate prediction of potential failure for structures in numerical modeling requires abundant knowledge about materials deformation and fracture behavior under various loading conditions. This knowledge is synthesized in the so-called constitutive model of material behavior. A common problem is that a material model used in one particular loading condition may not be fully applicable for the others due to the loading difference. A material fracture model adaptable to various loading conditions is a key foundation for research of material mechanical response with numerical simulation analyses. Its development is of great significance in engineering applications.

Although a number of studies on material dynamic deformation has been conducted over recent decades, the modeling of material dynamic fracture strain considering the effect of strain rate has not been as extensive as that with the static fracture strain. One of the prime reasons is that, compared with the static or low

strain rate loading, the realization of high strain rate tests and subsequent modeling are more complex, time-consuming, and require an appropriate testing method/equipment. Among the above-mentioned fracture strain models, only the Johnson-Cook (hereafter JC) fracture strain model takes the strain rate into consideration. As a result, the JC fracture strain model is widely used in research of high velocity impact problems. However, the testing conditions for the calibration of the model parameters and the applicable range for JC model have not yet been well established. For example, it is not clear whether the material parameters of this fracture strain model calibrated within the strain rate order of $10^2$/s could be used in engineering applications with the strain rate higher than $10^3$/s. A general fracture strain model covering a wider range of strain rates will be helpful in solving the dynamic fracture problems. Moreover, the coupling effect between the strain rate and stress state on the material dynamic fracture strain is also unclear and urgent to be researched.

Dr. Astakhov current research aims at a better understanding of the deformation and fracture behavior of engineering materials, particularly in their manufacturing. A rectangular hat-shaped specimen has been developed to accommodate material deformation with different stress triaxialities. A technique combining SHPB test and high speed Digital Image Correlation (DIC) measurement has been developed. A comprehensive set of mechanical tests was performed, which covers strain rates from quasi-static to $10^3$/s and stress triaxialities ranging from−0.31 to 0.50. The fracture strain of Ti6Al4V as a function of a wide range of loading conditions was established. A general fracture strain model was proposed. The failure mechanisms at micro-scale for Ti6Al4V under varied loading conditions were investigated through observation of cross-sectional microstructure and fracture surface morphology. Currently, the influence of temperature on the material fracture is under active investigation.

See Wang B., Xiao X, Astakhov V.P., Liu Z. The effects of stress triaxiality and strain rate on the fracture strain of Ti6Al4V. Engineering Fracture Mechanics, Volume 219, 1 October 2019, 106627; Cheng, W., Outeiro J., Costes J-P, M'Saoubib R, Karaounic H., Astakhov V. A constitutive model for Ti6Al4V considering the state of stress and strain rate effects. Mechanics of Materials, Volume 137, October 2019, 103103.

# Structuring and Functionalization of Materials in Green Energies and Biosensing Systems

## by Changming Li, Member EUAS

Short Biography

*Professor, Research Institute Directors in both Suzhou University of Science and Technology and Southwest University, China; the Foreign Member of the European Academy of Science, the Foreign Member of Russian Academy of Engineering, the Fellow of the American Institute for Medical and Biological Engineering, the Fellow of Royal Society of Chemistry and the Fellow of International Thin Film Society.*

***Education***

*1987 Ph.D. in Electrochemistry, Wuhan University, China*
*1983 MS in Electrochemistry, Wuhan University, China*
*1970 BS in Chemistry, University of Science and Technology of China (USTC), China*

***Employment***

| | |
|---|---|
| *2018-present* | *Professor; Director of Institute for Clean Energies and Advanced Materials in Southwest University; Director of Materials and Devices in Suzhou University of Science and Technology, China* |
| *2013-2017* | *Professor; Dean for Faculty of Materials & Energy, Director of Institute for Clean Energies and Advanced Materials in Southwest University, China* |
| *2003-2012* | *Nanyang Technological University, Singapore: Professor, Head of Bioengineering Division, Director of Center for Advanced Bionanotechnology* |
| *1994-2003* | *Motorola, USA: Distinguished Member of Technical Staff, Senior Engineering Manager and Member of Science Advisory Board of Motorola* |
| *1991-1993* | *WPI, USA: Senior Staff Engineer and R&D manager* |
| *1989-1990* | *University of Illinois at Urbana-Champaign, USA, Postdoctoral Research Fellow* |
| *1987-1988* | *Wuhan University, China: Lecturer* |
| *1971-1979* | *Hubei Chem Inc. China: Engineer, Director of Technology Division* |

***Main Professional Achievement Highlights***

- *700+ peer-reviewed high impact SCI papers including Nature Mater, Nature Energy, JACS, Phys Rev Let, Nanolett, ACS Nano, Adv Mater, Adv Energ Mater, Adv Funct Mater, Environ Energ Science etc., 262 USA, Singapore and China patents, 184 plenary/keynotes presentations and 8 book chapters.*
- *SCI cites more than 37,000, H-index: 90, 17 SCI Highly Cited Scientific Articles, 70+ SCI papers cites are over 100 times.*
- *Thomson Reuters World's Most Highly Cited Researchers. 2108, 2019 - Clarivate Analytics World's Most Highly Cited Researchers and 2014, 2015, 2016, 2017, 2018 and 2019 Elsevier World's and Chinese Most Cited Researchers in Materials.*
- *Editor in Chief for Materials Report: Energy, Advisory Members of Nanoscales and Nanoscales Advances (RSC), Advisory Board Member of Joule (Cell)*
- *Main research area: Nanoscience and Nanoengineering, green energies including batteries, fuel cells, supercapacitors, solar cells, OER/HER, sensors/lab-on-a chip and bioengineering*

***Selected Awards and Honors***

1. *Fellow of the American Institute for Medical and Biological Engineering*
2. *Foreign member of the European Academy of Science*

3. *Foreign Member of Russian Academy of Engineering*
4. *Member of EU Academy of Science*
5. *Fellow of Royal Society of Chemistry*
6. *Fellow of International Thin Film Society*
7. *Member of American Electrochemical Society*
8. *Member of National Science Foundation Review Panel for Sensors, USA*
9. *Member of NIH Multidisciplinary Study Section, USA*
10. *Panel Member for China National Critical Research Program, China*
11. *Panel Member of the Review Panel for the President's Young Science Award, Singapore*
12. *Panel Member of Singapore NRF Grant, Singapore*
13. *Member of Singapore Medical Council (SMC) Complaints Panel*
14. *Member of Public Sector Funding Panel of the Science and Engineering Research Council, Singapore*
15. *Chinese National Award in Medical Science and Technology (2019)*
16. *Chinese National Innovation Award for Research and Industrialization (2017)*
17. *China National Overseas Master Professor Award (2012)*
18. *China National Overseas Chinese Innovation Award (2012)*
19. *Nanyang Research and Innovation Award, Singapore (2017)*
20. *Motorola Master Innovator Award, USA (1997)*
21. *Motorola Distinguished Innovation Award, USA (1994, 1995, 1996, 1998)*
22. *Australian National University Craig Visiting Professor, Australia (2012)*
23. *Honorary professor of University of Wollongong, Australia (2012).*
24. *Honorary Professor of University of Electronics Science and Technology of China (2015).*
25. *Honorary Professor of the Institute of Process Engineering, Chinese Academy of Science (2013)*
26. *Honorable Professor of Peking University, China (2004)*
27. *Honorable Professor of Wuhan University, China (2004)*
28. *Visiting Professor of Wuhan University, China (2004)*
29. *Member of Strategy Advisory Board of Institute of Chongqing Green & Intelligent Technologies, Chinese Academy of Science (2013)*
30. *University Senator and Senate Steering Committee Member of Nanyang Technological University, Singapore (2004-2011)*
31. *Senior Advisor for Institute of Science and Technology of Chongqing, China (2013)*
32. *Chairman for Chongqing Information and Biological Science Association (2016).*
33. *Chairman for Chongqing Association of Commercialization, Education and Research (2016).*

Prof Changming Li has been implementing astonish convergence using functionalization of materials in micro-nanoscales with micro-nano-bio integration to carry out interdisciplinary research in life sciences, biomedical engineering and green energies, which not only greatly contribute to fundamental science, but also significantly advances important practical applications. He has established a world-renowned education and research programs when he served as Division Head and his followed Dean and directors in the universities. In more detail, he intensively studied nanoscience and nanoengineering, by which, for example, he has innovated arts of nanoengineering such as self-assembly to construct unique structured interfaces in applications of green energies and biosensors (Fig.1) He has fundamentally investigated biomimetic sensing method by delicately design materials nanostructures while modifying the surface electronic structure with high bio-interactions for highly sensitive and selective enzyme-free biomimetic biosensing platforms, holding great promise for new generation of artificial intelligent biosensors and rendering scientific insights from investigations of the enhancement mechanisms (Fig. 2). He creatively employs soft materials to architecting superior intelligent micro-nanostructure for various applications. (Fig. 3). He has pioneered the droplet-based digital microfluidic system by enabling totally digitally control, operation and analysis for micro/nano-synthesis and digital lab-on-a chip (Fig. 4). To understand the efficient charge-

separation mechanism for photo/electro conversion, he has devoted to design various delicate high performance solar devices (Fig. 5). He has used synthetic biology investigated conductive microbes for direct electron transfer process while shedding lights on rationally designing pore structure to increase the power density of microbial fuel cells by almost 2 orders of magnitude (Fig. 6). He has intensively investigated batteries, fuel cells and solar cells as well as other energy storage devices, warranting many valuable patents and industrializing them, while exploring the electrode kinetics and thermodynamics insights (Fig. 7). He has also studied target drug delivery systems, producing high loading capacity and long release time of proteins drugs by nanoengineering state-of-the-arts layer-by-layer self-assembled nanoporous structures. Because of his contributions to Science, Engineering Practices and Technology development as well as his protruding services to the profession and society, he is highly recognized as a pioneer and leader in the field of nanotechnologies and applications in green energies/biosensing technologies with numerous prominent awards and as the most visible face in nanoscience and nanoengineering,

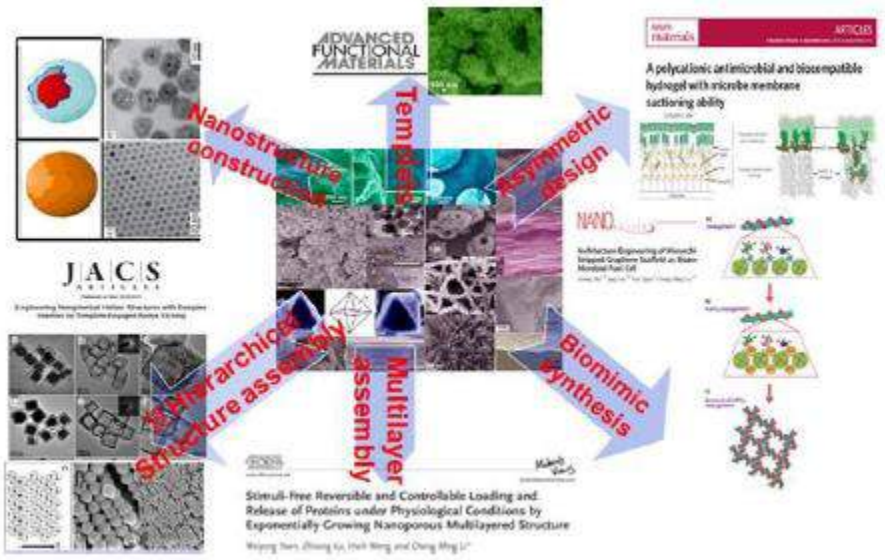



**Fig. 1** Self-assembly for unique structured interfaces

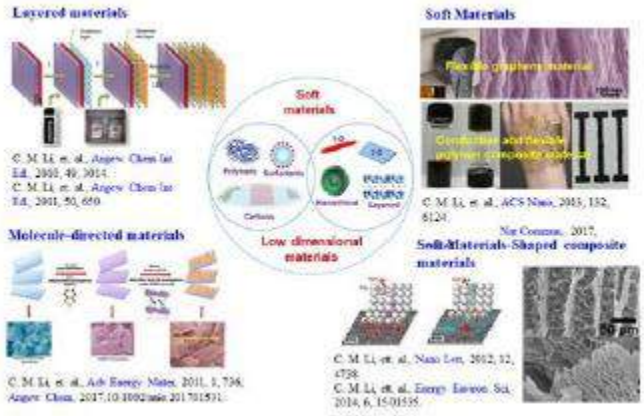



**Fig. 2** Soft materials-Architecting superior intelligent interfaces

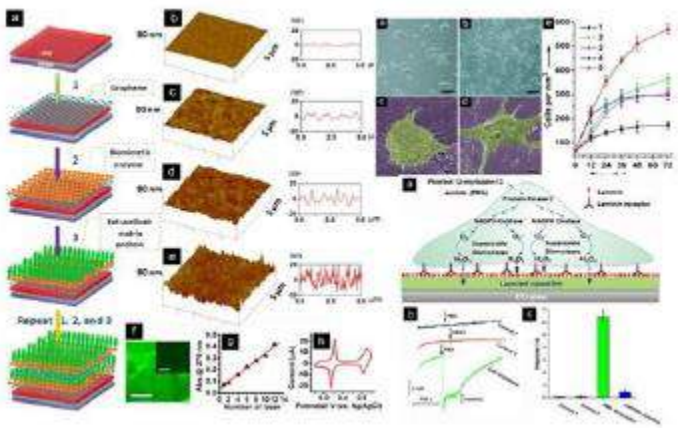


**Fig.3** Graphene-biointerface for amplified biomimetic molecular detection
(C. M. Li, et al, Adv Mater, 22, 5164-5167, 2010.)

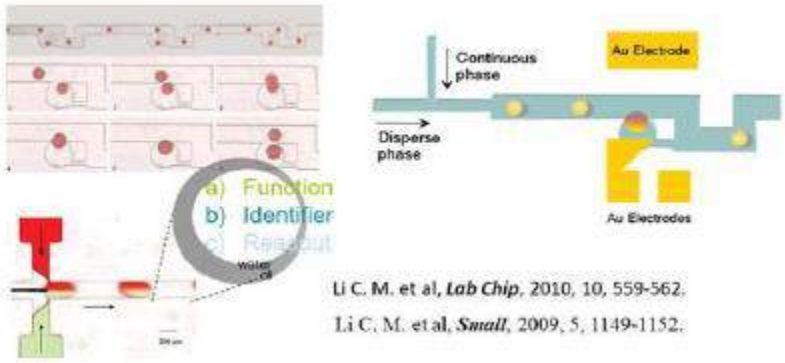



**Fig. 4** Droplet-based digital microfluidics

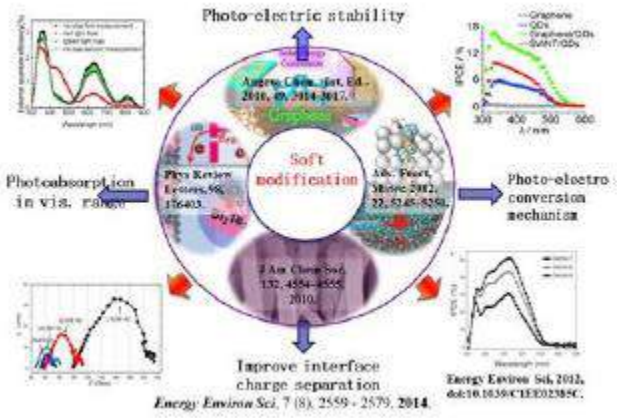



**Fig.5** Photo/electro conversion

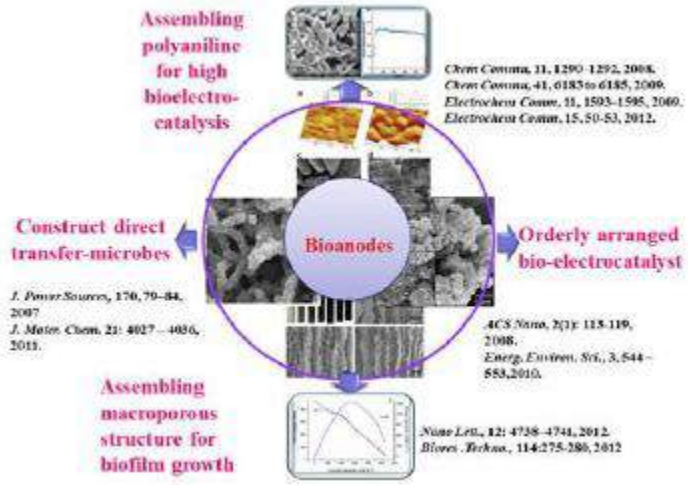



**Fig. 6** Biofuel Cells

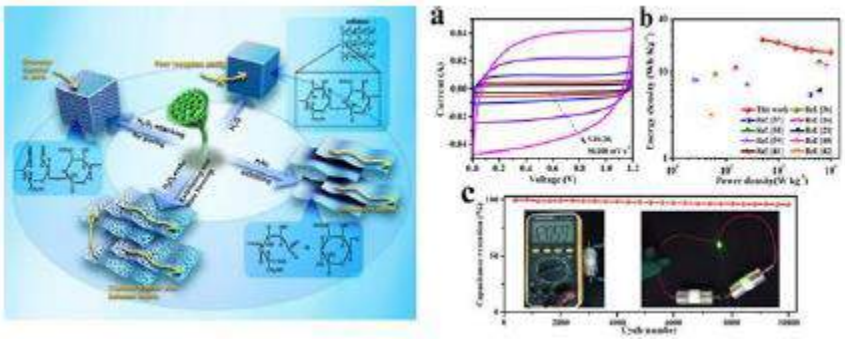



**Fig. 7** Graphene-like porous active carbon for supercapacitor
(C. M. Li* et al, Advanced Energy Materials, 99, 603-611, 2017.)

# New Aspects of Advanced Materials for Energy Storage & Conversion

## by Zongping Shao, Member EUAS

Short Biography

*Zongping Shao is a professor of chemical engineering at Nanjing Tech University, China and Curtin University, Australia. He obtained his PhD from Dalian Institute of Chemical Physics, China in 2000. He worked as a visiting scholar at Institut de Researches Sur La Catalyse, CNRS, France from 2000 to 2002, and a postdoc at California Institute of Technology, USA from 2002 to 2005.*

***Research Activities and Publications***

*Professor Shao's research interests include oxygen permeable membranes, solid oxide fuel cells (SOFCs), oxygen reduction, oxygen evolution and hydrogen evolution reactions (ORR, OER and HER), lithium-ion batteries, supercapacitors, polymer-electrolyte membrane fuel cells, solar cells, etc. He has published more than 600 international journal papers with a total citation of >30000 and an H-index of 81 (Google Scholar). He was selected by Clarivate Analytics as one of the highly cited researchers (2014, 2017-2019). He was also awarded as one of the highly cited Chinese researchers by Elsevier China (2015-2018).*

***Selected Awards and Honors***

1. *Highly Cited Researcher, Clarivate Analytics, 2019*
2. *Ten-Thousand Talents Program of China, 2019*
3. *Highly Cited Researcher, Clarivate Analytics, 2018*
4. *Ministry of Science and Technology Innovative Talents Promotion Plan, 2018*
5. *Second Prize in Hubei Province Science and Technology Award, China, 2017*
6. *Highly Cited Researcher, Clarivate Analytics, 2017*
7. *The Member of EU Academy of Sciences, 2017*
8. *Millions of Talent Projects National Candidates, China, 2017*
9. *Special Government Allowances of the State Council, China, 2016*
10. *Second Prize in Jiangsu Province Science and Technology Award, China, 2015*
11. *Highly Cited Researcher, Clarivate Analytics, 2014.*
12. *Distinguished Award for Novel Materials and their Synthesis by IUPAC& NMS, 2013*
13. *ARC Future Fellowships, 2011*
14. *The Changjiang (Yangtze River) Scholar Award, Chinese Ministry of Education, 2011*
15. *National Science Foundation for Distinguished Young Scholars of China, 2010*
16. *Young Researcher New Star Scientist Award (Scopus), 2010*
17. *"New Century Scientist" Awarded by Chinese Ministry of Education, 2008*
18. *Outstanding Young Scholar Award from Jiangsu Province, China, 2008*
19. *One Hundred Most Influential Papers of China, Chinese Institute of Scientific Information, 2008*
20. *Fok Ying Tung Research Grant for Excellent Scientist under 35, Education Foundation, Hong*

*Kong, 2007*

21. *One Hundred Most Influential Papers of China, Chinese Institute of Scientific Information, 2007*
22. *First Prize of Advance in Science and Technology of Liaoning Province, China, 2006*

**Major Research Areas**

1. Mixed conducting membranes for oxygen permeation
2. Key materials for SOFCs
3. Electrocatalysts for the ORR, OER and HER
4. Lithium-ion batteries, lithium-sulfur batteries, sodium-ion batteries and supercapacitors

**Typical Researches**

$Ba_{0.5}Sr_{0.5}Co_{0.8}Fe_{0.2}O_{3-\delta}$ (BSCF), a mixed oxygen-ionic and electronic conductor, was initially developed by Z. P. Shao as a ceramic membrane for oxygen separation from air. In 2004, Z. P. Shao applied BSCF, for the first time, as a cathode material for SOFCs operated below 600 °C. Since then, extensive research has been conducted on intermediate temperature (IT)-SOFCs all over the world. Actually, BSCF has become the hottest cathode material of IT-SOFCs nowadays. This is clearly indicated by the high citations of the paper (***Nature***, 2004, *431*, 170-173; 2254 times as of March, 2020). Afterwards, Prof. Shao's group continues to develop novel cathode materials for IT-SOFCs, for example, $SrSc_{0.2}Co_{0.8}O_{3-\delta}$ and $SrCo_{0.9}Nb_{0.1}O_{3-\delta}$. The operation temperature of SOFCs was further reduced to the range of 400-600 °C, promoting the development of low-to-intermediate temperature SOFCs.

For protonic ceramic fuel cells (PCFCs), Prof. Shao has developed an oxygen ion/proton/electron conducting nanocomposite, $BaCo_{0.7}(Ce_{0.8}Y_{0.2})_{0.3}O_{3-\delta}$ (BCCY), as a high-performance cathode for PCFCs. Self-assembly during high-temperature calcination results in the formation of a nanocomposite consisting of a mixed $H^+/e^-$ conducting $BaCe_xY_yCo_zO_{3-\delta}$ (P-BCCY) phase, mixed $O^{2-}/e^-$ conducting $BaCo_xCe_yY_zO_{3-\delta}$ (M-BCCY) and $BaCoO_{3-\delta}$ phases. The interplay between these phases promotes the ORR kinetics of this composite cathode and improves its thermo-mechanical compatibility by mitigating the mismatch in thermal expansion coefficient. The ORR activity of this BCCY composite was much higher than most of the reported cathodes for PCFCs, greatly accelerating the commercialization of this technology.

Prof. Shao has also developed perovskite-based anode materials for SOFCs that can address the coking/sulfur poisoning of the conventional nickel-based anode. The use of a water-storable proton-conducting perovskite oxide as the ceramic phase in the nickel-based

anode was found to rapidly eliminate the as-deposited carbon/sulfur, leading to the regeneration of the nickel surface and the prevention of the carbon/sulfur accumulation. Furthermore, the potential of combining nanocatalysts and water-storable materials in advanced anodes for SOFCs was demonstrated by using a facile impregnation and limited reaction protocol. A hierarchical anode composed of nickel nanoparticles, water-storable $BaZr_{0.4}Ce_{0.4}Y_{0.2}O_{3-\delta}$ perovskite, and amorphous BaO exhibited high hydrogen electro-oxidation activity, excellent operational stability, and superior sulfur tolerance.

For the room-temperature ORR, Prof. Shao introduced an effective strategy to boost the electrocatalytic activity of palladium (Pd) by stabilizing its unusual oxidation states. $LaFe_{1-x}Pd_xO_3$ (x = 0.05 and 0.1), which contain perovskite-type ionic $Pd^{3+/4+}$ species, were prepared by doping Pd into the perovskite oxide lattice, showing higher mass activity, better durability, and stronger methanol tolerance than the benchmark Pt/C (platinum supported on carbon). In addition, the introduction of A-site cation deficiency was demonstrated as another approach to enhancing the ORR activity of $LaFeO_3$, which is associated with the creation of oxygen vacancies and $Fe^{4+}$ species.

For the OER electrocatalysis, Prof. Shao utilized a doping or co-doping strategy to develop several highly active and stable perovskite electrocatalysts, such as $SrNb_{0.1}Co_{0.7}Fe_{0.2}O_{3-\delta}$, $BaCo_{0.9-x}Fe_xSn_{0.1}O_{3-\delta}$, and $SrCo_{0.95}P_{0.05}O_{3-\delta}$. These catalysts feature well-tailored catalytically active sites and show OER activities that are comparable to or even better than the state-of-the-art precious metal-based $IrO_2$. A magnetron sputtering method was further adopted by Prof. Shao to construct amorphous perovskite nanofilms loaded on nickel foam substrate, which gave rise to two orders of magnitude enhancement in OER mass activity. Such amorphous nanofilms can undergo fast reconstruction during electrocatalysis, which was proved to be a universal strategy toward the design of efficient OER catalysts. Very recently, Prof. Shao found that antiperovskite materials (e.g., $CuNNi_3$) represent another type of active catalysts for the OER.

For the HER electrocatalysis, Prof. Shao was the first to demonstrate the capability of perovskite oxides in catalyzing the HER in an alkaline solution. Through a facile A-site praseodymium (Pr) doping into the parent BSCF, he developed $Pr_{0.5}(Ba_{0.5}Sr_{0.5})_{0.5}Co_{0.8}Fe_{0.2}O_{3-\delta}$ with well-tuned surface electronic structures and properties, performing competitively with other non-Pt catalysts. Furthermore, novel synthetic methods (e.g., electrospinning, exsolution) were used to develop several nanostructured perovskite-based HER catalysts, which leads to even better catalytic performance. Prof. Shao has also developed Ruddlesden-Popper-type $Sr_2RuO_4$ as a high-performance

electrocatalyst for HER in an alkaline solution, which is comparable to those of the best electrocatalysts ever reported.

**Career-Best Research Outputs**

[1] **Shao, Z.**; Haile, S.M.; **Nature**, 431, **2004**, 170-173.

[2] **Shao, Z.**; Haile, S.M.; Ahn, J.; Ronney, P.; Zhan, Z.; Barnett, S.A.; **Nature**, 435, **2005**, 795-798.

[3] **Shao, Z.**; Zhang, C.; Wang, W.; Su, C.; Zhou, W.; Zhu Z.; Park, H.J.; Kwak, C.; **Angew. Chem. Int. Ed.**, 50, **2011**, 1792-1797.

[4] **Shao, Z.**; Zhou, W.; Zhu, Z.; **Prog. Mater. Sci.**, 57, **2012**, 804-874.

[5] Wang, W.; Su, C.; Wu, Y.; Ran, R.; **Shao, Z.**; **Chem. Rev.**, 113, **2013**, 8104-8151.

[6] Yang, B.; Ran R.; Zhong, Y.; Su, C.; Tadé, M.O.; **Shao, Z.**; **Angew. Chem. Int. Ed.**, 54, **2015**, 3722-3725.

[7] Zhu, Y.; Zhou, W.; Chen, Z.; Chen, Y.; Su, C.; Tadé, M.O.; **Shao, Z.**; **Angew. Chem. Int. Ed.**, 54, **2015**, 3897-3901.

[8] Zhu, Y.; Zhou, W.; Chen, Y.; **Shao, Z.**; **Angew. Chem. Int. Ed.**, 55, **2016**, 8988-8993.

[9] Xu, X.; Chen, Y.; Zhou, W.; Zhu, Z.; Su, C.; Liu, M.; **Shao, Z.**; **Adv. Mater.**, 28, **2016**, 6442-6448.

[10] Zhu, L.; Liu, Y.; Su, C.; Zhou, W.; Liu, M.; **Shao, Z.**; **Angew. Chem. Int. Ed.**, 55, **2016**, 9576-9579.

[11] Chen, G.; Zhou, W.; Guan, D.; Sunarso, J.; Zhu, Y.; Hu, X.; Zhang, W.; **Shao, Z.**; **Sci. Adv.**, 3, **2017**, e1603206.

[12] Zhu, Y.; Chen, G.; Zhong, Y.; Chen, Y.; Ma, N.; Zhou, W.; **Shao, Z.**; **Nat. Commun.**, 9, **2018**, 2326.

[13] Zhu, Y.; Tahini, H.A.; Hu, Z.; Dai, J.; Chen, Y.; Sun, H.; Zhou, W.; Liu, M.; Smith, S.C.; Wang, H.; **Shao, Z.**; **Nat. Commun.**, 10, **2019**, 149.

[14] Guan, D.; Zhou, J.; Huang, Y.; Dong, C.; Wang, J.; Zhou, W.; **Shao, Z.**; **Nat. Commun.**, 10, **2019**, 3755.

[15] Song, Y.; Chen, Y.; Xu, M.; Wang, W.; Zhang, Y.; Yang, G.; Ran, R.; Zhou, W.; **Shao, Z.**; **Adv. Mater.,** 32, **2020**, 1906979.

# Sluggish Kinetics of the Oxygen Reduction Reaction (ORR) & the Oxygen Evolution Reaction (OER)

## by Shaojun Guo, Member EUAS

Short Biography

***Shaojun GUO, Principal Investigator***

*Professor*
*Department of Materials Science and Engineering*
*Department of Energy and Resources Engineering*
*The Beijing Innovation Center for Engineering Science and Advanced Technology (BIC-ESAT)*
*College of Engineering, Peking University*
*Beijing 100871, China*
*Google Scholar: http://scholar.google.com/citations?user=9MRznZ0AAAAJ&hl=en*
*H-index: 101; Citation: >35,000 (Google Scholar)*

***Education***

*2005 – 2010, Ph.D., Changchun Institute of Applied Chemistry, Chinese Academy of Sciences*
*2001 – 2005, B.S., College of Chemistry, Jilin University*

***Professional Experience***

*2019-present, Professor, Department of Materials Science & Engineering, College of Engineering, Peking University.*
*2016 – present, PI, BIC-ESAT, College of Engineering, Peking University.*
*2015 –2018, Tenure Track Associate Professor, Department of Materials Science & Engineering, College of Engineering, Peking University. 2016 – Present, PI, The Beijing Innovation Center for Engineering Science*
*2013 – 2015, J. Robert Oppenheimer Distinguished Fellow, Los Alamos National Laboratory (LANL).*
*2011 – 2013, Postdoctoral Research Associate, Chemistry Department, Brown University*

***Awards***

*2019. Member of the European Union Academy of Sciences*
*2019. Xplorer Prize*
*2019. Chinese Chemical Society-Royal Society of Chemistry Young Chemist Award*
*2019. World Highly Cited Researchers (Clarivate Analytics)*
*2019. Elsevier-EnergyChem Young Investigator Award*
*2018. Fellow of the Royal Society of Chemistry*
*2018. World Highly Cited Researchers (Clarivate Analytics)*
*2018. Journal of Materials Chemistry Lectureship*
*2018. Young Analyst Awards*
*2017. World Highly Cited Researchers (Clarivate Analytics)*
*2017. Elsevier Chinese Most Cited Researchers*
*2017. Young Scientist Prize for China Electrochemical Society*
*2016. World Highly Cited Researchers (Clarivate Analytics)*
*2016. International Society of Electrochemistry (ISE)-Elsevier Prize for Applied Electrochemistry*
*2015. World Highly Cited Researchers (Thomson Reuters)*
*2014. World Highly Cited Researchers (Thomson Reuters)*
*2014. The Recruitment Program of Global Youth Experts, China*
*2013. J. Robert Oppenheimer Distinguished Fellowship (Los Alamos National Lab)*

## Research Interests

Nanochemistry for Metal, Carbon and Semiconductor Nanomaterials

Nanoenergy (Fuel Cells, Batteries and Artificial Photosynthesis)

Nanomaterials-based Analytical Sensors

Multi-functional Nanomaterials for Bioimaging and Biotherapy

## Main Contribution

The sluggish kinetics of the oxygen reduction reaction (ORR) and the oxygen evolution reaction (OER) has long posed one of the biggest challenges in the fields of proton exchange membrane fuel cells and water splitting devices. In order to tackle these challenging issues, we focus our research on rationally designing and engineering catalytic nanomaterials for renewable energy devices such as fuel cells and water electrolysers, and also deepen the understanding by establishing structure-performance relationship. We first created a class of PdMo 'bimetallene'—a palladium–molybdenum alloy in the form of a highly curved and sub-nanometre-thick metal nanosheet, which shows the world-recording electrocatalytic activity for ORR.

We revealed that the alloying effect, the strain effect due to the curved geometry, and the quantum size effect due to the thinness of the sheets could precisely tune the electronic structure of the materials for optimized oxygen binding, thus the unprecedented ORR performance of fuel cells. We also reported on a class of platinum-lead/platinum core/shell nanoplate catalysts that exhibit large biaxial strains. The biaxial strained nanoplates exhibit superior ORR specific and mass activities to commercial C/Pt catalyst. They are very stable for ORR, which can undergo 50,000 voltage cycles with negligible activity decay and no apparent structure and composition changes. These findings pave new avenues for future breakthroughs in electrocatalysts that enable the wide adoption of renewable energy technologies, such as fuel cells and water electrolysers. These important results were published in Nature, Science, Nature Reviews Materials and Nature Communications, *etc*.

## A list of 15 relevant publications

**(1)** Mingchuan Luo, Zhonglong Zhao, Yelong Zhang, Yingjun Sun, Yi Xing, Fan Lv, Yong Yang, Xu Zhang, Sooyeon Hwang, Yingnan Qin, Jing-Yuan Ma, Fei Lin, Dong Su, Gang Lu and **Shaojun Guo***, PdMo Bimetallene for Oxygen Reduction Catalysis, ***Nature***, 2019, 574, 81.

**(2)** Lingzheng Bu, Nan Zhang, **Shaojun Guo***, Xu Zhang, Jing Li, Jianlin Yao, Tao Wu, Gang Lu, Jing-Yuan Ma, Dong Su* and Xiaoqing Huang*, Biaxially Strained PtPb/Pt Core/Shell Nanoplate Boosts Oxygen Reduction Catalysis, ***Science***, 2016, 354, 1410.

**(3)** Mingchuan Luo and **Shaojun Guo***, Strain-Controlled Electrocatalysis on Multimetallic Nanomaterials, ***Nature Reviews Materials***, 2017, 2, 17059.

**(4)** Jianping Lai, Bolong Huang, Yonghua Tang, Fei Lin, Peng Zhou, Xu Chen, Yingjun Sun, Fan Lv and **Shaojun Guo***, Barrier-free Interface Electron Transfer on PtFe-$Fe_2C$ Janus–like Nanoparticles Boosts Oxygen Catalysis, ***Chem***, 2018, 4, 1153.

**(5)** Peng Zhou, Ning Li, Yuguang Chao, Weiyu Zhang, Fan Lv, Kai Wang, Wenxiu Yang, Peng Gao, **Shaojun Guo***, Themolysis of noble metal nanoparticle into electron-rich phosphorus-coordinated noble metal single atoms at low temperature, ***Angewandte Chemie International Edition***, 2019, 58, 14184.

**(6)** Mingchuan Luo, Yingjun Sun, Xu Zhang, Yingnan Qin, Mingqiang Li, Yingjie Li, Chunji Li, Yong Yang, Lei Wang, Peng Gao, Gang Lu and **Shaojun Guo***, Stable High-index Faceted Pt Skin on Zigzag-like PtFe Nanowires Enhances Oxygen Reduction Catalysis, ***Advanced Materials***, 2018, 30, 1705515.

**(7)** Yingjun Sun, Xu Zhang, Mingchuan Luo, Xu Chen, Lei Wang, Yingjie Li, Mingqiang Li, Yingnan Qin, Chunji Li, Nuoyan Xu, Gang Lu, Peng Gao, **Shaojun Guo***, Ultrathin PtPd-based Nanorings with Abundant Step Atoms Enhance Oxygen Catalysis, ***Advanced Materials***, 2018, 30, 1802136.

**(8)** Yuguang Chao, Peng Zhou, Na Li, Jianping Lai, Yong Yang, Yelong Zhang, Yonghua Tang, Wenxiu Yang, Yaping Du, Dong Su, Yisheng Tan, and **Shaojun Guo***, Ultrathin Visible-light Driven Mo–incorporation $In_2O_3$-$ZnIn_2Se_4$ Z-scheme Nanosheet Photocatalysts, ***Advanced Materials***, 2019, 31, 1807226.

**(9)** Jianping Lai, Bolong Huan, Yuguang Chao, Xu Chen and **Shaojun Guo***, Strongly Coupled Nickel-Cobalt Nitrides/Carbon Hybrid Nanocages with Pt-like Activity for Hydrogen Evolution Catalysis, ***Advanced Materials***, 2019, 31, 1805541.

**(10)** Weiyu Zhang, Yong Yang, Bolong Huang, Fan Lv, Kai Wang, Na Li, Mingchuan Luo, Yingjie Li, Yingjun Sun, Zhikun Xu, Yingnan Qin, Wenxiu Yang, Jinhui Zhou, Yaping Du, Dong Su, **Shaojun Guo***, Ultrathin PtNiM (M = Rh, Os and Ir) Nanowires as Efficient Fuels Oxidation Electrocatalytic Materials, ***Advanced Materials***, 2019, 31, 1805833.

**(11)** Jianrui Feng, Fan Lv, Weiyu Zhang, Peihao Li, Kai Wang, Chao Yang, Bin Wang, Yong Yang, Jinhui Zhou, Fei Lin, Gui-Chang Wang and **Shaojun Guo***, Iridium-based Multimetallic Porous Hollow Nanocrystals for Efficient Overall Water Splitting Catalysis, ***Advanced Materials***, 2017, 29, 1703798.

**(12)** Zhonghong Xia, **Shaojun Guo***, Strain Engineering of Metal Nanomaterials for Energy Electrocatalysis, ***Chemical Society Reviews***, 2019, 48, 3265.

**(13)** Wenxiu Yang, Jinhui Zhou, Shuo Wang, Weiyu Zhang, Zichen Wang, Fan Lv, Kai Wang, Qiang Sun and **Shaojun Guo***, Freestanding film made by necklace-like N-doped hollow carbon with hierarchical pores for high-performance potassium-ion storage, ***Energy Environmental Science***, 2019, 12, 1605.

**(14)** Fan Lv, Jianrui Feng, Kai Wang, Zhipeng Dou, Weiyu Zhang, Jinhui Zhou, Chao Yang, Mingchuan Luo, Yong Yang, Yingjie Li, Peng Gao, and **Shaojun Guo***, Iridium-tungsten Alloy Nanodendrites as pH-universal Water Splitting Electrocatalysts, ***ACS Central Science***, 2018, 4, 1244.

**(15)** Peng Zhou, Qinghua Zhang, Zhikun Xu, Qiuyu Shang, Liang Wang, Yuguang Chao, Yiju Li, Hui Chen, Fan Lv, Qing Zhang, Lin Gu and **Shaojun Guo***, Atomically dispersed Co-$P_3$ on CdS nanorods with electron-rich feature boosts photocatalysis, ***Advanced Materials***, 2019, 31, 1904249.

# Ferritin - Conjugated Lectins for Cell Surface Carbohydrate Structures

## by Garth L. Nicolson, Member EUAS

Short Biography

***Professor Emeritus Garth L. Nicolson, PhD, MD (H)***

*Professor Emeritus Garth L. Nicolson is the Founder, President, Chief Scientific Officer and Emeritus Research Professor of Molecular Pathology at the Institute for Molecular Medicine in Huntington Beach, California. He is also a Conjoint Emeritus Professor at the University of Newcastle (Australia). He was previously the David Bruton Jr. Chair in Cancer Research and Professor and Chairman at the University of Texas M.D. Anderson Cancer Center in Houston, and he was Professor of Internal Medicine and Professor of Pathology and Laboratory Medicine at the University of Texas Medical School, Houston. Professor Nicolson has published over 700 medical and scientific papers, including editing 20 books, and he has served on the Editorial Boards of 30 medical and scientific journals and was Senior Editor of four of these. Professor Nicolson has won many awards, such as the Burroughs Wellcome Medal of the Royal Society of Medicine (United Kingdom), Stephen Paget Award of the Metastasis Research Society, U.S. National Cancer Institute Outstanding Investigator Award, the Innovative Medicine Award of Canada and the EU Academy of Sciences. He is also a Colonel (O6, Honorary) of the U. S. Army Special Forces and a U.S. Navy SEAL (Honorary) for his work on Armed Forces and veterans' illnesses.*

***Professional Experience:***

***Primary Appointment:***

*1996-Present, President and Founder, Chief Scientific Officer and Emeritus Professor of MolecularPathology, The Institute for Molecular Medicine, PO Box 9355, S. Laguna Beach, CA 92652*

***Secondary Appointments:***

*2003-Present, Conjoint Emeritus Professor, Faculty of Science and Technology, University of Newcastle, Newcastle, Australia*

***Previous Appointments:***

*1989-00, Professor, Department of Internal Medicine, The University of Texas Medical School, Houston, TX*
*1981-99, Adjunct Professor, Department of Pathology, School of Veterinary Medicine, Texas A & M University, College Station, TX*
*1982-99, Professor, Department of Pathology and Laboratory Medicine, The University of Texas Medical School, Houston, TX*
*1980-96, David Bruton Jr. Chair in Cancer Research, Professor and Chairman, Tumor Biology, The University of Texas M. D. Anderson Cancer Center, Houston, TX*
*1980-96, Professor, The Graduate School of Biomedical Sciences, The University of Texas Health Science Center, Houston, TX*
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*1978-80, Professor, Department of Physiology and Biophysics, College of Medicine, University of California, Irvine, CA*
*1977-80, Associate Director, Oncology Program, University of California, Irvine, CA*
*1975-80, Professor, Department of Developmental and Cell Biology, University of California, Irvine*
*1974-76, Chairman, Department of Cancer Biology, The Salk Institute, La Jolla, CA*
*1972-74, Head, Cancer Council Laboratory, Director, Electron Microscopy Laboratory, The Salk Institute, La Jolla, CA*
*1970-71, Senior Research Associate, Cancer Council Laboratory, The Salk Institute, La Jolla, CA*
*1967-70, USPHS Predoctoral Fellow University of California, San Diego, CA*

***Honors and Awards:***

*European Union Academy of Sciences, 2019-*
*Doctor of Medicine, M.D. (H), University of the Republic of Uruguay, 2015*
*Yanagimachi Distinguished Lectureship, University of Hawaii School of Medicine, 2012*
*John Drulle Memorial Lectureship, International Lyme and Associated Diseases Society (ILADS), 2008*
*Annual Award of the Common Cause Medical Research Foundation (Canada), 2006*
*Innovative Medicine Award (Canada), 2002*

*Stephen Paget Award, Metastasis Research Society, 1998*
*Albert Schweitzer Award (Portugal), 1998*
*First Norman N. Durham Lectureship, Environmental Institute, OSU, 1996*
*Indo-American Society for Health & Laboratory Professionals Award, 1996*
*Distinguished Presentation Award, Third International Cancer Molecular Biology Symposium, 1996*
*COLONEL (Honorary), U. S. Army Special Forces, 1995*
*SEAL (Honorary), U.S. Navy Special Forces, 1995*
*Haskel Visiting Professorship, University of Pennsylvania, 1995*
*Burroughs Wellcome Medal, Royal Society of Medicine Foundation, London, 1991*
*Outstanding Faculty Award, The University of Texas Health Science Center at Houston, 1991*
*U.S. National Cancer Institute U.S.S.R. Scientist Exchange Award for Collaborative Research on Molecular and Genetic Aspects of Tumor Metastasis, 1991*
*Evan and Marion Helfaer Distinguished Lectureship, The Cancer Center of the Medical College of Wisconsin, 1990*
*Dean's Teaching Excellence List, The University of Texas Health Science Center at Houston Graduate School of Biomedical Sciences, 1985-1994*
*Teaching Excellence Award for Best Course, The University of Texas Medical School at Houston, 1990*
*NCI/NIH Outstanding Investigator Award, 1987*
*Annual Award of the Japan Histochemical Society, 1976*
*Eli Nadel Memorial Lecture in Biochemistry, 1983*
*Rita Ferdinand Memorial Lectureship, 1982*
*Guy Lipscomb Memorial Lecture in Chemistry, 1980*
*Upjohn Biology Education Award, 1976*
*Presidential Award, Electron Microscopy Society of America, 1971*

## BRIEF CAREER RESEARCH COMPENDIUM

Professor Nicolson trained with Prof. S. J. Singer (University of California, San Diego), where he devised new techniques for elucidating the topographic distribution of cell components, their dynamics and structural organization into a biological membrane. This showed for the first time the random-dispersed topographic display of some surface antigens and non-random distributions of others. He was the first to synthesize and use ferritin-conjugated lectins for cell surface carbohydrate structures and was the first to show asymmetric distributions of plasma membrane and intracellular membrane glycoproteins, indicating the lack of significant flip-flop or trans-membrane rotation. This work led to the *Fluid-Mosaic Model of Membrane Structure* [1], which gained widespread support since its inception and was the most cited journal paper in the biomedical sciences for the following decade. After over 40 years this model of cell membrane structure has proven to be relevant for describing the basic structure of a variety of intracellular and cellular membranes of plant and animal cells and lower forms of life [2].

After moving to The Salk Institute in San Diego Nicolson found that certain membrane components were freely mobile in the membrane, while others were restrained by specific cellular or membrane mechanisms. This concept led to new proposals for trans-membrane regulation, where cytoskeletal elements played a central role in controlling the display and mobility of outer cell surface components [3]. Nicolson was the first to determine that the display of integral trans-membrane sialoglycoproteins in erythrocytes were under trans-membrane control by an inner membrane surface network containing actin and spectrin [4]. Similarly, for the first time bifunctional crosslinking agents were used to confirm that outer cell surface perturbation by polyvalent ligand binding (and clustering) can be translated across the cell membrane and reflected by the distributions of components on the inner membrane surface [5]. These experiments led to the theory of *Trans-Membrane Control of Membrane Components* [3], an important concept in membrane regulation found in many other cell systems. For example, Nicolson found that tumor cells lose at

least some ability to dynamically control their cell surface receptors [3, 6]. Using drugs, such as tertiary amine local anesthetics, a collaborative study confirmed that cytoskeletal components were involved in trans-membrane regulation in many cell systems [7].

After neoplastic transformation cytoskeletal control systems are altered, and transformed cells lose at least some of their cell surface trans-membrane controlling systems, which may account for some of their aberrant interactions [3, 6]. In other systems, such as mammalian spermatozoa, Nicolson found that cell surface receptors were differentially regulated in distinct regions along the single, continuous plasma membrane of the sperm [8]. This was the first example of the lateral control of cell surface components into particular membrane domains [2, 3]. Trans-membrane control was also found to be important in antibody-complement and toxin-mediated killing of cells. Using plant toxins, such as ricin, which was first affinity purified to homogeneity in Nicolson's laboratory [9-11], he showed that cell surface receptor dynamics determine whether toxin molecules enter cells, a necessary step for cytotoxicity. By selecting resistant variant tumor cell lines that bound, but did not transport toxin molecules into the cytoplasm, he showed that specific membrane glycoprotein receptors are responsible for toxin endocytosis [10, 11]. Similarly, derivation of resistant variants to antibody-complement-mediated killing allowed Nicolson to conclude that this process is also controlled, in part, by the dynamics of the antigen-antibody complexes on the cell surface [12]. Thus evidence on the importance of cell membrane dynamics in tumor escape from toxin killing and humoral immune surveillance was obtained.

When Nicolson arrived at the University of California, Irvine he concentrated on two important cell surface problems. The first was a collaboration with Prof. Ryuzo Yanagimachi on studying sperm-egg recognition, its role in fertilization, and the development of safe, specific immunological methods of control of fertilization. For example, an ovum-specific antigen was identified in the extracellular matrix of the mature egg, and antibodies were made against this antigen. These antibodies selectively homed to and concentrated in the ovaries after injection and specifically bound to the extracellular matrix (zona pellucida) of ova. The ova remained viable, but were incapable of subsequent fertilization by capacitated, activated sperm [13]. Such experiments were designed to develop a safe, effective, efficient and reversible method for controlling human fertility.

The second problem area concerned the spread of tumors or metastasis, the leading cause of clinical deaths due to cancer. Tumor metastasis can be thought of as a cell surface problem involving membrane alterations which result in improper cell-cell interactions and positioning in tissue, and subsequent malignant cell escape, transport, arrest and establishment or colonization at new and often distant sites [14, 15]. Nicolson used sequential *in vivo* selection techniques to obtain tumor cell lines with differing metastatic potentials. Certain of these variant tumor cell lines metastasized to very specific secondary sites, such as lung, liver, brain, ovary, etc. [15]. Using these models he was the first to propose that the organ distribution of metastases was determined, in part, by adhesive interactions between blood-borne tumor cells and host organ cells [16]. Subsequently several laboratories confirmed these observations.

In 1980 after moving to the University of Texas M. D. Anderson Cancer Center, Nicolson extended his studies on malignant animal tumors to clinical cancers metastatic to particular sites and developed his theories of the *Organ Tropism of Metastatic Colonization due to Specific Adhesion, Degradation, Migration and Growth of Metastatic Cells*. By comparing non-metastatic with highly metastatic tumor lines of common genetic origin, a great deal has been learned about the cellular characteristics essential for blood-borne metastasis. Nicolson was the first to show that microvessel endothelial cells in each

organ display unique cell surface glycoproteins *in vitro* as well as *in vivo* [17]. Metastatic cells also express multiple receptors for basement membrane components, and he found that different tumor systems use different arrays of such receptors to bind to various organ basement membranes.Thus he found that multiple cell adhesion components were involved in endothelial cell adhesion and implantation [18].

Highly metastatic tumor cells secrete and display on their surfaces several degradative enzymes that are essential in basement membrane invasion. Nicolson's labortory discovered enzymes, such as heparanase, specific for heparan sulfate proteoglycan degradation, and a new collagenase specific for basement membrane collagens, that can be used to monitor patients for the presence of highly metastatic cells [19, 20]. His laboratory later cloned the gene for heparanase.

In addition to degradative enzymes, cell surface glycoproteins, such as breast cancer metastasis-associated gp580, were discovered, isolated, and monoclonal antibodies used to detect the presence of metastases in clinical biopsy specimens [21]. Degradative enzymes in some highly metastatic cells are controlled by trophic factors, and Nicolson was the first to discover that organ trophic factors, such as nerve growth factor (NGF), are important in metastasis and can control invasion of certain tumor cells by regulating certain degradative enzymes [22].

Another important discovery was the isolation and characterization of the first paracrine growth factor that differentially stimulated the growth of highly metastatic tumor cells at particular organ sites. Nicolson's finding and isolation of lung-derived growth factor 1 (LDGF-1) was the first report on *Metastasis-Associated Organ Paracrine Growth Factors* [23]. Sequencing data indicated that LDGF-1 was related to transferrin, and it was released by endothelial cells as an important step in stimulation of malignant cell growth at secondary sites. Recently Nicolson's lab has identified several different human transferrin-like genes. In contrast to systemic transferrin, the paracrine transferrins are encoded by separate genes and seem to be related to wound healing. In the brain, transferrin-like factor-3 is an important developmentally regulated growth factor.

Microvessel endothelial cells appear to be involved in several steps of metastasis, and Nicolson was the first to show that in addition to cell adhesion of blood-borne metastatic cells microvessel endothelial cells also released paracrine motility factors [24] and paracrine growth factors [25]. Some of these paracrine factors have been isolated and sequenced. For example, a major motility factor for liver-metastatic cells was identified as a novel factor that is involved in normal brain development and wound healing, and a major lung-derived motility factor for lung-metastatic cells was isolated and characterized as monocyte chemotactic protein-1 [26].

In 1996 Nicolson moved to assume the post of President and Chief Scientific Officer of the Institute for Molecular Medicine in Huntington Beach, California. Nicolson's laboratory was involved in identifying several differentially expressed genes in highly metastatic cells. For example, in breast cancer dozens of genes were found to be differentially expressed in highly metastatic cells. Some of these genes were sequenced and compared. Most of the *Metastasis-Associated Genes* encoded known molecules, such as adhesion molecules, degradative enzymes, transcription factors, cytoplasmic proteins and cell surface molecules. At least two of the genes were novel. One of these, named *mta1*, encoded a 703 amino acid putative signal transduction molecule that is related to enhanced invasion of metastatic cells [27].

Determining how each of the *Metastasis-Associated Genes* was being controlled and related to the different steps of metastasis as well as their role in tumor progression and malignancy is important in understanding cancer and developing new methods of

treatment. In some metastatic systems, differences in gene expression were related to escape from host surveillance, and Nicolson was the first to describe that certain mitochrondrial genes can be overexpressed in order to allow malignant cells to escape cytostatic responses of macrophages and other host effector cells that inhibit tumor cell respiration [28]. Nicolson also examined the role of genes and gene complexes in the progression of highly metastatic cells, events that could help explain malignant cell properties, genetic instabilities and propensity to diversify and generate heterogenous phenotypes [29]. In some tumor systems oncogene expression was found to be destabilizing and enhanced the diversification of some of these cells to metastatic cells, eventually yielding heterogeneous malignant cell populations at rapid rates [30]. The failure of cells within tissues to stabilize could be due, in part, to the loss of cell communication via gap junctions. Nicolson found that metastatic epithelial cells lost gap junctional communication in relation to their metastatic properties and also their stabilities [31]. By characterizing the differences in malignant cell surface molecules, enzymes, receptors and growth factors and inhibitors that are important in metastatic tumor spread and ultimately the genes that control these molecules, more effective and selective means for identifying, monitoring and destroying cancer metastases could be developed.

The Institute for Molecular Medicine was founded by Nicolson to study chronic illnesses, such as Chronic Fatigue Syndrome, Fibromyalgia Syndrome, Gulf War Illness, Arthritis, Inflammatory Bowel Disease, Asthma and other conditions. As a part of these studies Nicolson began studying the role of particular viruses and bacteria as *Chronic Infections in Various Chronic Diseases* [32]. For example, he found with his late wife Nancy Nicolson a very pathogenic Mycoplasma and other infections as an important source of morbidity in chronically ill patients [33-35]. The Nicolson group has published procedures for the identification of Mycoplasma infections and their successful treatment in chronically ill patients [34-36]. These infections have become important in neurodegenerative diseases like amyotrophic lateral sclerosis [37] and autism spectrum disorders [38] as well as various fatiguing and rheumatic illnesses [39-42].

The recent direction of Nicolson is furthering his interests in medicine and membrane structure and dynamics by his new proposal and development of *Membrane Lipid Replacement* for treatment of mitochondrial dysfunction and some of the symptoms found in chronic illnesses. This approach uses all-natural dietary membrane lipids to repair the damage to cellular membranes that occurs during most diseases, and especially chronic diseases, cancer and aging [43, 44]. By using a protected oral mixture of membrane glycerolphospholipids Nicolson has been able to restore mitochondrial function and reduce fatigue in various clinical conditions [43, 44]. This natural membrane supplement has also been useful in reducing pain and other symptoms in fibromyalgia and diabetic neuropathy [45]. Recently membrane replacement molecules have been shown to increase sperm motility and fertilization capacity [46]. Clinical and experimental studies are underway in several institutions around the world using *Membrane Lipid Replacement* to treat autism spectrum disorders, fatiguing illnesses, neurodegenerative diseases, chemical detoxification, pain disorders and digestive diseases. These various projects are a direct outcome of the original 1972 *Fluid-Mosaic Model of Membrane Structure* [1, 2].

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# Science and Technology of a Multifunctional Oxide and Nanocarbon Thin Films and Application to Development and Commercialization of a New Generation of Multifunctional Industrial, High-Tech and Implantable Medical Devices

**by Orlando Auciello, Member EUAS**

Short Biography

***Orlando Auciello: Distinguished Endowed Chair Professor, University of Texas-Dallas (Materials Science/Engineering and Bioengineering Departments, 2012 - present).***

*Auciello graduated with M.S. (1973) and Ph.D. (1976) degrees in Physics from the Physics Institute "Dr. Balseiro" (Universidad Nacional de Cuyo, Argentina). Electronic Engineering at the University of Cordoba-Argentina (1964-1970).*

*Auciello was Postdoctoral at Mc Master University (Canada, 1976-1979), Research Scientist at the University of Toronto-Canada (1979-1984), Associate Professor at North Carolina State University (1985-1988), Senior Research Scientist at the Microelectronics Center of North Carolina (1988-1996), Senior Scientist (1996-2005) and Distinguished Argonne Fellow (2005-2012).*

*Auciello is directing basic and applied research programs on different fields, involving multi-component oxide thin films and application to systems and devices (ferroelectric memories, high-k dielectric oxide films, resistive change memories, nanoscale CMOS devices, photovoltaic energy generation / super-capacitors for energy storage devices, high-frequency devices, piezoelectric thin films for MEMS/NEMS sensors and actuators); and nanocarbon thin films (ultrananocrystalline diamond (UNCD), nanocrystalline diamond (NCD), and microcrystalline diamond (MCD) and graphene films) and applications to industrial, high-tech and medical devices. Auciello's work on ferroelectric films contributed to the development of nonvolatile memories now in the market in smart cards.*

*The UNCD film technology developed and patented by Auciello and colleagues is now commercialized by three companies co-founded by him and colleagues:*

*• Advanced Diamond Technologies (ADT), spun-off from Argonne National Lab (top company spun-off from a DOE Laboratory in 2003 / Profitable in 2014 /sold for profit to a large company in 2019) is commercializing industrial components and systems (UNCD-coated mechanical pump seals and bearings, and water purification systems based on electrolysis with corrosion resistant electrodes based on electrically conductive B-doped UNCD-coated metal electrodes) (Auciello is co-founder, equity holder, investor, and worked closely to develop new UNCD coated industrial products for ADT).*

*• Original Biomedical Implants (OBI)-USA / 2013-prsent), and (OBI-Mexico / 2016-present), developing and commercializing a new generation of UNCD-based high-tech and implantable medical devices / prostheses and medical treatments based on nanotechnology. Products in advanced state of development by OBI-USA and OBI-Mexico include: i) new generation of Li-ion batteries with anodes, cathodes, membranes, and inner walls of battery cases coated with corrosion resistant UNCD coatings, enabling LIBs with ≥ 10x longer life and safer than current LIBs, for applications to defibrillators/pacemakers, cell phones, computers, battery-*

*powered electronic devices, and electric cars; ii) Biocompatible UNCD-coated dental implants with practically no corrosion induced in current metal-based dental implants by oral fluids (Clinical trials implanting UNCD-coated DI in 10 people, in México, demonstrated the superior performance over current commercial metal DIs ; iii) UNCD-coated metal prostheses (hips, knees) with no failure due to the protective UNCD coating; iv) new retina reattachment procedure, using biocompatible super-paramagnetic nanoparticles injected inside the eye attracted by an external temporary magnet to push the retina back into place (clinical trials performed in Argentina between 2015-2106 restored full vision to two patients (2 patents granted in USA and Japan in 2016).*
*Auciello has published 31 books and about 550 articles in the fields described above, holds 26 patents, and organized, chaired, and lectured at numerous national and international conferences. He was Associate Editor of Appl. Phys. Lett (2000-2019), Journal of Materials Research (2002-2010), and currently Associate Editor of the International Journal "Coatings" (2019-present), Member of Vacuum Board (1994-2010), Integrated Ferroelectrics Board (1997-2019). Editor of two book series on thin films and applications to devices (Academic Press). He was member of the Materials Research Society (MRS) Board of Directors (2000-2003), Chair of the MRS International Relations Committee 2005-2010,* ***Vice President of the MRS (2012), President of the MRS (2013), and Past President of the MRS (2014).***
*He has numerous Awards, including seven R&D 100 Awards, 2003 Hispanic Engineering National Achievement Award, 2006 Federation of National Laboratories Award, 2008 University of Chicago Distinguished Performance Award, and is a* ***Fellow of the AAAS and MRS.***

**Brief Research**

**1986-1996**. O. Auciello (North Carolina State University (NCSU) and Microelectronics Center of North Carolina (MCNC)) and colleagues were one of the first two groups in producing Y-Ba-Cu-O High Temperature Superconductors (HTSC) Films based on the bulk YBCO material discovered in the late 1980's. This work opened the way for science/technology of HTSC thin films from the 90's until today.
J. Narayan, N. Biunno, R. K. Singh, O.W. Holland, and **O. Auciello**, "Formation of Thin Superconducting Films by Laser Processing Method," Appl. Phys. Lett. **vol. 51,** 1845-1847 (1987). **ISI Citation: 1000.**

**1986-2008.** O. Auciello (NCSU and Argonne National Laboratory (ANL)) and colleagues pioneered the development of conducting oxide electrodes ($RuO_2$ was patented as the first oxide electrode for Ferrolectric Random Access Memories (FeRAMS) to eliminate the 30-year old problem of polarization fatigue in $PbZr_xTi_{1-x}O_3$ (PZT) ferroelectric capacitors for FeRAM, through a careful control of oxygen vacancies at the electrode-ferroelectric interface. This was a critical step in the development of reliable FRAMs based on PZT thin films. Fujitsu and Texas Instruments are currently using the conducting oxide ($IrO_2$) electrode approach for commercialization of FeRAMs based on PZT thin films.

A.I. Kingon, **O. Auciello**, H.N. Al-Shareef, D.J. Lichtenwalner, and R. Dat,"Hybrid Metal / Metal-Oxide Electrodes for Ferroelectric Memories," US Patent #5,555,486; (1996).

**O. Auciello**, J.F. Scott, R. Ramesh, "The Physics of Ferroelectric Memories," Physics Today, p. 22, July 1998. **ISI citation as of 2020: 2354.**
**Importance:** this paper showed the physics and future of ferroelectric memories for insertion in the market.

**In the 2000s**, Auciello and colleagues conducted pioneering research, using the unique one of two worldwide highest energy/intensity X-Ray synchrotron (Advanced Photon Source-Argonne National Laboratory) to demonstrate that the limit of ferroelectricity in Perovskite PbTiO Films is three Atomic Units. This R&D opened the way for the science and technology of nanoferroeletrics.

D.D. Fong, G.B. Stephenson, S.K. Streiffer, J.A. Eastman, **O. Auciello**, P.H. Fuoss, C. Thompson, "Ferroelectricity in Ultrathin Perovskite Films," Science, **vol. 304**, 1650-1653 (2004). **ISI Citation Information: Times Cited: 500.**

**1995-present.** O. Auciello and A. Gruverman demonstrated a new technique (Piezoresponse Force Microscopy (PFM)) based on Atomic Force Microscopy to study ferroelectric domains and dynamics, at the nanoscale, in ferroelectric films. This technique measures the atomic scale displacement of atoms on the surface of ferroelectric materials, upon application of a voltage between the top and bottom surface of the ferroelectric layer, which induces polarization due to displacement of ions in the lattice. Many groups now use the PFM technique worldwide, and several companies are commercializing AFM-PFM systems for research.

A. Gruverman, **O. Auciello,** and H. Tokumoto "Imaging and control of domain structures in ferroelectric thin films via scanning force microscopy,", Annual Rev. of Materials Science, **vol. 28**, (1999) 101-123,
**ISI Citation: 500.**

**Importance:** this paper showed the importance of the new piezoresponse imaging technique to study ferroelectric domains at the nanoscale and open the new field of PFM imaging of ferroelectric domains and contributed to develop a new market of PFM instrumentation.

**1996-present** O. Auciello pioneered the development of a unique multifunctional material in thin film form. The material is based on a novel TiAl alloy layer, for which Auciello's group demonstrated several functionalities, namely: 1) oxygen diffusion barrier to integrate oxides (e.g., $BaSr_xTi_{1-x}O_3$ (BST)) films (grown at high-temperature in oxygen-rich environments) with copper electrode layers (without oxidation of the electrode) to achieve the highest performance BST based capacitors with the highest electrical conductivity electrodes for high frequency devices demonstrated today. Auciello's group latter used the TiAl film barrier to integrate oxide piezoelectric thin films with a novel multifunctional material in thin film form, named ultrananocrystalline diamond (UNCD), to develop a new generation of low voltage piezoelectrically actuated diamond microelectromechanical/nanoelectromechanical systems (MEMS/NEMS) with the highest performance demonstrated today.
The observation that TiAL formed a thin oxide layer (~3 to 4 nm thick) lead to another breakthrough functional use of TiAl alloys, as an amorphous $TiAlO_x$ layer with relatively high-dielectric constant and bandgap for application as a novel amorphous high-k dielectric to replace $SiO_2$ ion the next generation of nanoscale CMOS devices. The idea came from observing that $Al_2O_3$ is the material with the highest bandgap (~ 8 ev)) closest to $SiO_2$ (~ 9 eV), although with relatively low K- 10, while $TiO_2$ exhibits the highest K among all amorphous oxides explored for the new generation of high-K CMOS gates, but with relatively low bandgap (3.3 eV). Auciello postulated that by producing a $Ti_xAl_{1-x}O_3$ with the appropriate stoichiometry, this material can provide a better alternative to $HfO_2$, which is currently used in all gates of CMOS devices in the market today.

**O. Auciello**, W. Fan, B. Kabius, S. Saha, and J.A. Carlisle, C. Lopez and E.A. Irene, R.A. Baragiola "A New Hybrid $Ti_xAl_{1-x}O_y$ Gate Dielectric Layer for Next Generation Ultra-High Capacitance Density CMOS Gates,", Appl. Phys. Lett **86** (2005).
**Importance:** this paper shows that the new TiAlOx dielectric layer exhibits the highest dielectric constant (~ 35) among all known amorphous oxides, including $HfO_2$, which replaced $SiO_2$ in CMOS devices in 2006.

Following the R&D on $Ti_xAl_{1-x}O_3$ films described above, Auciello's group pioneered another

breakthrough in the high-K dielectric thin film field, which consisted in the development of a new material science approach based on growing $TiOx/Al_2O_3$ nanolaminates (NLs) that produced he highest dielectric constant oxide thin films known today. For 150 nm thick $TiOx/Al_2O_3$ NLs with sub-nanometer thick sublayers, few Angstrom change in sublayer thickness dramatically increases relaxation cut-off frequency by more than 3 orders of magnitude with high dielectric constant ($k \geq 1000$). This unusual phenomenon was demonstrated to be based on the two-phase Maxwell-Wagner relaxation phenomena.

G. Lee, B-K Lai, C. Phatak, R.S. Katiyar, and **O. Auciello**, "Tailoring Dielectric Relaxation in Ultra-Thin High-Dielectric Constant Nanolaminates for Nanoelectronics", Appl. Phys. Lett **102,** 142091 (2013).

W. Li, Z. Chen, R. N. Premnath, B. Kabius, and **O. Auciello**, "Controllable Giant Dielectric Constant in $Al_2O_3/TiO_2$ Nanolaminates", J. Appl. Phys. **110,** 024106-1-8 (2011).
**Importance:** The two papers cited above open the way for the new field of science and technology of multifunctional oxide nanolaminates.

The concept of $TiOx/Al_2O_3$ nanolaminates was subsequently extended by Auciello's group to investigate and develop $BiFeO_3$ (BFO)/ $SrTiO_3$ (STO)/BFO nanolaminates (BSB-NLs). By introducing the nanoscale STO layer in between two nanoscale BFO layers, the leakage current density was reduced by two orders of magnitude with respect to relatively high leakage currents of single BFO layers (from $10^{-5}$ A/cm$^2$ to $10^{-7}$ A/cm$^2$). The BSB-NL also shows very high piezoelectric response, which is ~ 5 times higher than that of the pure BFO with the same thickness. The highly strained state of the BFO layers concurrently with the chemical/crystallographic state of the interfaces between the BFO and STO layers contribute to the very high values of piezoresponse and very low leakage current observed in the BSB-NLs.

G. Lee, E. M. A. Fuentes-Fernandez, G. Lian, R. S. Katiyar, and **O. Auciello**, "Hetero-epitaxial $BiFeO_3/SrTiO_3$ Nanolaminates with Higher Piezoresponse Performance Over Stoichiometric $BiFeO_3$ Films", Appl. Phys. Lett. **106**, (2015) 022905.

**Importance:** this paper opened the way for a new field focused on R&D on piezoelectric nanolaminates with superior piezolectric properties over those of single phase BFO films.

**1996-present**. O. Auciello and two colleagues (D. M. Gruen and A. R. Krauss) started a whole new field of research and technological development focused on the science and technology of a novel material in thin film form defined as ultrananocrystalline diamond (UNCD). They developed a unique patented plasma chemistry involving Ar (the lowest cost inert gas) and $CH_4$ as the source of C atoms to grow diamond films with the smallest grains demonstrated today (2-5 nm). UNCD films exhibit a unique combination of exceptional mechanical, tribological, physical, chemical, electronic, thermal transport, and biocompatible properties. They performed pioneering research to understand the fundamentals underlying the growth and the properties of UNCD, and in the process obtained several key patents to enable the commercialization of the UNCD technology. Auciello lead the work to demonstrate that UNCD films can be used in a wide range of technologies, and to do so, he co-founded Advanced Diamond Technologies (ADT) in 2003, jointly with J.A. Carlisle. The multifunctionalities of UNCD enables a broad range of commercial applications, namely: a) UNCD coatings are now in commercial mechanical pump seals (marketed by ADT), making a major impact in enabling pumps in the chemical, the oil and car industries run with 20% savings in energy usage, and in UNCD-coated bearings for Merck-Millipore machines mixing chemicals to produce pharmaceutical drugs; b) Atomic Force Microscope UNCD tips now in

the market provides wear-free AFM tips for much higher resolution AFM analysis as compared with wear prone Si tips (ADT became profitable in 2014 and sold for profit to a large company in 2019); c) New diamond-based MEMS/NEMS technologies to replace the current Si-based technology that is hindering the development and commercialization of MEMS and NEMS devices, due to the poor mechanical and tribological properties of Si (new RF MEMS switches, using UNCD as a dielectric with controlled charging have been developed and are in the process of being inserted in a new generation of RF communication devices, electronic radars and more); d) New UNCD-based field electron emission cathodes for application to field emission displays, cold cathodes for mass spectrometer for deep space exploration and more.

**2000-2010**: Auciello was a member of a multidisciplinary team of scientist, medical doctors, and surgeons, developing an artificial retina to restore vision to people blinded by genetically induced degeneration of retina photoreceptors (retinitis pigmentosa). Auciello developed a hermetic bioinert/biocompatible UNCD coating encapsulating a Si microchip implantable inside the eye as an artificial retina– the Argus II device, marketed by Second Sight in Europe and the USA, since 2011, returns partial vision to people blind by retinitis pigmentosa, and they can read letters and recognize objects again, although diffusively, via a Si microchip receiving images from a CCD camera and injecting electronic charges into the retina ganglion cells, for transmission to the brain to form images);
**2011-present:** Auciello founded Original Biomedical Implants (OBI-USA / 2013-present) and (OBI-México / 2016-present) with Dr. J.L. Rubio (MD) (Founder and CEO of Rubio Pharma and NICDET), the latter functional in a facility of four floors with clean rooms class 1-1000, developing new generation of UNCD-coated implantable medical devices and prostheses, namely:

a) Auciello is now directing R&D focused on developing a new generation of UNCD-coated metal-based prostheses (dental implants (DI), hips, knees and many others), for which the biocompatible/body fluids corrosion resistant/lowest coefficient of friction UNCD coating eliminates the degradation produced in current metal-based prostheses, requiring early than desired replacement. Clinical trials on UNCD-coated DI have been conducted during the last two years in the World Class clinic of Dr. Gilberto López-Chávez in Queretaro-México, implanting UNCD-coated commercial Ti-alloy DI in 10 people, demonstrating that UNCD-coated DI eliminates the failure of metal implants due to chemic al corrosion by oral fluids. UNCD-coated DI represent a revolution in DI technology.
b) Auciello and researchers and MDs colleagues, in Argentina, are developing a new treatment for retina reattachment based on injecting a solution of superparamagnetic nanoparticles inside the eye, which are attracted by a magnetic field produced by a UNCD-coated magnet outside the eye, attracting the particles, pushing the retina back to the eye wall for laser treatment for reattachment. Clinic al trials on two patients demonstrated that this new treatment will be transformational.
c) Auciello's group recently demonstrated that UNCD surfaces support an efficient growth of stem cells, and they are now investigating the feasibility of differentiating those cells into photoreceptors to replace the dead photoreceptors in the retina of people blinded by the death of photoreceptors, and in the future differentiation into spinal cord cells to eventually restore motion to people paralyzed by trauma of those cells, brain cells, to control or eliminate brain degradation conditions, such as Parkinson decease, and improvements in many other human conditions. This research started a new field of developmental biology based on the UNCD biocompatibility.

The new UNCD-coated implantable medical devices and prostheses will produce a revolution in the medical device and prostheses industry worldwide.

W. Yang, **O. Auciello**, J.E. Butler, W. Cai, J.A. Carlisle, J.E. Gerbi, D.M. Gruen, T. Knickerbocker, T. Lasseter, J.N. Russell, L. M. Smith, R. J. Hamers "DNA Modified Nanocrystalline Diamond Thin Films as Stable, Biologically, Active Substrates,", *Nature Mater.* **1** (2002) 253-257.
**Importance:** This is the first paper that demonstrated that the surface of UNCD films can be functionalized to express DNA and other biomolecules, opening the field of diamond-based developmental biology.

X. Xiao, J. Birrell, J.E. Gerbi, **O. Auciello** and J.A. Carlisle, "Low Temperature Growth of Ultrananocrystalline Diamond," J. Appl. Phys. 96 (2004) 2232-2239.
**Importance:** Demonstration that the UNCD films are the only diamond films that can be synthesized at 400 ˚C, opening the pathway to using UNCD for fabrication of monolithically integrated diamond MEMS/NEMS with CMOS devices to enable a whole new hybrid diamond MEMS/NEMS /CMOS technology.

S. Sudarsan, J. Hiller, B. Kabius, and **O. Auciello**, "Piezoelectric/Ultrananocrystalline Diamond Heterostructures for High-Performance Multifunctional Micro/Nanoelectromechanical Systems," Appl. Phys. Lett. **90** (2007) 134101.
**Importance:** this is the first paper demonstrating the possibility of integrating an oxide based piezoelectric film (PZT) with a carbon based material (UNCD) to produce a new generation of high-performance piezoelectrically actuated diamond MEMS/NEMS, opening the way for a new generation of advanced MEMS/NEMS devices driven by CMOS.

"*In Vitro* and *In Vivo* Evaluation of Ultrananocrystalline Diamond for Coating of Implantable Retinal Microchips," X. Xiao, J. Wang, J. A. Carlisle, B. Mech, R. Greenberg, R. Freda, M. S. Humayun, J. Weiland, and **O. Auciello**, J. Biomedical Materials **77B (2)** (2006) 273-281.
**Importance:** This paper shows that UNCD coatings enable implantation of a Si microchip in the human eye as the key component of an artificial retina to restore sight to people blinded by retina photoreceptors' degeneration.

B. Shi, Q. Jin, L. Chen and **O. Auciello,** "Fundamentals of ultrananocrystalline diamond (UNCD) thin films as biomaterials for developmental biology: Embryonic fibroblasts growth on the surface of (UNCD) films," Diamond and Related Materials, **vol. 18** (2-3), 596-600 ) (2009).
**Importance** this is the first paper that demonstrates that UNCD surfaces are excellent for growing stem cells, thus opening the field for developmental biology based on diamond.

**G. Auciello, P. Gurman, M. B. Guglielmotti, D.G. Olmedo, A. Berra and M. J. Saravia, "Biocompatible Ultrananocrystalline Diamond Coatings for Implantable Medical Devices", MRS Bulletin, vol. 39 (07), 621 – 629 (2014).**
**O. Auciello**, "Novel Biocompatible Ultrananocrystalline Diamond Coating Technology for a New Generation of Medical Implants, Devices, and Scaffolds for Developmental Biology", Biomaterials and Medical Applications Journal, **vol 1** (1), 1000103 (2017).

# Stability and Barrier Systems of Municipal Waste Deposits

## by Heinz Brandl, Member EUAS

Short Biography

*Em.O.Univ.-Prof.Dipl.-Ing.Dr.techn.Dr.h.c.mult. Heinz Brandl*

*Prof. H. Brandl has been Full Professor for Soil and Rock Mechanics and Foundation Engineering (including Tunnelling) since 1977, chairing until 2009 the prestigious Institute for Soil Mechanics and Geotechnical Engineering, which was founded by Prof. Karl Terzaghi in 1928 at the Vienna University of Technology. Since 2008 he is Prof. Emeritus, but still worldwide active.*

*Professor Brandl authored about 590 scientific publications (including 21 books), partly published in 18 languages. The subjects cover laboratory and field testing, soil and rock mechanics, foundation engineering, slope engineering, earthworks, tunnelling, urban undergrounds, restoration of historical buildings, road and railway engineering, hydro/hydraulic engineering and environmental engineering, geosynthetics, geothermal engineering ("energy foundations", "energy tunnels" etc.), natural disaster mitigation and rehabilitation, etc. He also published on philosophical aspects and on ethics in the profession.*

*From the very outset of his professional work H. Brandl has been bridging the gap between theory and practice. He has been fully responsible for nearly 4000 projects of civil engineering, geotechnical, transportation, hydro and environmental engineering in Austria and elsewhere.*

*Prof. Brandl has been active world-wide since 1968 as chairman, general reporter, state-of-the-art reporter, special-, keynote- and opening lecturer, discussion leader and panellist at numerous international conferences on geotechnical engineering, environmental and transportation engineering, geosynthetics, etc. He delivered more than 600 lectures, was Rankine Lecturer (2001), M.Rocha Lecturer (2008), Giroud Lecturer (2010), and he created the prestigious "Vienna Terzaghi Lecture".*

*He was Vice-President ISSMGE (1997 - 2001), ISSMGE Council Member from 1968 to 2015 (i.e. longest serving member in ISSMGE history). and from 1973 to 2015 President of the Austrian Geotechnical Society. Moreover, he is a member of the Royal Academy of Sciences of Belgium, of the International Academy of Engineers (Moscow) and other Scientific Academies. Since June 2003 he has been President of the Austrian Society for Engineers and Architects (founded in 1848). He received numerous national and international awards (e.g. Kevin Nash Gold Medal), 20 honorary doctorates and other honours.*

***Stability and barrier systems of municipal waste deposits.***

Proceedings of the XVII European Conference on Soil Mechanics and Geotechnical Engineering. Reykjavik, Sept. 2019.

**ABSTRACT**

The paper underlines that an appropriate pre-treatment of waste is crucial to avoid the passing-on of environmental impacts of today's landfills to future generations. Morover, multi-barrier systems are recommended, especially in case of hazardous waste. For geotechnical stability analyses of waste deposits a compatibility investigation of the sometimes fundamentally different shear stress-strain behavior of waste and subsoil is recommended. Horizontal barriers commonly require composite liner systems, unless pre-treated or mono-waste of low risk potential is deposed. Assumptions for risk analyses are presented in this paper.

***Long-term settlement (creeping) of soft soils, and ground improvement.***

Proceedings of the 3rd International Congress and Exhibition on Sustainable Civil Infrastructure – GeoMEast Cairo 2019. Springer Nature.

**ABSTRACT**

This keynote paper focuses on the long-term settlement (creeping) of highly compressible soils, considering also soft sludge. Long-term oedometer tests lasted up to 42 years and were performed on silty sand, (organic) clayey silt, peat and (pre-treated) sewage sludge. Secondary consolidation (creep) could be observed in all cases, lasting over many years and occurring widely linear with the logarithm of time. However, temporary acceleration may also be observed, indicating a discontinuous nature of internal deformations due to accelerated rearrangement in the fabric – mainly in very soft soils with peaty components. This long-term phase is followed by tertiary creeping with a long lasting fading out period. In both phases microcrystalline sliding occurs.

In addition to the laboratory tests results of comprehensive field measurements are summarized, showing the influence of different ground improvement methods on the creeping behaviour of highly compressible fine-grained soils (partly organic). Most data were collected from a highway junction with embankments on very soft, heterogeneous ground (locally 15 m deep and with a natural water content up to 1000%), constructed between 1972 and 1974, and monitored since. Different ground improvement methods were compared, disclosing details of primary, secondary and tertiary

settlement: Deep dynamic compaction/consolidation (heavy tamping), vibroflotation (piled embankments), temporary surcharge loading, and local combinations of the previous methods, including also vertical drains.Keywords: settlement, creeping, highly compressible soils, oedometer tests, heavy tamping, deep ground improvement, sludge.

# Nanostructured Electrode Materials for Energy Applications

## by Haitao Huang, Member EUAS

Short Biography

*Professor, Department of Applied Physics, the Hong Kong Polytechnic University*

***Education:***

*Ph.D, Materials Science (2000), Nanyang Technological University, Singapore*

*M.Eng., Materials Physics (1993), Shanghai Institute of Metallurgy, Chinese Academy of Sciences*

*Double Bachelor's Degrees in Applied Physics and Applied Mathematics (1990), Shanghai Jiao Tong University*

***Current Position:***

*Professor (Jul. 2019-present), Department of Applied Physics, Hong Kong Polytechnic University*

***Positions Held:***

*Associate Professor (Jul. 2014—Jun. 2019), Department of Applied Physics, Hong Kong Polytechnic University*

*Assistant Professor (Jul. 2008—Jun. 2014), Department of Applied Physics, Hong Kong Polytechnic University*

*Lecturer (Sept. 2004—Jun. 2008), Department of Applied Physics, Hong Kong Polytechnic University*

*University Postdoctoral Fellow (May 2003—Sept. 2005), Department of Mechnical Engineering, Hong Kong Polytechnic University*

*Research Fellow (Oct. 2002—Apr. 2003), School of Electrical and Electronic Engineering, Nanyang Technological University, Singapore*

*Postdoc. Fellow (Oct. 2000—Oct. 2002), School of Materials Engineering, Nanyang Technological University, Singapore*

***Selected Awards and Honors:***

*Natural Science Award (2nd Class), the Ministry of Education, P.R.China, 2019.*

*Science and Technology Award, (2nd Class), the Ministry of Land and Resources, P.R.China, 2017.10*

*Minjiang Scholar Award (Minjiang Chair Professor, 2016.12)*

*Outstanding Achievement Award, Asia Pacific Society for Materials Research, Jul. 2014*

*Being selected in Marquis Who's Who in Asia (2007 and 2012), Marquis Who's Who in the World (2007, 2010, 2012 and 2014), and Marquis Who's Who in Science and Engineering (2011-2012, 11th Edition; 2016-2017, 12th Edition)*

***Professional Service and Memberships:***

*Advisory Board Member, Journal of Materials Chemistry C, 2014.01 to 2017.08*
*Editorial Board Member, Scientific Reports, 2015.06 to date*
*Editorial Board Member, Composites Communications, 2015.09 to date*
*Editorial Board Member, Materials Reports: Energy, 2019 to date*
*Editorial Board Member, Science of Advanced Materials, 2009.02 to date*
*Guest Editor, Journal of Applied Electrochemistry, 2018*
*Guest Editor, Composites Part A, 2008.*
*Guest Editor, Key Engineering Materials, 2007*
*Board Committee Member of the International Academy of Electrochemical Energy Science (IAOEES), 2019.05—*
*Professional Member, Chinese Society for Composite Materials, 2017.12-2022.12.*
*Member, EU Academy of Sciences, 2020*

Prof. Huang obtained his double B.Sc. degrees in Applied Physics and Applied Mathematics from Shanghai Jiao Tong University, M.Eng. in Materials Physics from Shanghai Institute of Metallurgy and Ph.D in Materials Science from Nanyang Technological University, Singapore. He is currently the Professor and Program Leader of postgraduate studies in the Department of Applied Physics, the Hong Kong Polytechnic University. His current research interests include materials for energy storage and conversion (such as supercapacitors, rechargeable batteries and solar cells), and ferroelectric materials for energy applications. He has published over 260 refereed papers in top journals, including *Nature*, *Nature Photonics*, *Joule*, *Chem*, *Nature Communications*, *Energy & Environmental Science*, and *Advanced Materials*, etc. He obtained the *Outstanding Achievement Award* from the Asia Pacific Society for Materials Research in 2014, the *Science and Technology Award* (2nd class) from the Ministry of Land and Resources of the People's Republic of China in 2017, and the *Natural Science Award* (2nd Class) from the Ministry of Education, P.R.China, in 2019. He was awarded the Chair Professorship under the "Mingjiang Scholar" scheme in 2016. He has been a Guest Editor for *Composites Part A*, *Journal of Applied Electrochemistry*, and *Key Engineering Materials*, and an advisory board member of *Journal of Materials Chemistry C* during 2014-17. He is currently on the editorial board of *Scientific Reports*, *Composites NCommunications*, *Science of Advanced Materials*, and *Materials Reports: Energy*. He is also the board committee member of the International Academy of Electrochemical Energy Science (IAOEES).

**Current Research Areas**

1. Ferroelectric Materials for Energy Applications: (1) Electric energy storage in physical capacitor using ferroelectric/antiferroelectric materials with high saturation polarization and high breakdown field. (2) Polarization-assisted pyro-/piezo-catalysis for hydrogen evolution reaction and decomposition of organic pollutants. (3) Solid-state cooling using electrocaloric effect and Olsen cycles.
2. Electrochemical Energy Storage and Electrocatalysis: (1) Flexible/wearable supercapacitors. (2) Electrocatalysts for HER, OER, and $CO_2$RR, etc.
3. Rechargeable Batteries: (1) High energy density layered oxide cathode materials for lithium-ion batteries. (2) Electrospinning of carbon-based nanostructured anode materials for batteries.
4. Solar Cells: (1) Perovskite solar cells. (2) $TiO_2$ nanotube photonic crystals for photon management of dye-sensitized solar cells.

**Book and Book Chapters**

1. H.Huang and J.F.Scott, "Ferroelectric Materials for Energy Applications", Wiley-VCH, 2018 (ISBN: 978-3-527-34271-6).
2. Y.Chen, X.Li, L.Zhou, Y.-W.Mai and H.Huang, "High-Performance Electrospun Nanostructured Composite Fiber Anodes for Lithium-Ion Batteries", *Multifunctionality of Polymer Composites: Challenges and New Solutions* (Editors: Klaus Friedrich and Ulf Breuer), Elsevier, 2015 (ISBN: 978-0-323-26434-1).
3. H.Huang, G.Zhang, H.Liang and L.Zhou, "Anodic $TiO_2$: Fabrication, Current Applications and Future Perspectives", *Nanostructured Materials for Electrochemical Biosensors* (Editors: U. Yogeswaran, S. Kumar, and S. Chen), Nova Science Publishers, Inc., NY, USA, 2009 (ISBN: 978-1-60741-706-4).

**Selected Journal Publications** (>260 in total, with a total citation >9200 times, H-index=54 according to Google Scholar as of 2020.03.26)

1. Y.Chen, Z.Wang, X.Li, X.Yao, C.Wang, Y.Li, W.Xue, D.Yu, S.Y.Kim, F.Yang, A.Kushima, G.Zhang, H.Huang, N.Wu, Y.-W.Mai, J.B.Goodenough and J.Li, "Li Metal Deposition and Stripping in a Solid-State Battery via Coble Creep", *Nature* 578, 251(2020)
2. L.Ye, Y.Ying, D.Sun, Z.Zhang, L.Fei, Z.Wen, J.Qiao and H.Huang, "Highly Efficient Porous Carbon Electrocatalyst with Controllable N-Species Content for Selective $CO_2$ Reduction", *Angew.Chem.Int.Ed.* 59, 3244 (2020). Selected as Very Important Paper (VIP).
3. H.You, Z.Wu, L.Zhang, Y.Ying, Y.Liu, L.Fei, X.Chen, Y.Jia, Y.Wang, F.Wang, S.Ju, J.Qiao, C.-H.Lam and H.Huang, "Harvesting the Vibration Energy of $BiFeO_3$ Nanosheets for Hydrogen Evolution", *Angew.Chem.Int.Ed.* 58, 11779 (2019).
4. Y.Liu, Y.Ying, L.Fei, Y.Liu, Q.Hu, G.Zhang, S.Y.Pang, W.Lu, C.L.Mak, X.Luo, L.Zhou, M.Wei and H.Huang, "Valence Engineering via Selective Atomic Substitution on Tetrahedral Sites in Spinel Oxide for Highly Enhanced Oxygen Evolution Catalysis", *J.Am.Chem.Soc.* 141, 8136 (2019) Selected as Supplementary.
5. B.Peng, Q.Zhang, B.Gang, G.Leighton, C.Shaw, S.Milne, B.Zou, W.Sun, H.Huang and Z.L.Wang, "Phase-Transition Induced Giant Negative Electrocaloric Effect in a Lead-Free Relaxor Ferroelectric Thin Film", *Energy & Environ. Sci.* 12, 1708 (2019).
6. X.Li, K.Li, S.Zhu, K.Fan, L.Lyu, H.Yao, Y.Li, J.Hu, H.Huang, Y.-W.Mai and J.B.Goodenough, "Fiber-in-Tube Design of $Co_9S_8$-carbon/$Co_9S_8$ Enables Efficient Sodium Storage", *Angew.Chem.Int.Ed.* 58, 6239 (2019) Selected as Very Important Paper (VIP).
7. K.Yao, S.Leng, Z.Liu, L.Fei, Y.Chen, S.Li, N.Zhou, J.Zhang, Y.-X.Xu, L.Zhou, H.Huang and A.K.-Y.Jen, "Fullerene-Anchored Core-Shell ZnO Nanoparticles for Efficient and Stable Dual-Sensitized Perovskite Solar Cells", *Joule* 3, 417 (2019).
8. H.You, Y.Jia, Z.Wu, F.Wang, H.Huang and Y.Wang, "Room-Temperature Pyro-Catalytic Hydrogen Generation of 2D Few-Layer Black Phosphorene Under Cold-Hot Alternation", *Nature Commun.* 9, 2889 (2018) Selected as Editors' Highlights of recent research on Energy Materials.
9. X.Xu, L.Xiao, Y.Jia, Z.Wu, F.Wang, Y.Wang, N.O.Haugen and H.Huang, "Pyro-catalytic Hydrogen Evolution by $Ba_{0.7}Sr_{0.3}TiO_3$ Nanoparticles: Harvesting Cold-Hot Alternation Energy Near Room-Temperature", *Energy & Environ. Sci.* 11, 2198 (2018) Highlighted by Royal Society of Chemistry's magazine *Chemistry World*.
10. M.Xu, L.Fei, W.Lu, Z.Chen, T.Li, Y.Liu, G.Gao, Y.Lai, Z.Zhang, P.Wang and H.Huang, "Engineering Hetero-Epitaxial Nanostructures with Aligned Li-Ion Channels in Li-Rich Layered Oxides for High-Performance Cathode Application", *Nano Energy* 35, 271 (2017)
11. M.Xu, L.Fei, W.Zhang, T.Li, W.Lu, N.Zhang, Y.Lai, Z.Zhang, J.Fang, K.Zhang, J.Li and H.Huang, "Tailoring Anisotropic Li-Ion Transport Tunnels on Orthogonally Arranged Li-Rich Layered Oxide Nanoplates Toward High-Performance Li-Ion Batteries", *Nano Lett.* 17, 1670 (2017)
12. Y.Liu, N.Fu, G.Zhang, M.Xu, W.Lu, L.Zhou and H.Huang, "Design of Hierarchical Ni-Co@Ni-Co Layered Double Hydroxide Core-Shell Structured Nanotube Array for High-Performance Flexible All-Solid-State Battery-Type Supercapacitors", *Adv.Funct.Mater.* 27, 1605307 (2017).
13. Y.Chen, X.Li, K.Park, L.Zhou, H.Huang, Y.-W.Mai and J.B.Goodenough, "Hollow Nanotubes of N-Doped Carbon on CoS", *Angew.Chem.Int.Ed.* 55, 15831 (2016) Selected as *Hot paper*.

14. C.T.Yip, X.Liu, Y.Hou, W.Xie, J.He, S.Schlücker, **D.**Lei and H.Huang, "Strong Competition Between Electromagnetic Enhancement and Surface-Energy-Transfer Induced Quenching in Plasmonic Dye-Sensitized Solar Cells: A Generic yet Controllable Effect", *Nano Energy* 26, 297 (2016).
15. J.Lin, M.Guo, C.T.Yip, W.Lu, G.Zhang, X.Liu, L.Zhou, X.Chen and H.Huang, "High Temperature Crystallization of Free-Standing Anatase $TiO_2$ Nanotube Membranes for High Efficiency Dye-Sensitized Solar Cells", *Adv.Funct.Mater.* 23, 5952 (2013).
16. G.Zhang, W.Li, K.Xie, F.Yu and H.Huang, "A One-Step and Binder-Free Method to Fabricate Hierarchical Nickel-Based Supercapacitor Electrodes with Excellent Performance", *Adv.Funct.Mater.* 23, 3675 (2013)
17. M.Guo, K.Xie, J.Lin, Z.Yong, C.T.Yip, L.Zhou, Y.Wang and H.Huang, "Design and Coupling of Multifunctional $TiO_2$ Nanotube Photonic Crystal to Nanocrystalline Titania Layer as Semi-Transparent Photoanode for Dye-Sensitized Solar Cell", *Energy Environ. Sci.* 5, 9881 (2012)
18. Y.Chen, Z.Lu, L.Zhou, Y.-W.Mai and H.Huang, "Triple-Coaxial Electrospun Amorphous Carbon Nanotubes with Hollow Graphitic Carbon Nanospheres for High-Performance Li Ion Batteries", *Energy Environ. Sci.* 5, 7898 (2012)
19. C.T.Yip, H.Huang, L.Zhou, K.Xie, Y.Wang, T.Feng, J.Li, and W.Y.Tam, "Direct and Seamless Coupling of $TiO_2$ Nanotube Photonic Crystal to Dye-Sensitized Solar Cell: A Single-Step Approach", *Adv.Mater.* 23, 5624 (2011) (Selected as *Frontispiece article*)
20. H.Huang, "Solar Energy: Ferroelectric Photovoltaics", *Nature Photonics* 4, 134 (2010)

**On-going Projects**

1. Flexible High Temperature and High Energy Density Dielectric Materials Based on PTFE (Shenzhen Science, Technology and Innovation Commission), RMB3,000,000, Nov.1, 2019—Apr.30, 2022 (PI).
2. Surface Plasmon Enhanced Pyro-Catalytic Water Splitting by Ferroelectric Materials (General Research Fund, Research Grants Council, Hong Kong), HK$869,898, Jan.1, 2020—Dec.31, 2022 (PI).
3. High Performance Battery Materials (Hong Kong Polytechnic University), HK$315,000, Jan.7, 2019—Jan.6, 2021 (PI).
4. Multifunctional Nanocoating for High-Performance Nickel-Rich Layered Oxide Cathode Materials (General Research Fund, Research Grants Council, Hong Kong), HK$632,421, Jan.1, 2019—Dec.31, 2021 (PI).
5. Controllabe Engineering of Layered/Spinel Heterostructure in 3D High-Capacity/Voltage Cathode Towards Ultrahigh Areal Energy Density Solid-State Thin Film Li-ion Battery (Hong Kong Polytechnic University), HK$645,000, Aug.1, 2018—Jul.31, 2020 (PI).

# Material Model to Capture the Damage Effects in a Football Player's Brain

## by Mark F. Horstemeyer, Member EUAS

Short Biography

***Mark F. Horstemeyer, Dean of Engineering, Liberty University***

*As a fellow of four societies (ASME, ASM, SAE, and AAAS) Dr. Mark F. Horstemeyer has published close to 500 journal articles, conference papers, books, and technical reports with a citation impact h-factor over 60 with a total of over 12,000 citations; he has been invited to give over 150 lectures throughout the world (was named as honorary professor of Xihua University, Chengdu, China); and has won many awards (R&D 100 Award, AFS Best Paper Award, Sandia Award for Excellence, Ralph E. Powe Research Award, Ohio State's Thomas French Alumni Achievement Award); and has mentored over 120 graduate students and post-doctoral researchers. He has started two start-up companies in trying to put predictive science into engineering designs: Predictive Design Technologies, LLC; Advanced Technology Associates, LLC. He earned a B.S. degree (with honors) from West Virginia University in Mechanical Engineering in 1985, a M.S. degree from Ohio State University in Eng. Mechanics in 1987, and a Ph.D. from Georgia Institute of Technology in Mech. Eng. and Math & Matls (minors) in 1995. He is currently Dean of Engineering at Liberty University. Previous to that, he worked at Sandia National Labs (1987-2002) and Mississippi State University (2002-2018), where he held a Chair position for the Center for Advanced Vehicular Systems (CAVS) in Computational Solid Mechanics. He couples multidiscale, multiphysics research of mechanics and materials in three synergistic areas: theoretical modeling, experimentation, and large scale parallel computational simulation.*

Regarding concussions in American football, Dr. Horstemeyer has recently developed a material model to capture the damage effects in a football player's brain (Horstemeyer, M.F., Berthelson, P.R., Moore, J., Persons, A.K., Dobbins, A. and Prabhu, R.K., 2019. A mechanical brain damage framework used to model abnormal brain tau protein accumulations of National Football League players. *Annals of biomedical engineering*, *47*(9), pp.1873-1888.). A mechanics-based brain damage framework was used to model the abnormal accumulation of hyperphosphorylated p-tau associated with Chronic Traumatic Encephalopathy (CTE) within the brains of deceased National Football League (NFL) players studied at Boston University and to provide a framework for

understanding the damage mechanisms. P-Tau Damage is formulated as the multiplicative decomposition of three independently evolving damage Internal State Variables (ISVs): nucleation related to number density, growth related to the average area, and coalescence related to the nearest neighbor distance. The ISVs evolve under different rates for three well known mechanical boundary conditions, which in themselves introduce three different rates making a total of nine scenarios, that we postulate are related to brain damage progression: 1) monotonic overloads, 2) cyclic fatigue which corresponds to repetitive impacts, and 3) creep which is correlated to damage accumulation over time. Different NFL player positions are described to capture the different types of damage progression. Skill position players, such as quarterbacks, are expected to exhibit a greater p-tau protein accumulation during Low Cycle Fatigue (LCF) (higher amplitude impacts with a lesser number), and linemen who exhibit a greater p-tau protein accumulation during High Cycle Fatigue (HCF) (lower amplitude impacts with a greater number of impacts). This mechanics-based damage framework presents a foundation for developing a multiscale model for Traumatic Brain Injury (TBI) that combines mechanics with biology. Figure 1 shows four different levels of the brain damage of four different NFL players who died. Figure 2 shows the comparison of the Horstemeyer brain damage model with the experimental data representing different deceased NFL players who incurred brain damage.

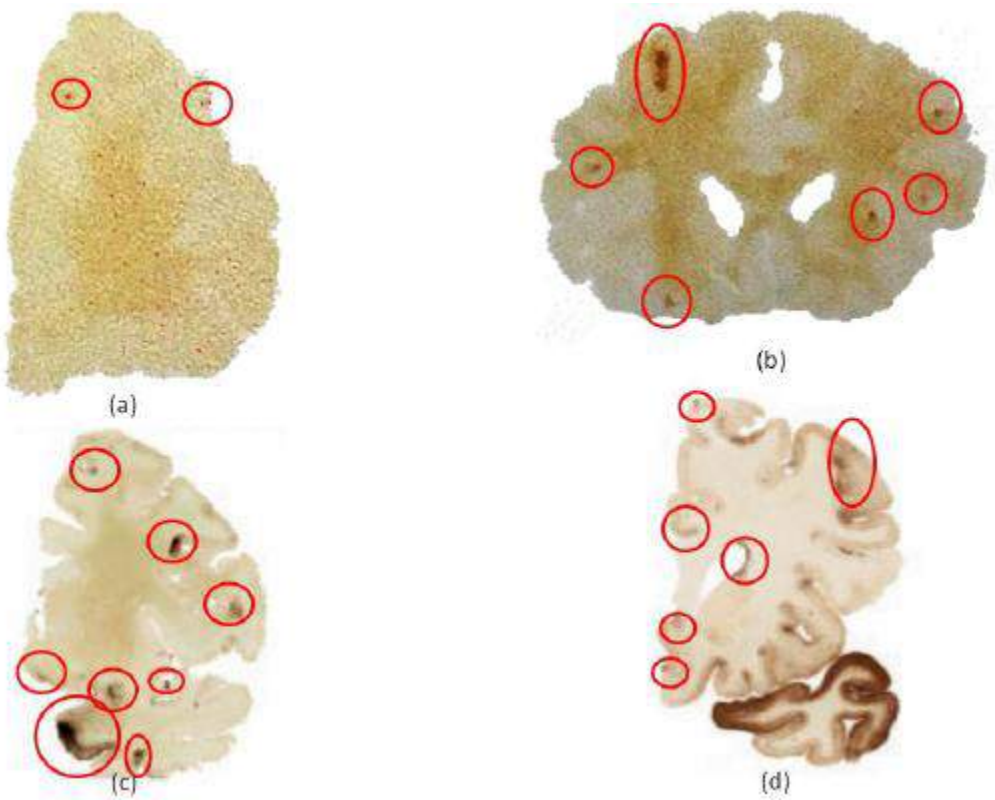


**Figure 1**. Comparison of Tau Protein stages found in the brains of deceased athletes analyzed by McKee *et al.* illustrating each stage of damage: (a) Stage 1 shows a Tau Protein area fraction of 0.03% with two nucleation sites at an age of 28.3+13 years; (b) Stage 2 shows a Tau Protein area fraction of 0.59% with six nucleation sites at an age of 44.3+16 years; (c) Stage 3 shows a Tau Protein area fraction of 2.87% with eight

nucleation sites at an age of 56.0+14 years; and (d) Stage 4 shows a Tau Protein area fraction of 20.85% with twenty three nucleation sites (we did not circle them all because there are too many) at an age of 77.4+12 years. Note that scales and brain regions differ in the four images.

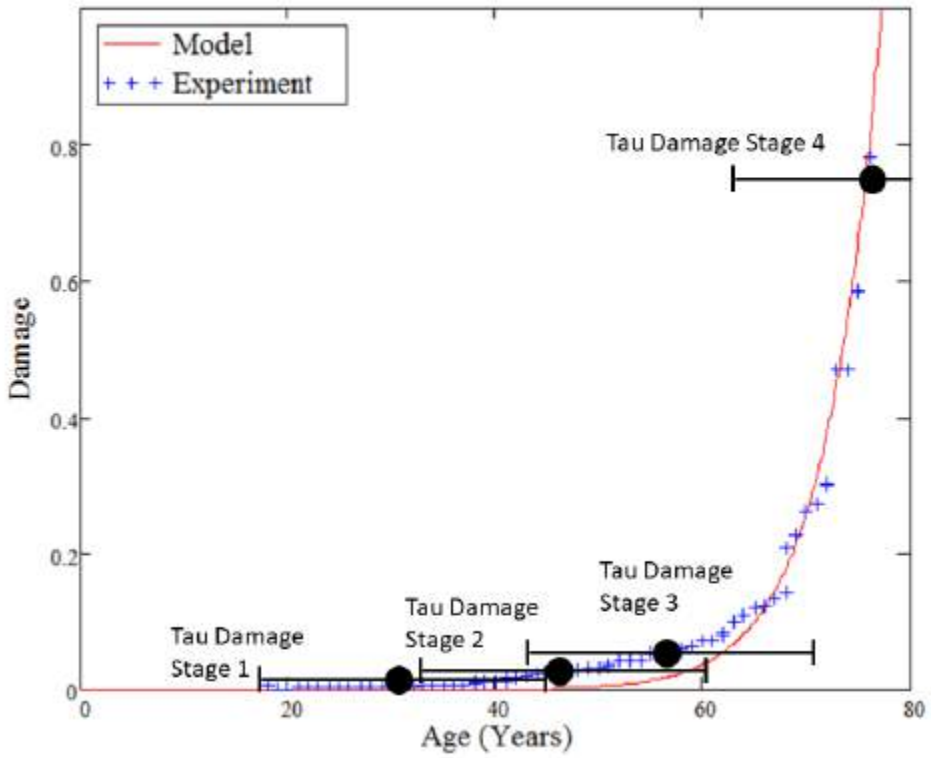


**Figure 2.** The damaged Tau protein region sorted in ascending order from experimental data. The damage model (red line) of Horstemeyer captures the relationship between the tau protein damage sorted in ascending order. The multiplication of the nucleation, growth, and coalescence functions gives rise to the Tau protein area fraction curve (red line). The blue plus signs are experimental data representing a different NFL player who died with TBI.

# Transforming Liquefied Natural Gas (LNG) Plant Construction Productivity through Mobile Computing Technologies

**by Xiangyu Wang, Member EUAS**

Short Biography

***Work Experience***

*Professor (Personal Chair) (2011 to presence), Curtin University, Australia*
*Curtin-Woodside Chair Professor for Oil, Gas & LNG Construction and Project Management (July 2013-July 2018), Curtin University, Australia*
*College of Experts, ARC (Australian Research Council) (January 2016 – Dec 2018), Australian Government*
*Acting Woodside Chair Professor of LNG Construction (February 2012 – July 2013), Curtin University, Australia*
*Curtin Director of Australasian Research Centre for Building Information Modelling (BIM) (March 2012 - presence), Curtin University, Australia*
*Editor-in-Chief, Visualization in Engineering: an International Journal, Springer-Verlag (2012 - presence)*

***Education***

*Ph.D., Purdue University, 2005*
*Master, University of Washington, 2002*
*Bachelor, Tongji University, 2000*

***Recognitions***

*Member, EU Academy of Sciences, since 2018*
*Keynote and Plenary Speakers for over 50 International conferences/forums*
*World Top 100 Engineers, 2014*
*External judge for Innovation and Technology award, 2013 Woodside Awards*
*The impact of his work was reported over 40 times by a wide range of international and domestic prestigious media. His work with his industry partners was featured twice in the Australian newspaper,* Energynewsbulleting.net, *ScienceWA magazine, LNG World News, Business News, Western Australian Energy Research Alliance, CNN, the Conversation, and Energy Publications*
*Editor-in-chief, Visualization in Engineering: an International Research Journal, Springer Verlag*
*Editorial Board Member, Journal of Construction Engineering and Management, American Society of Civil Engineers (ASCE) (2007-present), Journal of Information Technology in Construction (ITcon), Engineering, Construction and Architectural Management (ECAM), since 2015, The Open Construction and Building Technology Journal, Bentham Science Publisher, since 2011, Journal of Frontiers in Construction Engineering (FCE), since 2012, Journal of Construction Engineering, Science and Engineering Publishing Company, since 2012, International Journal of Oil and Gas, since 2014, Journal of Frontiers of Information and Communication Technology, since 2014*
*Guest Editor, Automation in Construction, Elsevier, 2009, 2012, 2013, 2014, Journal of Operational Research Society, 2012, Journal of Information Technology in Construction (ITcon) 2012, 2014, International Journal of Advanced Robotic Systems, 2012, Journal of Industrial and Management Optimization, 2013, 2014, Archives of Computational Methods in Engineering, 2014, Journal of Intelligent and Robotic Systems, 2014, Scientific World Journal, 2014.*
*Book Editor, for over 10 books for Springer Verlag, Wiley, IGI Global, and Bentham eBook*

**MOST RECENT SIGNIFICANT RESEARCH**

**1. ARC (Australian Research Council) Linkage Project 2013-2016 (#LP130100451)**

**Title:** Transforming Liquefied Natural Gas (LNG) Plant Construction Productivity through Mobile Computing Technologies

**Abstract:** Australia's liquefied natural gas (LNG) construction industry is plagued by major cost blowouts. This project will investigate a new mobile computing approach for streamlining LNG construction projects, thus yielding significant productivity gains

**Representative Publications:**

- Chi, H. L., Kang, S. C., & Wang, X. (2013). Research trends and opportunities of augmented reality applications in architecture, engineering, and construction. Automation in construction, 33, 116-122.
- Park, C. S., Lee, D. Y., Kwon, O. S., & Wang, X. (2013). A framework for proactive construction defect management using BIM, augmented reality and ontology-based data collection template. Automation in Construction, 33, 61-71.
- Jun Wang, Wenchi Shou, Xiangyu Wang & Peng Wu(2016),Developing and evaluating a framework of total constraint management for improving workflow in liquefied natural gas construction, Construction Management and Economics, 34:12,859-874

**2. ARC Linkage Project 2014-2017 (#LP140100873)**

**Title:** Boosting Up Productivity: Optimizing Scaffolding Life Cycle Management with Virtual Design and Construction

**Abstract:** This project aims to innovatively integrate a decision support system, virtual design and construction, and onsite monitoring into one dynamic scaffolding planning system to significantly lift productivity. The emphasis is on producing optimal solutions for planning, design, erection, dismantling, and relocation of scaffolding, so that productivity is maximised subject to satisfying required cost and safety constraints.

**Representative Publications:**

- Hou, L., Zhao, C., Wu, C., Moon, S., & Wang, X. (2016). Discrete firefly algorithm for scaffolding construction scheduling. Journal of Computing in Civil Engineering,31(3), 04016064.
- Moon, S., Xu, S., Hou, L., Wu, C., Wang, X., & Tam, V. W. (2017). RFID-aided tracking system to improve work efficiency of scaffold supplier: stock management in Australasian supply chain, Journal of Construction Engineering and Management,144(2), 04017115.
- Lopez, R., Chong, H. Y., Moon, S., & Wang, X. (2017). Case study on subcontracting arrangements in the scaffolding supply chain of a Liquefied Natural Gas infrastructure project. Journal of Civil Engineering and Management,23(8), 1136-1147.

**3. ARC Linkage Project 2016-2019 (#LP160100528)**

**Title:** Bridge Performance Assessment through Advanced Sensing and Modelling

**Abstract:** The aim of this project is to develop an innovative approach for bridge infrastructure performance assessment and reserve capacity estimation based on advanced sensing and modelling. The proposed approach consists of: (1) Laser Scanning, (2) Optimal Wireless Sensing, (3) In-situ Data Interpretation and (4) Building Information Modelling (BIM).

**Representative Publications:**

- Liang, R., Dong, Z., Sheng, Z., Wang, X., & Wu, C. (2017). Case study of selecting decision-making schemes in large-scale infrastructure projects. Journal of Infrastructure Systems,23(4), 06017001
- Zhu, J., Wang, X., Wang, P., Wu, Z., & Kim, M. J. (2019). Integration of BIM and GIS: Geometry from IFC to shapefile using open-source technology. Automation in Construction,102, 105-119.
- Zhu, J., Wang, X., Chen, M., Wu, P., & Kim, M. J. (2019). Integration of BIM and GIS: IFC geometry transformation to shapefile using enhanced open-source approach. Automation in Construction,106, 102859.

**4. ARC Discovery Project 2017-2019 (#DP170104613)**

**Title:** Automatic Construction Monitoring through Semantic Information Modelling

**Abstract:** This project aims to develop computational algorithms and methods for automatic as-built construction monitoring through semantics-based Building Information Modelling (BIM). Construction as–built monitoring is crucial for the cost, time, quality and safety of projects. Methods for generating as-built status are primarily manual. There are gaps in sophistication of automation, and recognition for semantic construction information during the process is low. The project is expected to provide efficient and accurate solutions for as-built construction monitoring.

**Representative Publications:**

- Chong, H. Y., Lee, C. Y., & Wang, X. (2017). A mixed review of the adoption of Building Information Modelling (BIM) for sustainability. Journal of Cleaner Production, 142, 4114-4126.
- Song, Y., Wang, X., Tan, Y., Wu, P., Sutrisna, M., Cheng, J. C., & Hampson, K. (2017). Trends and opportunities of BIM-GIS integration in the architecture, engineering and construction industry: a review from a spatio-temporal statistical perspective. ISPRS International Journal of Geo-Information,6(12), 397.
- Tan, Y., Song, Y., Liu, X., Wang, X., & Cheng, J. C. (2017). A BIM-based framework for lift planning in topsides disassembly of offshore oil and gas platforms. Automation in construction,79, 19-30.

**5. ARC Discovery Project 2017-2019 (#DP170104612)**

**Title:** A Multi-agent System for Stakeholder Management in Off-site Construction

**Abstract:** This project aims to investigate a socio-technology model for stakeholders and informatics to improve off-site construction (OSC) productivity in infrastructure construction. A multi-agent system for OSC could drive down cost,but requires highly integrated collaboration among stakeholders. The project's quantitative approaches include large-scale social network analysis, multi-agent consensus modelling and an optimisation algorithm for collaborative planning. The project outcomes are expected to secure long-term economic benefits by enhancing performance in complex projects.

**Representative Publications:**

- Teng, Y., Mao, C., Liu, G., & Wang, X. (2017). Analysis of stakeholder relationships in the industry chain of industrialized building in China. Journal of Cleaner Production,152, 387-398.
- Hu, X., Chong, H. Y., & Wang, X. (2019). Sustainability perceptions of off-site manufacturing stakeholders in Australia. Journal of Cleaner Production,227, 346-354.
- Hu, X., Chong, H. Y., Wang, X., & London, K. (2019). Understanding Stakeholders in Off-Site Manufacturing: A Literature Review. Journal of Construction Engineering and Management,145(8), 03119003.

**6. ARC Industrial Training Centre 2016-2021 (#IC150100023)**

**Title:** ARC Training Centre for Advanced Manufacturing of Prefabricated Housing

**Abstract:** The training centre aims to unlock the potential potential growth of Australia's prefabricated building industry by creating a sustainable training ecosystem including both industry and universities.

**Representative Publications:**

- Chai, J., Wu, C., Zhao, C., Chi, H. L., Wang, X., Ling, B. W. K., & Teo, K. L. (2017). Reference tag supported RFID tracking using robust support vector regression and Kalman filter. Advanced Engineering Informatics,32, 1-10.
- Hou, L., Chi, H. L., Tarng, W., Chai, J., Panuwatwanich, K., & Wang, X. (2017). A framework of innovative learning for skill development in complex operational tasks. Automation in Construction,83, 29-40.
- Wu, C., Wang, X., Chen, M., & Kim, M. J. (2019). Differential received signal strength based RFID positioning for construction equipment tracking. Advanced Engineering Informatics,42, 100960.

**7. ARC Linkage Project 2019-2022 (#LP180100222)**

**Title:** Asset Intelligence: Maximising Operational Effectiveness for Digital Era

**Abstract:** The primary aim of this project is to develop an innovative lifecycle semantic-based decision making approach through asset intelligence so as to maximise the operational effectiveness maintenance, repair and rehabilitation planning of infrastructure assets.

# Vascular Dysfunction in Cardiovascular (CV) Disease

## by Thomas F. Lüscher, Member EUAS

Short Biography

*Professor Lüscher studied medicine at the University of Zurich and obtained his post-graduate training in internal medicine, clinical pharmacology and cardiology at this institution. He then moved, as Research Associate in Cardiovascular Pharmacology, to the Mayo Clinic and Mayo Foundation in Rochester, Minnesota where he started his research on endothelial function and CVD and also further pursued his clinical training. He moved to the University of Basel, as a consultant in cardiology and research group leader in vascular biology and later became Professor of Pharmacotherapy at this institution. In 1993 he moved to the University of Bern as Co-Director of Cardiology, before being nominated Professor and Chairman of the University Heart Center at Department of Cardiology of the Uni-versity Hospital, Zurich, Switzerland in 1996. In 2017 he accepted the position of Director of Research, Education and Development at the Royal Brompton and Harefield Hospitals and Professor of Cardiology at Imperial College, London. Simultaneously, he holds a part-time position as Professor of Cardiology and Chairman of the Center for Molecular Car-diology at the University of Zurich.*

*Important other activities of Professor Thomas F. Lüscher are in publishing as Editor-in-Chief of the European Heart Journal, the ESC Textbook of Cardiovascular Medicine and other educational products for students and physicians. He is also President of the Zurich Heart House - Foundation for Cardiovascular Research, which organizes important educational events such as the London Postgraduate Course in Heart Failure and Cardiology Update*

*Postgraduate courses in Davos, Switzerland; London, UK and Mumbai, India.*

**Research and Science**

Research has focused on understanding vascular dysfunction in cardiovascular (CV) disease. Indeed, blood vessels and their function and structure play an essential role in maintaining CV haemostasis, while their dysfunction is crucially involved in the development of angina pectoris, myocardial infarction and stroke. An crucial regulator are endothelial cells, which are strategically located between the circulating blood and smooth muscle cells, where structure and function of blood vessels is regulated. Important mediators of endo-thelial control of the circulation are nitric oxide, prostaglandins, endothelium-derived hyper-polarizing factors on the one hand and endotheliumderived contracting factors such as en-dothelin and prostanoids on the other hand. They not only regulate vasomotion, but also structural changes related to migration and proliferation of smooth muscle leading to vas-cular stiffening and increased resistance. Their luminal release inhibits or activates circu-lating platelets. Endothelial cells produce tissue factor when exposed to cytokines leading to thrombus formation. Endothelial mediators regulate the human CV system under normal conditions and their dysfunction is involved in hypertension, induced by lipoproteins and glucose as well as mechanical forces. Endothelial dysfunction is an early stage of CV disease, leading eventually to structural changes, i.e. medial hypertrophy and remodelling and plaque formation. Endothelial function is also regulated by longevity and aging genes; their interplay not only affects lifespan, but is a final common pathway of CV disease. The translation of molecular pathways in isolated cells and animal

models into human CV disease including coronary artery disease and the reversal of endothelial dysfunction by ACE inhibitors and calcium antagonists was a major achievement.

More recently, inflammation in acute coronary syndromes (ACS) was a major topic. At sites of coronary occlusion, interleukin-6 and other cytokines are upregulated leading to the expression of matrix metallopeptidases and fibrin activating protein and in turn to plaque rupture and thrombus formation. Novel proteins involved in ACS were characterized such as Cyr-61 and gut microbiome derived molecules such as trimethylamine (TMAO) as well as trimethyllysine (TML) which are highly predictive of outcomes in ACS.

Finally, we characterized a new ACS, i.e. Takotsubo syndrome (TTS), a microcirculatory disturbance induced by a sympathetic surge originating in the mid-brain, mainly in post-menopausal women, leading to left ventricular dysfunction with apical ballooning. Of note, TTS has an in-hospital mortality of around 4% and major adverse coronary events thereafter.

Thus, our research is a paradigmatic translational endeavor to understand molecular mechanism in cells, tissue and animal models and translating it into a clinical context with potential therapeutic applications. As such, the group has importantly contributed the understanding of cardiovascular disease and is among the most highly cited ones with an h-index of 128.

# Improvements in Watershed Science

## by Jeffrey J. McDonnell, Member EUAS

Short Biography

***EDUCATION***

*1989* ***Ph.D., Forest Hydrology****. University of Canterbury, Christchurch, New Zealand. Thesis: "The age, origin and pathway of subsurface stormflow in a steep humid headwater catchment", 270p.*

*1985* ***M.Sc., Watershed Ecosystems Graduate Program****, Trent University, Peterborough, Canada. Thesis: "Snowcover ablation and meltwater runoff on a small Precambrian Shield watershed", 127p.*

*1983* ***B.Sc. (Honors), Physical Geography*** *(now Physical & Environmental Sciences), University of Toronto, Toronto, Canada. Thesis: "Storm waves, sediment flux and beach morphodynamics in a barred nearshore zone, Wymbolwood Beach, Ontario", 110p.*

***PROFESSIONAL EXPERIENCE***

*2012-* ***Professor****, School of Environment and Sustainability;* ***Associate Director (International)****, Global Institute for Water Security, University of Saskatchewan, Saskatoon, Saskatchewan.*

*1999-2012* ***Richardson Chair in Watershed Science*** *(1999-12);* ***University Distinguished Professor*** *(2009-12), Department of Forest Engineering, Resources and Management;* ***Director*** *(2010-12), Institute for Water and Watersheds, Oregon State University, Corvallis Oregon.*

*1993-99* ***Associate Professor*** *(1993-97);* ***Professor*** *(1997-99), SUNY College of Environmental Science and Forestry, Syracuse, New York.*

*1989-93* ***Assistant Professor****, Department of Forest Resources, Utah State University, Logan Utah.*

*1989-90* ***Research Hydrologist****, NASA Marshall Space Flight Center, Universities Space Research Assoc., Huntsville, Alabama.*

***EXECUTIVE SUMMARY***

*GS h index = 83 March 2020 (Total citations 26,580) i10 index = 240, WOS h index = 69 (as of April 20, 2020)*

***MAJOR HONORS and AWARDS***

*2017* *Leonardo Lecture, European Geophysical Union, EGU Leonardo Conference, Saig, Germany*

*2016* *Gallagher Lecturer, Department of Geoscience, University of Calgary, Alberta*

*2016* *International Hydrology Prize (Dooge Medal), International Association of Hydrological Sciences/UNESCO/World Meteorological Organization.*

*2015* *Elected to the Royal Society of Canada (Canada's National Academy of Science)*

*2015* *Boussinesq Award Lecture, Royal Netherlands Academy of Arts and Sciences, Amsterdam, Netherlands*

*2015* *EGU Dooge Award for best paper in Hydrology and Earth System Science "Hydrological connectivity inferred from diatom transport through the riparian system".*

*2014* *Elected Fellow, Geological Society of America*

*2013* *Nannerl Keohane Distinguished Lecture and Award, UNC Chapel Hill and Duke University*

*2012* *Borland Lecture Award, Hydrology Days, Colorado State University, Fort Collins*

| | |
|---|---|
| *2011* | *Birdsall-Dreiss Distinguished Lecturer, Geological Society of America (50 university lecture tour)* |
| *2009* | *Doctor of Science (DSc), University of Canterbury* |
| *2009* | *John Dalton Medal, European Geosciences Union* |
| *2009* | *Woo Lecturer, Canadian Geophysical Union* |
| *2009* | *Elected Fellow, American Geophysical Union* |

**BRIEF RESEARCH**

Jeffrey McDonnell was the first endowed chair in Watershed Science in the USA and was awarded the highest distinction of the Oregon State University as University Distinguished Professor. In 2016 he received the International Hydrology Prize (Dooge Medal) from the International Association of Hydrological, UNESCO and the World Meteorological Organization (2016). His work includes two studies highlighted on the cover of *Nature Geoscience* (2010; 2017) and further international recognition including the election as Fellow of the Royal Society of Canada (Canada's National Academy of Science), Fellow of the American Geophysical Union (2009), Fellow of the Geological Society of America (2014), Fellow and Life Member, International Water Academy (2005) and Fellow of the European Union Academy of Sciences (2019). He has received the Dalton Medal (2009) from the European Geophysical Union and the Birdsall-Dreiss Distinguished Lecturer Award (2011) from the Geological Society of America and the Gordon Warwick Medal (1998) from the British Society for Geomorphology. He has delivered the Penman Lecture to the British Hydrology Society, the Woo Lecture to the Canadian Geophysical Union and the Boussinesq Award Lecture to the Royal Netherlands Academy of Arts and Sciences. Most recently, he was awarded the University of Saskatchewan's Distinguished Researcher Award and the J.W. George Ivany Internationalization Award where he is now Professor of Hydrology and Associate Director of the Global Institute for Water Security.

Over the past thirty years, McDonnell and colleagues' work has expanded the fundamental understanding of hillslope hydrology with implications for our understanding of catchment hydrology and models of rainfall-runoff:

- Pioneering approaches in stable isotope tracing of water infiltrating into and transiting catchments—from the first field deployment of laser spectrometer for rainfall-runoff analysis to the first lab intercomparison of soil water extraction techniques.
- Discovery of common runoff behavior across diverse hillslope systems, leading to the first recognition that all runoff is the same and leading the development of a new theory of "fill-and-spill" for runoff generation across scale.
- Discovery of ecohydrological separation—that different pools of water supply plant transpiration vs groundwater recharge and streamflow generation, with related publications in Nature-Geoscience and Nature.
- Transforming understanding of the age of streamflow from some of the first work on soil water residence times to the first incorporation of transit times into

conceptual rainfall-runoff models and discovery of scaling relations between streamwater transit time and flowpath length and gradient.

Beyond his science, McDonnell has served as President of the AGU Hydrology Section and served as President of the IAHS International Commission on Tracers. He has also been an ardent early career supporter with seven early mentoring articles that have appeared in Science and Nature with a combined Altmetric score of over 3000. All this has culminated in his 2020 book *Navigating an Academic Career: A Brief Guide for PhD Students, Postdocs and Early Career Faculty*, published by John Wiley and Sons.

## SELECTED PAPERS LAST TWO YEARS

### *2019*

Benettin, P., P. Queloz, M. Bensimon, J.J. McDonnell and A. Rinaldo, 2019. Velocities, residence times, tracer breakthroughs in a vegetated lysimeter: a multitracer experiment. Water Resources Research, DOI:10.1029/2018WR023894

Blöschl, G., M. Bierkens, A. Chambel, C. Cudennec, G. Destouni, A. Fiori, J. Kirchner, J.J. McDonnell, H. Savenije, M. Sivapalan, C. Stumpp, E. Toth, E. Volpi, G. Carr, J. Salinas, B. Széles, A. Viglione and 200 others, 2019. 23 unsolved problems in hydrology – a community perspective. Hydrological Sciences Journal, 64:10, 1141-1158, DOI:10.1080/02626667.2019.1620507

Coles, A.E., B. McConkey and J.J. McDonnell, 2019. Fifty years of recorded hillslope runoff on seasonally-frozen ground: The Swift Current, Saskatchewan, Canada dataset. Earth System Science Data, in press.

Evaristo, J., M. Kim, J. van Haren, L. Pangle, C. Harman, P. Troch and J.J. McDonnell, 2019. Characterizing the fluxes and age distribution of soil water, plant water, and deep percolation in a model tropical ecosystem. Water Resources Research, DOI:10.1029/2018WR023265.

Evaristo, J. and J.J. McDonnell, 2019. Global analysis of streamflow response to forest management. Nature, DOI:10.1038/s41586-091-1306-0 (retracted Feb 2020 in issue 578:326, DOI: 10.1038/s41586-020-1945-1)

Fan, Y, M. Clark, D. Lawrence, S. Swenson, L. Band, S. Brantley, P. Brooks, W.E. Dietrich, A. Flores, G. Grant, J. Kirchner, D. Mackay, J.J. McDonnell, P. Milly, P. Sullivan, C. Tague, H. Ajami, N. Chaney, A. Hartmann, P. Hazenberg, J. McNamara, J. Pelletier, J Perket, E. Rouholahnejad-Freund, T. Wagener, X. Zeng, E. Beighley, J. Buzan, M Huang, B. Livneh, B.
Mohanty, B. Nijssen, M. Safeeq, C. Shen, W. van Verseveld, J. Volk and D Yamazaki, 2019. Structures and functions of hillslope hydrology with relevance to Earth System Modeling: Syntheses and testable hypotheses. Water Resources Research, DOI:10.1029/2018WR023903.

Gaj, M. and J.J. McDonnell, 2019. Soil tension controls the isotopic fractionation factor for evaporation from soil. Hydrological Processes, DOI:10.1002/hyp.13418.

Gaj, M., A. Lamparter, S. Woche, J. Bachmann, J.J. McDonnell and F. Stange, 2018. The role of matric potential, solid interfacial chemistry and wettability on isotopic equilibrium fractionation. Vadose Zone Journal, DOI:10.2136/vzj2018.04.0083.

Lazo, P., G. Mosquera, J.J. McDonnell and P. Crespo, 2019. The role of vegetation, soils, and precipitation on water storage and hydrological services in Andean Páramo catchments. Journal of Hydrology, DOI:10.1016/j.jhydrol.2019.03.050.

Li, H., B. Si, P. Wu and J.J. McDonnell, 2019. Water mining from deep critical zone by apple trees growing on loess in monsoonal climate. Hydrological Processes, DOI:10.1002/hyp.13346.

López-Días, V., N. Martínez-Carreras, F. Barnich, T.Wirtz, J.J. McDonnell and L. Pfister, 2019. Fractionation of 2H/H and 18O/16O isotopic ratios in water through nafion membranes. Journal of Membrane Science, 752:128-139, DOI:10.1016/j.memsci.2018.11.003.

McDonnell, J.J., 2019. Step up to leadership for mid-career growth. Nature, DOI:10.1038/d41586-019-01936-7.

Nehemy, M., C. Millar, K. Janzen, M. Gaj, D. Pratt, C. Laroque and J.J. McDonnell, 2019. $^{17}O$- excess as a detector for co-extracted organics in vapor analyses of plant isotope signatures. Rapid Communications in Mass Spectrometry, 33(16): 1301-1310.

Pfister, L., C. Grave, J. Beisel and J.J. McDonnell, 2019. A global assessment of freshwater mollusk shell oxygen isotope signatures and their relation to precipitation and stream water. Scientific Reports, DOI:10.1038/s41598-019-40369-0.

Sprenger, M., C. Stumpp, S. Allen, P. Benettin, M. Dubbert, A. Hartmann, M. Hrachowitz, J. Kirchner, J.J. McDonnell, N. Orlowski, D. Penna, S. Pfahl, M. Rinderer, N. Rodriguez, C. Werner and M Weiler, 2019. The demographics of water: A review of water ages in the critical zone. Reviews of Geophysics, DOI:10.1029/2018RG000633

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# Publication Ethics in the Open-Access Era

## by George Perry, Member EUAS

Short Biography

*George Perry is Professor of Biology and Chemistry, Semmes Foundation Distinguished University Chair in Neurobiology, and former Dean of Sciences at The University of Texas at San Antonio. Perry has studied Alzheimer's disease since 1982 and was the first to discover that oxidative stress is a key feature of this and related neurodegenerative diseases. His studies identified oxidative damage, its source from metabolic/mitochondria failure and catalysis by iron and copper. This work led to a novel interpretation of the role of amyloid—that instead of causing Alzheimer's disease, it is a protective antioxidant response, and the reason all the amyloid-based therapies have failed.*

*Perry received his Bachelor of Arts degree in zoology with high honors from University of California, Santa Barbara. After graduation, he headed to Scripps Institution of Oceanography and obtained his Ph.D. in marine biology under David Epel in 1979. He then received a postdoctoral fellowship in the Department of Cell Biology in the laboratories of Drs. Bill Brinkley, Anthony Means and Joseph Bryan at Baylor College of Medicine where he laid the foundation for his observations of abnormalities in cell structures.*

*He is distinguished as one of the top Alzheimer's disease researchers with over 1000 publications, one of the top 100 most-cited scientists in neuroscience and behavior and one of the top 25 scientists in free radical research.*

*Perry has been cited over 92,000 times and is recognized as an ISI highly cited researcher (H=153). Perry is editor-in-chief for the Journal of Alzheimer's Disease, the most cited journal in the field. He is a fellow of the American Association for the Advancement of Sciences, Texas Academy of Sciences, and the Microscopy Society of America. He is past-president of the Southwestern and Rocky Mountain Division of the American Association for the Advancement of Science and past-president of the American Association of Neuropathologists. He was awarded the Society for the Advancement of Chicanos and Native American in the Sciences' (SACNAS) Distinguished Professional Mentor Award, the Senior Investigator Award of the International College of Geriatric Psychoneuropharmacology (ICGP), Martin Goland Award of the Alamo Chapter of Sigma Xi, and Senior Fulbright Scholar. He was elected a Foreign Corresponding Member of the Academy of Sciences of Lisbon, Foreign Correspondent Member of the Spanish Royal Academy of Sciences, Corresponding Member of the Mexican Academy of Sciences, and Member of the Dana Alliance for Brain Initiatives.*

*For over a decade, Perry hosted the Texas Science and Engineering Fair. He has mentored over a hundred students and fellows in research.*

## Abstract

As new scientific journals seem to be born hourly, the process of selecting in which to publish can bewilder. The open-access journal revolution of knowledge dissemination creates opportunities, while at the same time, threats from "predatory" journals undermine scientific rigor. We need to look back centuries for a similar challenge: the printing press, which made laborious hand copying no longer necessary but created the opportunity for disinformation. *Imprimatur* was then used to validate information. Religious authority during the Age of Enlightment was ceded to the scientific academies that produced collections of letters, the precursor of the journal article. Each academy set its standards for publication based on their illustrious members. Using the academies as models, other learned societies also developed journals, lending their reputation and society standards. It was only 150 years ago that Nature arose as a leading, entirely private and for profit, journal. These private venues had to establish their own standards and validation: the cost and complexities of publication required a certain discipline and these private publications existed on this platform. Open-access journals have disposed of the cost and complexity of publication. While many established publishers embrace open-access, poorly resourced companies continue to enter with limited peer review and even more limited business practices. Identifying "predatory" journals has been difficult because many of their features overlap with established journals. Recently, publishers have made a concerted effort to define standards for open-access that can guide authors.

## Introduction

The internet has revolutionized scientific exchange, and one of the primary mechanisms is through Open Acess (OA). We have certainly experienced our lives completely transitioned to virtuality during COVID-19, and OA is doing the same. With every advance there is co-evolution of pathogens that diminish the benefits, and it is important to minimize their impact. In scientific publishing, one of the most glaring is the predatory journal. This review will provide a historical context of the balance between authoritative validation versus freedom for emergent ideas. The definition of the "predatory" journal can be as simple as "you can recognize it when you see it". Yet at a December 2019 meeting of leading publishers there was no more than a guideline definition of what constituted a "predatory" journal, and no clear consensus.[(1)] Membership in the Committee on Publication Ethics, PubMed listing, Web of Science listing, none of these assure a journal is "non-predatory".

Understanding why predatory journals emerged can benefit from examining the history of scientific publishing, coinciding with the printing press, the Renaissance, and eventually the Enlightment. This opened an era of broad dissemination of ideas relatively unrestrained by authority, mirroring what we are now seeing through internet publishing.

## History of Scientific Publishing

Prior to the printing press, scribes laboriously produced books that few could afford. In the mid-15$^{th}$ century the invention of movable type changed everything. Mark Twain remarked that everything good and bad resulted from printing. While the printing press opened the Bible and knowledge to the masses and led to the Reformation, its first use was to print Catholic indulgences. Technology had unintended consequences, and authority

controlled the dissemination through *imprimatur* and other forms of validation.

Violating authority was serious: Galileo was forced to recant heliocentrism. Galileo is in the direct scientific lineage of most modern scientists, who at their core work toward finding unbiased truth. This internal conflict is intrinsic to science from Copernicus to my own studies of amyloid.

Authority validation was transferred from the church to the scientific academies during the Renaissance/Enlightment following a similar rule of *imprimatur.* The oldest continuous academy, the Royal Society of London, formed in 1660, but was predated by earlier societies in the 1500s. Newton's books have the *imprimatur* mark of Samuel Pepys, President of the Royal Society. The first scientific journal, Philosophical Transactions of the Royal Society[(2)], consisted of members passing letters among other members, reporting discoveries and soliciting comment, much like the current review system. The academies provided authority. Other more specialized societies also regulated their memberships and organized journals and meetings to promote scientific discoveries. A similar pattern developed in the US with the National Academy of Sciences, State Academies, AAAS, and prior to them at least a couple of independent academies, American Academy of Arts & Science and American Philosophical Society, all publishing and validating scientific inquiry.

It was only 150 years ago that the first successful private/independent journal formed: Nature. Private journals followed a similar peer review process to the academies, except the reviewers were members of the editorial boards or other experts chosen by the editors. The substantial expertise and cost of manuscript evaluation, publication, and distribution served as a major barrier to entry for any but the most organized publishers. In fact Nature lost money during many of its early years.[(3)]

Aside from minor technical developments, the great evolution in all journals was in 1960 with their numeric evaluation by the Institute of Scientific Information, founded by Eugene Garfield. Since then, most journals have focused on increasing their impact factor, the number of citations of a journal's articles in the following two years. This metric has dictated library subscription, the prior major revenue source for survival and reputation of a journal. It has had the unintended consequence of equating short-term popularity with quality that has often led fields astray for decades by following the highest impact journals.

## Development of Open Access Publication

This system worked in equilibrium, until a confluence of technology and concepts met in the late 1990s and early 2000. First, Harold Vamus, director of the NIH, was concerned that research results were behind pay walls blocking those who paid for the research from reading it. Second, scientists were beginning to provide access to data in the public domain as a model of what was to come. Computer scientists and physicists were increasingly posting pre-reviewed content in websites and archives (http://arxiv.org).

These efforts led to major consensus statements from the Budapest Open Access Institute 2002, Bethesda Statement on Open Access Publishing 2003, Berlin Declaration on Open Access to Knowledge in the Sciences and Humanities 2003, World Summit on the Information Society 2003.

The first broadly known commercial OA family of over 50 journals was Biomed Central in 2000, initially owned by Current Science Group, headed by Vitez Tracz. It was modeled after Varmus's vision. Tracz later founded Faculty of 1000, Current Opinions, The Scientist, Current Drugs, and others. He is considered a visionary. In the following years other groups developed, including Public Library of Sciences (PLOS) by Varmus,

Frontiers by Markram (leader of the European Brain Initiative), and others.

While these journal groups were focused around open dissemination of research results, as a result of being open access the primary income of journals, library and personal subscription, and reprints, was gone. The income had to come from other sources, usually authors. This left some publishers with an incentive to accept articles with minimum peer review, and others to provide few services after acceptance, simply ”they had their money”. It must be remembered that traditional publishers also often charge authors in advance of publication for submission, page charges, reprints, and color figures.

As printing indulgences and the Bible laid the tracks for the reformation, OA had unintended consequences because it greatly lowered the resources for entry into scientific publishing. No longer were there large journal offices with staff filling envelopes to send to reviewers. Typesetting was no longer a physical activity, and most important, the work was moving internationally. European and US publishers did most of the back-end work in other countries, mostly developing countries. With aspects of publishing moving offshore, one can think that the whole enterprise could be moved with similar results, yet many OA publishing companies did not have the historical organization or financial backing to develop solid peer review and manuscript processing, such as corrections and retraction. Some, as Bentham, followed a traditional model focused on indexing and increased impact factor, while others, e.g. Omics, followed unique business models that were greatly under-resourced in skill or capital.

## Ethical Standards

To bring ethical standards to the emerging OA journals, the Committee on Publication Ethics (COPE) formed to set guidelines. Similarly, PubMed, Web of Science, and others set standards with varying degrees of success. In 2015, Jeffrey Beall used 26 criteria to define the term “predatory journal”.[(4)] He published Beall’s list of those he judged as not following the guidelines. Frontiers, a prominent publisher, was on the list and sued Beall and the University of Colorado, resulting in the list being removed. This issue arose because defining a predatory journal is difficult even with 26 criteria; the increasing competition among journals has led many to follow similar paths to predatory journal practices. Nature is the owner of Biomed Central, Frontiers, and founded its own OA journals, Scientific Reports and Nature Communications. Science (AAAS) has Science Advances. Numerous well-respected professional societies have also launched OA journals.

There is now a strong movement to make all journals OA. In 2018, eleven European funders proposed Plan S, where all work must be in true open access publishers, and will not accept the hybrid model where specific articles can be made OA within print journals.

The issue of OA quality has become more pressing with the number of poorly resourced journals growing greatly in the past few years. As Nature points out, “It can be tough to distinguish a predatory journal from a journal that is under-resourced”.[(1)]

## Conclusions

This past December, a number of prominent publishers set to meet the issue head on. They were left struggling with how to define a predatory journal and came up with guidelines that are still under discussion.[(1)] This discussion should also include the movement of journals to equate short term impact factors with quality and the movement away from the rigorous peer review that historically made journals sources of reference rather than fueling the improducibility crisis. Until then, it is buyer beware, and the recent

guide of Think-Check-Submit is a start. (http://thinkchecksubmit.org)

Lost in the recent argument is the fundamental balance between sanction of authority (*imprimatur*) and the innovation that was at the heart of the Renaissance Enlightment and the new Information Age. Striking a balance that benefits scientific advancement requires adherence to the fundamental values of the scientific community, including peer review, while allowing development of ideas that change the center of the universe.

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# Global Change Impact on Deep-Sea Ecosystems

## by Roberto Danovaro, Member EUAS

Short Biography

*Roberto Danovaro was born in Genoa (degrees in 1988). PhD in Environmental Sciences at the University of Pisa in 1993. Full Professor in 2001 at the Polytechnic University of Marche. Director of the Department of Marine Sciences (2004 to 2010), Director of the Department of Life and Environmental Sciences (2011 to 2014) at the Polytechnic University of Marche. Pro-Rector (Delegated to the Research) at the Polytechnic University of Marche (2010-2013). President of the Scientific Council of WWF Italy, Steering Board Member of OECD (Fostering Innovation in Ocean Economy). Member of the Scientific Council of several research institutions and panels (IUCN, UNEP, EU), Editor in Chief of international journals and coordinator of several EU and international programs. President of the Italian Society of Ecology (2011-2013), and of the Italian Society of Limnology and Oceanography (2008-2011). President of the European Federation of Scientific Technological Societies (2008-2012). Member of the EU Academy of Sciences. RD received several Awards, including the World Prize BMC Biology (London, 2010), the Award of French Society of Oceanography (2011), and the ENI Award "Protection of the Environment" (2013). Nominated in 2013 by the Italian Ministry of Education University and Research (MIUR), President of the Stazione Zoologica Anton Dohrn (National Institute of Marine Biology Ecology and Biotechnology). In the 2018 was renewed as President of the SZN (2018-2022). (RD Scientometric data: H index - 80; articles on ISI journals with IF >450; citations>22.000; >2300 citations per year).*

## Selected Publications and their citations (Google Scholar®)

**Ecological variables for developing a global deep-ocean monitoring and conservation strategy.**

R Danovaro, E Fanelli, J Aguzzi, D Billett, L Carugati, C Corinaldesi, ...*Nature Ecology & Evolution* 2020, 4(2), 181-192 (IF:10.08)

The deep sea (>200 m depth) encompasses >95% of the world's ocean volume and represents the largest and least explored biome on Earth (<0.0001% of ocean surface), yet is increasingly under threat from multiple direct and indirect anthropogenic pressures. Our ability to preserve both benthic and pelagic deep-sea ecosystems depends upon effective ecosystem-based management strategies and monitoring based on widely agreed deep-sea ecological variables. Here, we identify a set of deep-sea essential ecological variables among five scientific areas of the deep ocean: (1) biodiversity; (2) ecosystem functions; (3)

impacts and risk assessment; (4) climate change, adaptation and evolution; and (5) ecosystem conservation. Conducting an expert elicitation (1,155 deep-sea scientists consulted and 112 respondents), our analysis indicates a wide consensus amongst deep-sea experts that monitoring should prioritize large organisms (that is, macro- and megafauna) living in deep waters and in benthic habitats, whereas monitoring of ecosystem functioning should focus on trophic structure and biomass production. Habitat degradation and recovery rates are identified as crucial features for monitoring deep-sea ecosystem health, while global climate change will likely shift bathymetric distributions and cause local extinction in deep-sea species. Finally, deep-sea conservation efforts should focus primarily on vulnerable marine ecosystems and habitat-forming species. Deep-sea observation efforts that prioritize these variables will help to support the implementation of effective management strategies on a global scale.

**Scientists' warning to humanity: microorganisms and climate change.**

R Cavicchioli, WJ Ripple, KN Timmis, F Azam, LR Bakken, M Baylis, ...*Nature Reviews Microbiology* 2019, 1, 69 (cit:69, IF:34.65)

In the Anthropocene, in which we now live, climate change is impacting most life on Earth. Microorganisms support the existence of all higher trophic life forms. To understand how humans and other life forms on Earth (including those we are yet to discover) can withstand anthropogenic climate change, it is vital to incorporate knowledge of the microbial 'unseen majority'. We must learn not just how microorganisms affect climate change (including production and consumption of greenhouse gases) but also how they will be affected by climate change and other human activities. This Consensus Statement documents the central role and global importance of microorganisms in climate change biology. It also puts humanity on notice that the impact of climate change will depend heavily on responses of microorganisms, which are essential for achieving an environmentally sustainable future.

**MERCES: Marine Ecosystem Restoration in Changing European Seas (H2020 funded project).**

R Danovaro (coordinator), C Gambi (Scientific Project manager) *PeerJ Preprints* 2018

MERCES "Marine Ecosystem Restoration in Changing European Seas" (GA 689518) is the first H2020 European project focused on the ecological restoration of degraded marine habitats and the recovering of their biodiversity and ecosystem services. Specific aims include a) improving existing, and developing new, restoration actions of degraded marine habitats; b) increasing the adaptation of EU degraded marine habitats to global change; c) enhancing marine ecosystem resilience and services; d) conducting cost-benefit analyses for marine restoration measures; e) creating new industrial targets and opportunities. To achieve these objectives MERCES created a multi-disciplinary consortium (28 Partners from 16 Countries) with skills in marine ecology, restoration, policy, socio-economics, knowledge transfer, dissemination and communication. MERCES is divided in 10 Work packages (including the project management) dedicated to: the inventory of EU degraded marine habitats (WP1); pilot restoration experiments on shallow soft and hard bottoms and deep-sea ecosystems (WPs2-3-4); the analysis of the restoration effects on ecosystem services (WP5); the legal, policy and governance outputs to make effective the potential of

marine restoration (WP6); the assessment of the socioeconomic returns of marine ecosystems' restoration (WP7) and the dissemination of the results to the widest audience including industrial stakeholders (WP8) and the general public (WP9).

**The deep-sea under global change.**

R Danovaro, C Corinaldesi, A Dell'Anno, PVR Snelgrove, *Current Biology* 2017, 27(11), R461-R465 (cit:50, IF:9.19)

The deep ocean encompasses 95% of the oceans' volume and is the largest and least explored biome of Earth's Biosphere. New life forms are continuously being discovered. The physiological mechanisms allowing organisms to adapt to extreme conditions of the deep ocean (high pressures, from very low to very high temperatures, food shortage, lack of solar light) are still largely unknown. Some deep-sea species have very long life-spans, whereas others can tolerate toxic compounds at high concentrations; these characteristics offer an opportunity to explore the specialized biochemical and physiological mechanisms associated with these responses. Widespread symbiotic relationships play fundamental roles in driving host functions, nutrition, health, and evolution. Deep-sea organisms communicate and interact through sound emissions, chemical signals and bioluminescence. Several giants of the oceans hunt exclusively at depth, and new studies reveal a tight connection between processes in the shallow water and some deep-sea species. Limited biological knowledge of the deep-sea limits our capacity to predict future response of deep-sea organisms subject to increasing human pressure and changing global environmental conditions. Molecular tools, sensor-tagged animals, in situ and laboratory experiments, and new technologies can enable unprecedented advancement of deep-sea biology, and facilitate the sustainable management of deep ocean use under global change.

**A submarine volcanic eruption leads to a novel microbial habitat.**

R Danovaro, M Canals, M Tangherlini, A Dell'Anno, C Gambi, G Lastras, ...*Nature Ecology & Evolution* 2017, 1(6), 1-9 (cit:17, IF:10.97)

Submarine volcanic eruptions are major catastrophic events that allow investigation of the colonization mechanisms of newly formed seabed. We explored the seafloor after the eruption of the Tagoro submarine volcano off El Hierro Island, Canary Archipelago. Near the summit of the volcanic cone, at about 130 m depth, we found massive mats of long, white filaments that we named Venus's hair. Microscopic and molecular analyses revealed that these filaments are made of bacterial trichomes enveloped within a sheath and colonized by epibiotic bacteria. Metagenomic analyses of the filaments identified a new genus and species of the order Thiotrichales, *Thiolava veneris*. Venus's hair shows an unprecedented array of metabolic pathways, spanning from the exploitation of organic and inorganic carbon released by volcanic degassing to the uptake of sulfur and nitrogen compounds. This unique metabolic plasticity provides key competitive advantages for the colonization of the new habitat created by the submarine eruption. A specialized and highly diverse food web thrives on the complex three-dimensional habitat formed by these microorganisms, providing evidence that Venus's hair can drive the restart of biological systems after submarine volcanic eruptions.

**An ecosystem-based deep-ocean strategy.**

R Danovaro, J Aguzzi, E Fanelli, D Billett, K Gjerde, A Jamieson, ...*Science* 2017, 355(6324), 452-454 (cit:79, IF:16.81)

Increasing exploration and industrial exploitation of the vast and fragile deep-ocean environment for a wide range of resources (e.g., oil, gas, fisheries, new molecules, and soon, minerals) raises global concerns about potential ecological impacts. Multiple impacts on deep-sea ecosystems (>200 m below sea level; ~65% of the Earth's surface is covered by deep ocean) caused by human activities may act synergistically and span extensive areas. Cumulative impacts could eventually cause regime shifts and alter deep-ocean life-support services, such as the biological pump or nutrient recycling. Although international law and national legislation largely ignore the deep sea's critical role in the functioning and buffering of planetary systems, there are promising developments in support of deep-sea protection at the United Nations and the International Seabed Authority (ISA). We propose a strategy that builds from existing infrastructures to address research and monitoring needs to inform governments and regulators.

**Virus-mediated archaeal hecatomb in the deep seafloor.**

R Danovaro, A Dell'Anno, C Corinaldesi, E Rastelli, R Cavicchioli, ...*Science Advances* 2016, 2(10), e1600492 (cit:51, IF12.80)

Viruses are the most abundant biological entities in the world's oceans, and they play a crucial role in global biogeochemical cycles. In deep-sea ecosystems, archaea and bacteria drive major nutrient cycles, and viruses are largely responsible for their mortality, thereby exerting important controls on microbial dynamics. However, the relative impact of viruses on archaea compared to bacteria is unknown, limiting our understanding of the factors controlling the functioning of marine systems at a global scale. We evaluate the selectivity of viral infections by using several independent approaches, including an innovative molecular method based on the quantification of archaeal versus bacterial genes released by viral lysis. We provide evidence that, in all oceanic surface sediments (from 1000- to 10,000-m water depth), the impact of viral infection is higher on archaea than on bacteria. We also found that, within deep-sea benthic archaea, the impact of viruses was mainly directed at members of specific clades of Marine Group I Thaumarchaeota. Although archaea represent, on average, ~12% of the total cell abundance in the top 50 cm of sediment, virus-induced lysis of archaea accounts for up to one-third of the total microbial biomass killed, resulting in the release of ~0.3 to 0.5 gigatons of carbon per year globally. Our results indicate that viral infection represents a key mechanism controlling the turnover of archaea in surface deep-sea sediments. We conclude that interactions between archaea and their viruses might play a profound, previously underestimated role in the functioning of deep-sea ecosystems and in global biogeochemical cycles.

**Macroecological drivers of archaea and bacteria in benthic deep-sea ecosystems.**

R Danovaro, M Molari, C Corinaldesi, A Dell'Anno *Science Advances* 2016, 2(4), e1500961 (cit:38, IF12.80)

Bacteria and archaea dominate the biomass of benthic deep-sea ecosystems at all latitudes,

playing a crucial role in global biogeochemical cycles, but their macroscale patterns and macroecological drivers are still largely unknown. We show the results of the most extensive field study conducted so far to investigate patterns and drivers of the distribution and structure of benthic prokaryote assemblages from 228 samples collected at latitudes comprising 34°N to 79°N, and from ca. 400 to 5570-m depth. We provide evidence that, in deep-sea ecosystems, benthic bacterial and archaeal abundances significantly increase from middle to high latitudes, with patterns more pronounced for archaea, and particularly for Marine Group I Thaumarchaeota. Our results also reveal that different microbial components show varying sensitivities to changes in temperature conditions and food supply. We conclude that climate change will primarily affect deep-sea benthic archaea, with important consequences on global biogeochemical cycles, particularly at high latitudes.

**Virus decomposition provides an important contribution to benthic deep-sea ecosystem functioning.**

A Dell'Anno, C Corinaldesi, R Danovaro *Proceedings of the National Academy of Sciences* 2015, 112(16), E2014-E2019 (cit:57, IF:9.58)

Viruses are key biological agents of prokaryotic mortality in the world oceans, particularly in deep-sea ecosystems where nearly all of the prokaryotic C production is transformed into organic detritus. However, the extent to which the decomposition of viral particles (i.e., organic material of viral origin) influences the functioning of benthic deep-sea ecosystems remains completely unknown. Here, using various independent approaches, we show that in deep-sea sediments an important fraction of viruses, once they are released by cell lysis, undergo fast decomposition. Virus decomposition rates in deep-sea sediments are high even at abyssal depths and are controlled primarily by the extracellular enzymatic activities that hydrolyze the proteins of the viral capsids. We estimate that on a global scale the decomposition of benthic viruses releases ∼37–50 megatons of C per year and thus represents an important source of labile organic compounds in deep-sea ecosystems. Organic material released from decomposed viruses is equivalent to 3 ± 1%, 6 ± 2%, and 12 ± 3% of the input of photosynthetically produced C, N, and P supplied through particles sinking to bathyal/abyssal sediments. Our data indicate that the decomposition of viruses provides an important, previously ignored contribution to deep-sea ecosystem functioning and has an important role in nutrient cycling within the largest ecosystem of the biosphere.

**Challenging the paradigms of deep-sea ecology.**

R Danovaro, PVR Snelgrove, P Tyler, *Trends in Ecology & evolution* 2014, 29(8), 465-475 (cit:168, IF:15.24)

Deep-sea ecosystems represent Earth's major ecological research frontier. Focusing on seafloor ecosystems, we demonstrate how new technologies underpin discoveries that challenge major ecological hypotheses and paradigms, illuminating new deep-sea geosphere–biosphere interactions. We now recognize greater habitat complexity, new ecological interactions and the importance of 'dark energy', and chemosynthetic production in fueling biodiversity. We also acknowledge functional hotspots that contradict a food-poor, metabolically inactive, and minor component of global carbon cycles. Symbioses appear widespread, revealing novel adaptations. Populations show

complex spatial structure and evolutionary histories. These new findings redefine deep-sea ecology and the role of Earth's largest biome in global biosphere functioning. Indeed, deep-sea exploration can open new perspectives in ecological research to help mitigate exploitation impacts.

**Chronic and intensive bottom trawling impairs deep-sea biodiversity and ecosystem functioning.**

A Pusceddu, S Bianchelli, J Martín, P Puig, A Palanques, P Masqué, ...*Proceedings of the National Academy of Sciences* 2014, 111(24), 8861-8866 (cit:175, IF:9.58)

Bottom trawling has many impacts on marine ecosystems, including seafood stock impoverishment, benthos mortality, and sediment resuspension. Historical records of this fishing practice date back to the mid-1300s. Trawling became a widespread practice in the late 19th century, and it is now progressively expanding to greater depths, with the concerns about its sustainability that emerged during the first half of the 20th century now increasing. We show here that compared with untrawled areas, chronically trawled sediments along the continental slope of the north-western Mediterranean Sea are characterized by significant decreases in organic matter content (up to 52%), slower organic carbon turnover (ca. 37%), and reduced meiofauna abundance (80%), biodiversity (50%), and nematode species richness (25%). We estimate that the organic carbon removed daily by trawling in the region under scrutiny represents as much as 60–100% of the input flux. We anticipate that such an impact is causing the degradation of deep-sea sedimentary habitats and an infaunal depauperation. With deep-sea trawling currently conducted along most continental margins, we conclude that trawling represents a major threat to the deep seafloor ecosystem at the global scale.

**Ecology: Protect the deep sea.**

EB Barbier, D Moreno-Mateos, AD Rogers, J Aronson, L Pendleton, ...*Nature* 2014 505 (7484), 475-477 (cit:72, IF:43.07)

More than 1 million square kilometers of the sea below 200 metres in depth are being ploughed by trawlers, according to estimates, and the next decade will see expansion of oil, gas and mineral extraction into deeper and deeper waters (see go.nature.com/brhbll). At risk are ecosystems that contribute to the health and productivity of the ocean, that challenge our ideas of the extremes at which life can exist (such as hydrothermal vents), and that are habitats and nurseries for fisheries (seamounts, for example). Our knowledge of deep-ocean biodiversity only hints at thousands of undiscovered organisms and their benefits. Some threatened species, such as cold-water corals, have lifespans of hundreds or even thousands of years; habitats, including rock concretions called manganese nodule beds, can take millennia to form. We call for formal governance structures and funds to be put in place by 2020 to create networks of deep-sea reserves that maintain and restore biodiversity and function in this vast and important biome. To support these efforts, a global strategy must be framed under the aegis of national governments and an international body. For areas that are beyond national jurisdiction, the International Seabed Authority (ISA) is best suited to this task.

# A Method for Design of High Strength Concrete Composition Considering Curing Temperature and Duration

## by Yuri Ribakov, Member EUAS

Short Biography

*Full Professor, Department of Civil Engineering, Faculty of Engineering, Ariel University, Ariel, Israel*

*Ph.D. 1998 – 2001 Department of Civil Engineering, Technion - Israel Institute of Technology, Haifa, Israel.*

*M.Sc. 1995-1998 Department of Civil Engineering, Technion - Israel Institute of Technology, Haifa, Israel.*

*B.Sc. 1984-1991 Faculty of Civil Engineering, Ukrainian Institute of Water Management Engineering, Rivne, Ukraine (with first class honors).*

***Professional Experience***

*I have a total more than 20 years of industrial, teaching and research experience in structural engineering.*

*2018 – present Head, Division of Structural Engineering, Department of Civil Engineering, Faculty of Engineering, Ariel University, Ariel, Israel.*

*2015 – present Full Professor, Department of Civil Engineering, Faculty of Engineering, Ariel University, Ariel, Israel.*

*2011 – 2014 Head, Department of Civil Engng, Faculty of Engineering, Ariel University,*

*2010 – 2015 Associate Professor, Department of Civil Engineering, Faculty of Engineering, Ariel University, Ariel, Israel.*

*2005 – 2010 Senior Lecturer, Department of Civil Engineering, Faculty of Engineering, Ariel University, Ariel, Israel.*

*2005 – 2008 Adjunct Senior Lecturer, Department of Civil Engineering, Faculty of Engineering, Ben Gurion University of Negev, Beer Sheva, Israel.*

*2000 – 2005 Lecturer, Department of Civil Engineering, Faculty of Engineering, Ariel University, Ariel, Israel.*

*1995 - 2000 Instructor, Structural Engineering Division, Faculty of Civil Engineering, Technion - Israel Institute of Technology, Haifa, Israel.*

*1992 - 1994 Deputy Chairman, Building Department, United Municipal Structures, Rivne, Ukraine.*

*1991 - 1992 Engineer - Researcher, Building Materials Division, Faculty of Civil Engineering, Ukrainian Institute of Water Management Engineering, Rivne, Ukraine.*

*1990–1991 Senior laboratory assistant, Division of Geomechanics and Foundations, Faculty of Civil Engineering, Ukrainian Institute of Water Management Engineering, Rivne, Ukraine.*

***Research Experience & Interests***

*Structural Engineering in general, Earthquake Engineering, Structural Dynamics, Seismic Design and Reinforced Concrete Structures and Elements in particular.*

***Honors & Awards***

*1999 Tuvia Netzer award – given for the research entitled "Influence of dampers on response of tall buildings to earthquakes".*

*2000 Abraham and Miriam Gutwirth Research Award.*

*2004 Award for excellence in research and teaching, Ariel University.*

*2005 Award for excellence in research and teaching, Ariel University.*

*2006 Award for excellence in research and teaching, Ariel University.*
*2007 Award for excellence in research and teaching, Ariel University.*
*2008 Award for excellence in research and teaching, Ariel University.*
*2010 Award for excellence in research and teaching, Ariel University.*
*2011 Award for excellence in research and teaching, Ariel University.*
*2012 Award for excellence in research and teaching, Ariel University.*
*2013 Award for excellence in research and teaching, Ariel University.*
*2013 Reviewing Excellence Award, Engineering Structures, Elsevier.*
*2014 Outstanding Reviewer Award, Engineering Structures, Elsevier.*
*2019 Award for excellence in research, Ariel University.*

***Research Grants***

*2008 – 2011* *Y. Ribakov (PI 1) and G. Agranovich (PI 2). Improving Seismic Response of Structures Using Optimal Dampers. Ministry of National Infrastructures, Israel.*

*2012* *Y. Ribakov (PI 1) and G. Agranovich (PI 2). Optimization of Hybrid Energy Dissipation Systems for Improving Structural Seismic Response. The Ministry of Energy and Water Resources of Israel.*

*2013* – 2015 *Y. Ribakov (PI 1) and S. Pushkar (PI 2). Seismic resistant of green buildings. The Ministry of Environmental Protection of Israel.*

*2014* – 2015 *M. Ben Chaim (PI 1) and Y. Ribakov (PI 2). Investigation of the Possible Impact on the Environment of Converting the Existing Vehicle Engines in Israel to Natural Gas. The Ministry of Environmental Protection of Israel.*

## A Method for Design of High Strength Concrete Composition Considering Curing Temperature and Duration

L. Dvorkin, V. Zhitkovsky, Y. Stepasyuk and Y. Ribakov

### Abstract

The paper deals with experimental results on temperature and curing duration influence on strength properties of high strength concrete (HSC). Dependences for calculating strength of high strength concrete at 12 h, 1, 7 and 28 days are developed for normal hardening conditions. Equations, allowing considering curing temperature in diapason between 5 and 40 °C as well as curing duration are proposed. The influence of steam curing parameters on HSC strength characteristics is investigated. Methodology for predicting concrete strength after steam curing and further normal hardening is proposed. The obtained calculation dependences and experimental-statistical models provide wide possibilities for design of effective high strength concrete compositions.

## Composite Binder Obtained by Using of Dust From Clinker Kilns

L. Dvorkin, V. Zhitkovsky, Y. Ribakov, O. Bordiuzhenko and A. Stepanuk

### Abstract

The paper deals with the features of obtaining a composite binder containing

cement kilns dust, blast furnace slag and Portland cement, in which increased complex activation of blast-furnace granulated slag is achieved, due to the increased content of alkalis in cement dust, as well as the effects of hydroxide and calcium sulphate, contained in the cement. The influence of composition, fineness of grinding and content of chemical additives on the hydration degree and strength of low water demand binders was studied. The optimal relationships between the binder composition and the required fineness of the grinding are established, which ensure the strength characteristics and the hardening speed. The influence of superplasticizers naphthalene formaldehyde and polycarboxylate types, which provide low water demand of binder and high fineness of its grinding, is studied. Using the method of the experiment mathematical planning, equations for the regression of compressive and flexural strengths in different compensations were obtained, which allow predicting strength, taking into account the composition and features of the technology for obtaining the binder.

# New Aspects by using Remotely Sensed Spatiotemporal Information to tackle Emerging Environmental Problems

## by Soe W. Myint, Member EUAS

Short Biography

***Education***

1. *Ph.D., Geography (GIScience), Louisiana State University*
2. *M.S., Natural Resources Program (Environmental Remote Sensing and Geoinformation for Development), Asian Institute of Technology*
3. *Post-Grad. Diploma, Forest Survey (Aerospace Remote Sensing Techniques), International Institute for Aerospace Survey and Earth Sciences (ITC), the Netherlands*
4. *B.S., Forestry, Rangoon University*

***Appointments***

*2013 – present:* *Professor, School of Geographical Sciences and Urban Planning, ASU*
*2008 – 2013:* *Associate Professor, School of Geographical Sciences and Urban Planning, ASU*
*2006 – 2008:* *Assistant Professor, School of Geographical Sciences, ASU*
*2001 – 2005:* *Assistant Professor, Department of Geography, University of Oklahoma*
*1994 – 1998:* *Research Specialist, United Nations Environment Program (UNEP/EAP-AP)*
*1983 – 1992:* *Dy Manager, National Forest Management/Inventory project, (UNDP/FAO/MYA/85/003)*

***Awards and Honors***

*(1) Fulbright Canada Research Chair in Water, Environment, and Clean Energy (2019-2020). https://asunow.asu.edu/20191009-asu-professor-heads-north-fulbright-canada-research-chair;https://www.uregina.ca/external/communications/feature-stories/current/2019/08-14.html; https://www.pressreader.com/canada/regina-leader-post/20190918/281500752960834; http://news.aag.org/2019/10/aag-newsletter-october-2019/.*

*(2) Keynote speech given at the 2019 conference banquet of the Canadian Association of Geographers' Prairie Division (Sept. 27-29, 2019).*

*(3) Graduation speech delivered at the 129$^{th}$ Asian Institute of Technology (AIT) Graduation Ceremony on May 18, 2018 - https://www.youtube.com/watch?v=-un1liwqPRo.*

*(4) Member, European Union Academy of Sciences (EUAS), elected 2018.*

*(5) Outstanding Paper in Landscape Ecology, 2017 (Co-author). United States International Association for Landscape Ecology, US-IALE annual meeting, Baltimore.*

*(6) Outstanding Achievement Award – American Association of Geographers (AAG) - Remote Sensing Specialty Group (RSSG), 2016 AAG Annual Meeting, San Francisco. According to AAG-RSSG, this Award is the most prestigious award for established remote sensing scholars at AAG.*

*(7) Prominent Alumnus of AIT - Received the title of Prominent Alumnus of Asian Institute of Technology (AIT), http://www.aitalumni.com/prominent-alumni-people.*

*(8) 2015 Best Imported Book Award given by the China Press Association – Chinese version of the book titled "Advances in Mapping from Aerospace Imagery: Techniques and Applications" My chapter contribution: Myint, S.W., 2012. The effects of the spatial pattern of vegetation cover on urban warming in a desert city, Advances in Mapping from Aerospace Imagery: Techniques and Applications (Editors X. Yang and J. Li), Taylor and Francis Group, LLC, pp 261-278.*

*(9) Success Story - Among those awarded as Prominent Alumni, my biography was published under 'Success Stories' of the Asian Institute of Technology (AIT) Alumni Association, http://www.aitalumni.com/success-stories-view/10.*

*(10) Nominated for the Zebulon Pearce Distinguished Teaching Award (given to tenured and tenure-track faculty members), 2017.*

*(11) Honored Guest (2009) College of Liberal Arts and Sciences Convocation ceremony, for making difference in multiple undergraduate students' education, Arizona State University.*

*(12) ASPRS Conference Management Award (2010) Recipient. Received at the 2010 American Society for Photogrammetry and Remote Sensing (ASPRS) annual conference in San Diego (April*

*26-30, 2010). The intent of this award is to recognize the great effort put forth by the individuals who volunteer their time to assist in the planning and execution of a successful annual conference.*

(13) *AITAA Distinguished Alumni Award (2007) for Academic and Research Excellence, Asian Institute of Technology.*
(14) *Best Paper Award for Early Career Scholars in Remote Sensing, Remote Sensing Specialty Group - AAG, 2007 - Published in PE&RS journal.*
(15) *CPGIS Scholar, 2005, selected by the Chinese Professionals in Geographic Information Science Abroad (CPGIS) to give lectures and research presentations at Jiangxi Normal University, Nanchang University, and Hubei University as part of the CPGIS Young Scholar Summit.*
(16) *CSISS Scholarship (Center for Spatially Integrated Social Science) to attend 2003 Geographically Weighted Regression workshop, University of California, Santa Barbara.*
(17) *Intergraph Young Scholar Award (UCGIS), 2002 UCGIS Summer Assembly, University of Georgia, Athens.*
(18) *USGS Scholar Award, First International Conference on GIScience, 2000, Savannah, GA, USA.*
(19) *Consultant (GIS) to World Health Organization (WHO), Geneva, Switzerland (1999) (while studying as a Ph.D. student).*
(20) *Best Student Paper Award – AAG - Remote Sensing Specialty Group, 2001 AAG meeting.*
(21) *Best Student Paper Award – American Society for Photogrammetry and Remote Sensing (ASPRS) – Mid-South Region Meeting at Clemson University, South Carolina, 2000.*
(22) *Best Student Paper Award (UCGIS-2000), 2000 UCGIS Summer Assembly, Portland, Oregon. Forty-two GIS/RS Graduate students from different Disciplines/Departments and Universities across the United States participated in the competition.*
(23) *Best Poster Presentation Award, 1998 - 18th Asian Conference on Remote Sensing, Kuala Lumpur, Malaysia.*
(24) *AAG Otis Paul Starkey Dissertation Research Award. Association of American Geographers, 2001.*
(25) *William G. Haag Award (2001). Most outstanding paper in professional meetings, Dept. of Geography & Anthropology, LSU.*
(26) *Best Student Paper Award (2nd place), 2000 South Western Division AAG meeting, Texas A&M University.*
(27) *Best Student Paper Award (2nd place), 1999 South Western Division AAG meeting at Texas State University, San Marcos.*
(28) *Robert C. West Field Research Award (November, 2000). Department of Geography and Anthropology, LSU.*
(29) *Student Oral Paper Presentation Award and Travel Award, UCGIS-2000. UCGIS Summer Assembly, Portland, Oregon.*
(30) *Scholars Enhanced Assistantship Award and Tuition Award (Graduate School), (9,000 US$, 1999 - 2001), LSU (1999 - 2001).*
(31) *Graduate School Travel Awards (3 awards): Graduate School, Louisiana State University [(October, 1999), (April, 2000), (October, 2000)].*
(32) *Best Student Award, 87th Public Service Officers Training Course (No. 87), Public Service Selection and Training Board, Myanmar, 1987.*
(33) *Best Student Award, Basic Officer Training Course No.1 – Myanmar Timber Enterprise, Ministry of Forestry, Myanmar, 1986.*
(34) *Netherlands Government's Fellowship, Post Graduate Diploma studies at ITC, the Netherlands (1988 - 1989).*
(35) *French Government Scholarship, M.S. - Asian Institute of Technology, Bangkok (1993 - 1994).*

His *research* focuses on deforestation, landscape modeling, simulation and growth prediction, urban climate change, land degradation, ecosystem services, water use, carbon release, atmospheric emission, climate adaptation, drought, land use land cover change, human-environment interactions, socio-economic analysis, variation, and extreme, urban heat island, climate adaptation, human-environment interactions, surface and ground water changes, crop water use, flood simulation, urban image classification, urban spatial modeling, risk analysis, mitigation, recovery, and monitoring, uncertainty, urban emission,

land fragmentation, evapotranspiration modeling, land fragmentation, regional climate change modeling, urban water use, urban growth prediction, local scale urban meteorological parameterization, urban heat island, degradation of ecosystem, carbon flux, aerosol assessment, disaster assessment, algorithm development, data mining, GIScience, spatial statistics, spatio-temporal analysis, and spatial model development.

Our planet has been experiencing significant changes in global population, urbanization, energy use, food security, water use, climate, and atmospheric conditions since the last few decades. These changes are emerging along with the rapid growth of data and advanced analysis approaches. The integrative space-time system of geographic information science, spatial pattern analysis, and geospatial algorithm development offer a unique and effective framework to investigate spatio-temporal processes, interactions in a wide range of environmental applications for informed decision-making, and large data analysis. Soe Myint has demonstrated if and how spatial-temporal image analysis, spatial pattern method, and advanced image analysis can be employed to tackle some emerging environmental issues in connection to evidence-based sustainable decision making. Example applications and their respective findings are given below.

**(1) Schaffer-Smith, D., S.W. Myint, R.L. Muenich, D. Tong, and J.E. DeMeester, 2020. Repeated hurricanes reveal risks and opportunities for social-ecological resilience to flooding and water quality problems, Environmental Science & Technology (accepted).**

Hurricanes that damage lives and property are accompanied by poor water quality that affects both human and natural communities, yet these water quality impacts are difficult to quantify. We developed an operational remote sensing-based hurricane flood extent mapping method, examined potential water quality implications of two '500-yr' hurricanes in 2016 and 2018, and identified options to increase social-ecological resilience in North Carolina. Flooding detected with synthetic aperture radar (>91% accuracy) extended beyond state-mapped hazard zones. Furthermore, the legal floodplain underestimated impacts for communities with higher proportions of older adults, disabilities, unemployment, and mobile homes, as well as for headwater streams with restricted elevation gradients. Pollution sources were repeatedly affected, including ~55% wastewater treatment plant (WWTP) capacity and swine operations that generate ~500 M tons/yr manure. We identified ~4.8 million $km^2$ of possible forest and wetland conservation and ~1.7 million $km^2$ of restoration or altered management opportunities. Results suggest that current hazard mapping is inadequate for resilience planning; increased storm frequency and intensity necessitate modification of design standards, land-use policies, and infrastructure operation. Implementation of interventions can be guided by a greater understanding of social-ecological vulnerabilities within hazard and exposure areas.

**(2) Wang, C., Y. Li, S.W. Myint, Q. Zhao, E.A. Wentz, 2019. Impacts of Spatial Clustering of Urban Land Cover on Land Surface Temperature across Köppen Climate Zones in the Contiguous United States, Landscape and Urban Planning, 192, 103668. (doi:10.1016/j.landurbplan.2019.103668).**

This study examines the combined impacts of spatial patterns of urban land cover types on land surface temperature (LST) by taking the regional climate background into consideration. Portland, Los Angeles, Chicago, Denver, Kansas City, Orlando, and Phoenix were selected metropolitan areas that represent major climate regions in the

contiguous U.S.. Urban land cover types were derived from the National Land Cover Database (NLCD) 2011. The summer mean LST images in 2011 were calculated using the Moderate Resolution Imaging Spectroradiometer (MODIS) LST products. Spatial patterns of the urban land cover types were quantified using Moran's *I*, and then analyzed against LST using multivariate regression analysis. Results indicate that clustered impervious surface can elevate LST for both daytime and nighttime across all the climate regions, except for Phoenix, which has a subtropical hot desert climate. The cooling effect of clustered vegetation cover was found to be significant in warm, dry and temperate regions. Clustered water bodies have a strong cooling effect during the daytime, but a heating effect at night, except for Los Angeles and Phoenix that have hot dry summers, and both are naturally scarce in large water bodies. Policy recommendations are put forward that reducing the size and aggregation of impervious surfaces while including more parks that have small, dispersed water bodies with large, clustered greenspaces can potentially become a widely adapted strategy to reduce urban warming in most cities in the contiguous U.S.

**(3) Liu, W., D. B. Agusdinata, and S. W. Myint, 2019. Spatio-temporal Patterns of Lithium Mining and Environmental Degradation in the Atacama Salt Flat, Chile, Journal: International Journal of Applied Earth Observations and Geoinformation, 80(2019):145-156.**

Emerging electric-driven vehicle technologies and the global transition to renewable energy has driven the production of lithium significantly in the past ten years. However, the potential impacts alongside this transition require closer scrutiny. The purpose of this research is to assess the environmental impact and its possible correlation with lithium mining in the Atacama Salt Flat, the world's largest lithium extraction site. Using both Landsat imagery and MODIS land products, we investigate the mining areas to (1) determine area and rate of change over time, (2) analyze spatiotemporal patterns of changes in key environmental parameters, and (3) perform regression analysis between lithium mining activities and environmental degradation between 1997 and 2017. We use five environmental parameters for our analysis: Normalized Difference Vegetation Index (NDVI), Daytime Land Surface Temperature (Day-LST), Soil Moisture Index (SMI), Nighttime Land Surface Temperature (Night-LST), and Net Evapotranspiration (ET). Our analysis shows that Lithium mining operations have expanded rapidly by 7.07% annually. Our pixel-based time-series trend analysis for each image stack, using the Mann-Kendall test and Sen's slope coefficient, shows some significant degradation over the past 20 years including (1) vegetation decline, (2) elevating daytime temperatures, (3) decreasing trend of soil moisture, and (4) increasing drought condition in national reserved lands. However, no substantial degradation in nighttime-LST and ET is observed in the study area. Our analyses of the relationship between mining activities and environmental degradation also indicate that the continuous expansion of lithium mining has strong negative correlations with the NDVI and SMI, and a strong positive correlation with LST. We identified lithium mining activities as one of the major stressors to the local environmental degradation. The results provide a baseline to evaluate future impacts of lithium mining in the region. We anticipate our analysis will help alarm mining regulators, local environmental regulators, lithium industry decision-makers, and national park managers provide better management of the world's largest lithium production sites for a sustainable future.

**(4) Fu, P., Y. Xie, , S.W. Myint, K. Meacham-Hensold, and C. Bernacchi, 2019. A physical model-based method for retrieving urban land surface temperatures under cloudy conditions, Remote Sensing of Environment, 230, 111191 https://doi.org/10.1016/j.rse.2019.05.010.**

Satellite-derived land surface temperature (LST), due to its synoptic coverage, has been widely used for understanding surface energy and carbon fluxes at local, regional, and global scales. Despite great achievements to develop practical algorithms to estimate LSTs from thermal infrared (TIR) data, the retrieval of LSTs for overcast moments has received much less attention. The existing techniques, such as passive microwave (PMW) approaches, surface energy balance (SEB) models, and reconstruction algorithms relying on spatial/temporal information, for estimating LSTs under cloudy skies may not fulfill the needs for a spatially and temporally consistent LST dataset. Inspired by the recent advancements in the physically based urban canopy models (UCMs), this study synergistically employed the coupled Weather Research and Forecasting Model (WRF)/UCM system and the random forest (RF) regression technique to effectively estimate LSTs under cloudy conditions. Taking the Baltimore-Washington metropolitan region as a test site, the WRF/UCM simulations (LSTs) were performed from April 28 to May 20, 2011. The MODIS LST images of the same period were downloaded and used to evaluate the effectiveness of the approach introduced in this study. LST pixelss under cloudy conditions for a partially cloudy or a fully cloud-contaminated image were retrieved using the RF model calibrated by the clear-sky pixels from the same image. Results suggested that the WRF/UCM system could well capture the diurnal temperature patterns but tended to underestimate air temperatures. The correlation coefficient value between the MODIS LSTs and simulated LSTs exhibited a wide range from 0.5 to 0.9 with the RMSE value varying from 1.0 K to 9.0 K across land covers. The utilization of the RF regression technique for estimating LSTs under cloudy conditions from a partially cloud-contaminated LST image greatly reduced the RMSE value to 1.7 K without compromising the correlation coefficient value. For a fully cloud-contaminated LST image, LSTs were estimated with the correlation coefficient and RMSE values of 0.74 and 2.1 K, respectively. Overall, the presented approach has potential to generate consistent and reliable LST dataset for various environmental applications. Further research efforts can be made to examine the impacts of the temporal distance between neighboring images and the target image on the performance of the developed approach.

**(5) Tran, T.V., D.X. Tran, S.W. Myint, C. Huang, H.V. Pham, T.H. Luu, T.M.T. Vo, 2019. Examining Spatiotemporal Salinity Dynamics in the Mekong River Delta Using Landsat Time Series Imagery and a Spatial Regression Approach, Science of the Total Environment, 687, 1087-1097.**

Most coastal areas globally face water shortages in the dry season due to salinization and drought. The Mekong River Delta (MRD) is recognized as the “Rice Bowl” in Vietnam but the negative effects of salinization and drought have damaged rice production in recent decades. However, regional assessment of the perturbation has been lacking. A Landsat-based satellite salinity index, the Enhanced Salinity Index (ESI), was developed in this study to explore patterns of annual salinity variations in agricultural land and their relationship to drought in the MRD from 1989 to 2018. The performance of the index was superior to that of other previously published remotely sensed indices, based on correlations with field measurements of electrical conductivity (i.e. groundwater and soil EC), which can be used as a proxy for salinity. The time-series ESI was then utilized to

explore the spatiotemporal dynamics of salinity in the study area using the Theil-Send median trend (TS) and Mann-Kendall significance tests (MK). In addition, temporal relationships with the Normalized Difference Water Index (NDWI) were used to investigate the relationship between drought and saline intrusion. Our results showed that freshwater and brackish areas increased inland, whereas those developed for shrimp farming may increase soil and groundwater salinity. A negative correlation between drought and salinity was also observed in surface water where fish and shrimp farming activities took place, while a positive relationship was discovered in rice and annual cropland areas. This study highlights the use of ESI as an effective parameter for modelling vegetation salinity and its relationship with cropland change. We also demonstrate the feasibility of integrating satellite imagery with spatiotemporal analyses to monitor and assess regional salinization dynamics.

# Activities in Materials Science and Engineering

## by Derek O. Northwood, Member EUAS

Short Biography

*Professor Derek O. Northwood is a Distinguished University Professor and Professor of Engineering Materials in the Department of Mechanical, Automotive and Materials Engineering at the University of Windsor, Windsor, Ontario, Canada. Professor Northwood has an earned doctorate in Chemical Physics (Crystallography) from the University of Surrey (UK) and a BSc (Eng) in Engineering Metallurgy from the Imperial College, University of London (UK). He is a licensed Professional Engineer in Ontario, Canada (PEng) and is a Chartered Professional Engineer (CPEng; NER), APEC Engineer, and International Professional Engineer (IntPE(AUS), in Australia. In the 40+ years as an academic, Professor Northwood has held various administrative positions including Department Head, Dean, Associate Dean of Research, Director of the Office of Research Services, President of the Industrial Research Institute, and, Research Leadership Chair, both at the University of Windsor and Ryerson University, Toronto, Canada. Professor Northwood has taught, researched and facilitated joint research and educational programs at 14 universities worldwide, including the UK, the USA, Australia, Taiwan, China, Singapore and Canada. He has published 687 papers in refereed international journals and conference proceedings, 9 chapters in books and has edited 7 books, on a wide range of topics including materials and their applications, and engineering and technology education. He has been elected Fellow of five international professional societies in Australia, Canada, the UK and the USA; namely, Fellow of the Royal Society of Canada (FRSC); Fellow of the Institution of Engineers Australia (FIEAust); Fellow of the World Institute for Engineering and Technology Education (FWIETE); Fellow of the Institute of Materials, Minerals and Mining (FIMMM); and Fellow of ASM International (FASM). On October 1, 2019 in Portland, Oregon, USA, Professor Derek O. Northwood was inducted as a Fellow of Alpha Sigma Mu (FAΣM), The International Professional Honor Society for Materials Science and Engineering.*

## RESEARCH ACTIVITIES AND PUBLICATIONS 2019

The research activities and associated publications have been divided into four primary areas, namely:

1. Developing the potential properties of traditional materials;
2. Innovation in Engineering Education
3. Plasma Electrolytic Oxidation (PEO) for the production of corrosion - and wear-resistant coatings on light metal alloys;
4. The "costs" of corrosion.

In addition to these four areas, work has been initiated on the electrospinning of polymer nanofibres. The electrospinning equipment has been built and a research program begun on the electrospinning of polyethylene oxide (PEO). PEO is a highly crystalline polymer that is non-toxic, biocompatible, biodegradable and can be produced as porous fibres. It is soluble in various organic solvents and water. In this research we are examining the effects of molecular weight, solvent, concentration and processing variables

on the product form which can vary from droplets to films including monolithic nanofibres and mattes.

## 1. Developing the potential properties of traditional materials

This is cooperative work that has been on-going for a number of years with Professor Cheng Liu, College of Mechanical Engineering, Yangzhou, Yangzhou, China. In this work, we have taken traditional materials, such as carbon steels and cast irons, and through the application of novel processing technologies have been able to form multi-scale, multi-phase microstructures that lead to stronger and tougher materials.

Research work has continued on austempered ductile iron (ADI) and the further development of a novel multi-step austempering heat treatment. The Research Group has also initiated a research program on high nitrogen stainless steels (HNSS) which are becoming an increasingly important engineering materials because of their excellent corrosion resistance and good mechanical properties. Present work is focused on the solution treatment stage of the thermo-mechanical processing of these steels. Example publications include:

Zhou, W., Yang, C., Cui, X., Liang, Z., Wang, X., Northwood, D.O., Liu, C.

High performance unalloyed ductile cast iron with multiphase structure
(2019) *Solid State Phenomena*, 295 SSP, pp. 43-48.

Abstract
An unalloyed ductile cast iron with a multiphase structure is designed by a novel austempering process. The designed austempering treatment consists of initial rapid quenching to 180°C after austenizing at 890°C for 20min, and finally austempering at 220°C for 240min. A multiphase structure comprising lenticular/needle-like prior martensite, fine needle bainitic ferrite and film retained austenite is obtained. The excellent mechanical properties, with a tensile strength of 1530MPa and an elongation of 3.1% can be achieved by controlling the matrix microstructure of 12% prior martensite, 15% retained austenite with 1.64% carbon content, and 73% bainitic ferrite. This is mainly attributed to prior marteniste which can promote refinement of multiphase colonies.

Zhuang, W., Jiang, Y., Zhou, W., Liang, Z., Northwood, D.O., Liu, C.

Influence of multi-step austempering temperature on tensile performance of unalloyed ductile iron
(2019) *Key Engineering Materials*, 803 KEM, pp. 3-7.

Abstract
Austempered ductile iron (ADI) has been widely used in various industries due to its excellent combination of high strength, ductility and good wear resistance. The tensile behavior of an unalloyed commercial ADI with a multiphase structure designed by a novel multi-step austempering treatment is investigated. The developed austempering process consists of austenitizing at 890°C for 20min, then initial rapid quenching to 180°C, and isothermal holding at 190, 220, 250°C for 120min, and finally air cooling to room temperature. The optimum mechanical properties with an ultimate tensile strength of 1350MPa, a yield strength of 1090MPa, as well as an elongation of 3.5% is achieved at 220°C. This is attributed to a synergistic strengthening effect of multiphase structure including a prior martensite with fine needle bainitic ferrite and film retained austenite.

Zhou, R., Wang, X., Liu, C., Northwood, D.O.

Self-organized Formation of Multilayer Structure in a High Nitrogen Stainless Steel during Solution Treatment
(2019) *MRS Advances*, 4 (5-6), pp. 271-276. Cited 1 time.

Abstract
Compared with traditional stainless steels, high nitrogen stainless steels (HNSS), have been widely used due to their high strength, toughness along with excellent corrosion resistance and low cost, formed by partial replacement of Ni (austenite-forming element) by N. The evolution of the microstructure of a

Cr19Mn19Mo2N0.7 stainless steel is investigated after solution treatment at 1010, 1060, 1200 or 1250°C for 30min. A complex multilayer structure has been found under a negative pressure vacuum. A white ferritic layer at the surface is formed, and a subsurface layer with full austenitic structure and a bulk microstructure comprising of austenite and ferrite are detected. With increasing solution temperature, the surface layer thickness increases. The formation of the multilayer structure is attributed to an outward diffusion, a diffusive retardation and an abnormal accumulation of nitrogen during solution treatment.

Dong, K., Zhou, R., Northwood, D.O., Liu, C.

Effect of solution treatment time on microhardness of high nitrogen austenitic stainless steel
(2019) *Key Engineering Materials*, 803 KEM, pp. 37-41.

Abstract
High nitrogen stainless steel (HNSS) is becoming an increasingly important engineering material because of its excellent corrosion resistance and good mechanical properties. A hot rolled Cr19Mn19Mo2N0.7 HNSS, having a microstructure consisting of banded ferrite and dotted/dendritic nitrides dispersed in the austenite matrix, was solution treated at 1160°C for various times. It is shown that the nitride can be dissolved, and the shape of ferrite can be changed by the solution treatment. The microhardness of both austenite and ferrite decreases with increasing solution treatment time. This is attributed to an increased grain size and a homogeneous distribution of alloying elements. The results are helpful in controlling the thermomechanical processing of HNSSs in commercial practice

Zhou, R., Northwood, D.O., Liu, C.

On nitrogen diffusion during solution treatment in a high nitrogen austenitic stainless steel
(2020) *Journal of Materials Research and Technology*, 9 (2), pp. 2331-2337.

Abstract
The generation and microstructural characteristics of the surface layer formed during solution treatment at 1200 °C of a high nitrogen austenitic stainless steel, have been investigated using optical microscopy, X-ray diffraction (XRD) and scanning electron microscopy (SEM) with energy dispersive X-ray spectroscopy (EDS). Contrasting with a bulk microstructure of austenite and ferrite, a multi-layer surface structure is obtained, which consists of a white outer-surface layer which is ferrite and a grey subsurface layer with austenite. Formation of the multi-layer structure occurs through phase transformations between austenite and ferrite due to the various levels of nitrogen diffusion. With increasing solution treatment time, the thicknesses of both the surface and the subsurface layer increase. Hardness tests show that the microhardness increases from the surface layer, to the subsurface layer and then to the bulk. This is attributed to the combined effects of solid solution strengthening from nitrogen and the grain size of austenite or ferrite.

## 2. Innovation in Engineering Education

Over the past six years, I have been working with Associate Professor Daniela Pusca, University of Windsor, on the challenges we face as educators in an engineering faculty. The emphasis has been on "Engineering Design", in particular for a first year foundation course.

In the 2018-2019 period, we have examined "creativity" in the context of engineering design education. It is considered that curiosity is a pre-requisite for creativity, as creative people are curious by default. Curiosity is inborn in children but it can be suppressed by the educational system. As famously quoted by Albert Einstein: "It is a miracle that curiosity survives formal education". Our role as instructors is to find ways to encourage and develop curiosity in students, because without curiosity, creativity will never follow. To do this we must both "teach creatively" and "teach for creativity" - by creating an engaging, stimulating teaching and learning environment that encourages curiosity, creativity, and intellectual diversity. The emphasis is on "learning" since "only the learner can learn". Example publications include:

Pusca, D., Northwood, D.O.

Curiosity, creativity and engineering education
(2018) *Global Journal of Engineering Education*, 20 (3), pp. 152-158. Cited 6 times.

Abstract
It has been stated that the need to know is an engine of discovery that motivates humanity to explore, experiment and achieve (Mario Livio and Robin Tatu). In this article, the authors discuss different opinions and definitions associated with curiosity as the need to know, its relation to creativity and the implication for the models of active learning. The purpose is twofold: 1) to better understand why curiosity, as a powerful human force for intellectual and creative expression, motivates stronger student engagement to find solutions for open-ended, complex problems; and 2) to analyse if curiosity and creativity can be cultivated, supported and encouraged or if they are suppressed by person-centred and context-centred factors or the education system itself. Instructors, when reflecting on what and how we teach, must place equal consideration on teaching creatively and teaching for creativity (Sir Ken Robinson). Case studies discuss the role of curiosity and creativity in engineering design courses at the University of Windsor and the instructor's role in creating an engaging, stimulating teaching and learning environment that encourages curiosity, creativity and intellectual dexterity.

Pusca, D., Northwood, D.O.

Creativity and its constraints in engineering education
(2019) *World Transactions on Engineering and Technology Education*, 17 (2), pp. 146-151.

Abstract
In this article, the authors discuss different opinions associated with creativity. There are various views as to whether constraints aid or harm creativity, including those who view that even the definition of creativity requires constraints. Using evidence, the authors argue that constraints trigger creativity, and examine the influencers of practical creativity in the context of engineering education. It is the authors' opinion that teaching and learning should be done creatively, and several practices for creative development are analysed in the context of engineering design courses at the University of Windsor, Windsor, Canada. As a result, not only the student experience is improved, but also the teaching moments become more enjoyable, and will trigger the instructor's enthusiasm in the process. The authors also examine why is creativity important to engineering and engineering education, how to practice creativity and what is the role of constraints on creativity.

## 3. Plasma-Electrolytic Oxidation (PEO) for the Production of corrosion and wear resistant coatings on light metals

Since 2008, I have been working with Dr. Riyad O. Hussein (now at Natural Sciences Division, Higher Colleges of Technology of Technology, United Arab Emirates and Professor Xueyuan Nie (University of Windsor) on the development of Plasma Electrolytic Oxidation (PEO) for the production of corrosion and wear resistant coatings on light metal alloys (Al, Mg, and Ti). The approach taken to this research has been multi-faceted and has involved both spectographic studies of the plasma to determine its temperature and composition, and detailed studies of the microstructure and composition of the resulting coating. These observations are related back to the PEO processing conditions (voltage, current mode, pulse timing, electrolyte composition and concentration) and substate composition. A model has been proposed for the ceramic coating growth mechanisms during PEO processing. Example publications include:

Hussein, R.O., Nie, X., Northwood, D.O.

An investigation of ceramic coating growth mechanisms in plasma electrolytic oxidation (PEO) processing
(2013) *Electrochimica Acta*, 112, pp. 111-119. Cited 200 times.

Abstract
To further our understanding of the plasma electrolytic oxidation (PEO) process, and to aid in the optimization of the process, it is important to identify the mechanisms of coating formation. In the present work, coatings up to 110 μm thick were produced on an AJ62 Mg-alloy substrate using the PEO process.

Optical emission spectroscopy (OES) was employed to follow the microdischarges and substrate and electrolyte elements present in the plasma discharge during the coating growth, and to determine plasma electron temperatures. During PEO processing of magnesium, some of the metal cations are transferred outwards from the substrate and react with anions to form ceramic coatings. Also, due to the high electric field in the discharge channels, oxygen anions transfer toward the magnesium substrate and react with Mg2+ cations to form a ceramic coating. In PEO process, the ceramic coating grows inwards to the alloy substrate and outwards to the coating surface simultaneously. The total coating thickness variation compared with the geometrical dimensions of the uncoated and coated samples were investigated. For the coating growth, there are three simultaneous processes taking place, namely the electrochemical reactions, the plasma chemical reactions and thermal diffusion. Oxygen diffusion occurring during PEO processing is discussed in terms of coating growth mechanisms.

Hussein, R.O., Nie, X., Northwood, D.O., Yerokhin, A., Matthews, A.

Spectroscopic study of electrolytic plasma and discharging behaviour during the plasma electrolytic oxidation (PEO) process
(2010) *Journal of Physics D: Applied Physics*, 43 (10), art. no. 105203, . Cited 300 times.

Abstract
In this study, a plasma electrolytic oxidation (PEO) process was used to produce oxide coatings on commercially pure aluminium (1100 alloy) at a pulsed dc power mode. The effects of process parameters (i.e. current density and treatment time) on the plasma discharge behaviour during the PEO treatment were investigated using optical emission spectroscopy (OES) in the visible and near ultraviolet (NUV) band (285-800 nm). The elements present in the plasma were identified. Stark shifts of spectral lines and line intensity ratios were utilized to determine the plasma electron concentrations and temperatures, respectively. The plasma electron temperature profile, coating surface morphology and coating composition were used to interpret the plasma discharging behaviour. The different coating morphologies and compositions at different coating surface regions are explained in terms of three types of discharge, which originate either at the substrate/coating interface, within the upper layer, or at the coating top layer. The high spike peaks on the plasma intensity and temperature profiles corresponded to discharges originated from the substrate/coating interface, while the base line and small fluctuations were due to discharges at the coating/electrolyte interface

Hussein, R.O., Nie, X., Northwood, D.O.

An investigation of ceramic coating growth mechanisms in plasma electrolytic oxidation (PEO) processing
(2013) *Electrochimica Acta*, 112, pp. 111-119. Cited 200 times.

Abstract
To further our understanding of the plasma electrolytic oxidation (PEO) process, and to aid in the optimization of the process, it is important to identify the mechanisms of coating formation. In the present work, coatings up to 110 μm thick were produced on an AJ62 Mg-alloy substrate using the PEO process. Optical emission spectroscopy (OES) was employed to follow the microdischarges and substrate and electrolyte elements present in the plasma discharge during the coating growth, and to determine plasma electron temperatures. During PEO processing of magnesium, some of the metal cations are transferred outwards from the substrate and react with anions to form ceramic coatings. Also, due to the high electric field in the discharge channels, oxygen anions transfer toward the magnesium substrate and react with Mg2+ cations to form a ceramic coating. In PEO process, the ceramic coating grows inwards to the alloy substrate and outwards to the coating surface simultaneously. The total coating thickness variation compared with the geometrical dimensions of the uncoated and coated samples were investigated. For the coating growth, there are three simultaneous processes taking place, namely the electrochemical reactions, the plasma chemical reactions and thermal diffusion. Oxygen diffusion occurring during PEO processing is discussed in terms of coating growth mechanisms

## 4. The "Costs" of Corrosion

The economic impact worldwide of corrosion has been shown to represent about 3.5% GDP and this percentage GDP lost to corrosion has remained constant over the years, despite the development of new materials and corrosion prevention methods. Furthermore, it is estimated that 25% to 35% of these costs would have been preventable using methods known at the time. In the paper, "Corrosion and Society", these economic costs are

examined further and the questions are asked: "Is this acceptable?" and "What, if anything, are we doing wrong?" These economic (financial) costs are only one aspect of how corrosion "costs" society. There are also the "social implications", namely "waste of natural resources" and "inconvenience to human beings, including loss of life." Taking the other "costs" into consideration leads to consideration of sustainability. The relation between corrosion and sustainability is examined in more detail in the paper, "Corrosion: The circular materials economy and design for sustainability." To do this we started with Ursula Franklin's contention (Franklin U, The Real World of Technlogy (CBC Massey lectures series), Anansi Press Limited, Concord, ON, Canada, 1992 ISBN 0-88784-531-2) that for us to make socially responsible decisions, and to develop and implement what she called "redemptive technologies", which turn harmful practices into less harmful ones, we need to use three sets of (accountancy and bookkeeping) books to examine the "costs" of corrosion. These 3 books were:

1. Dollars-and-Cents (economic)
2. People and Social Impacts
3. Environmental. Health and viability of nature, and the built environment

Examination of corrosion through these three "cost lenses" shows that both a 'Design for Sustainability' and a 'Circular Materials Economy' approach can help in addressing the "costs" challenges. However, when considering the three accounting books, it is important to identify:

WHO ARE THE STAKEHOLDERS?
WHO BENEFITS?
WHO PAYS?

The key element in the way forward to the use of "Redemptive" technologies, is "harm". The medical profession has the Hippocratic Oath as their guiding light". In essence the oath says:

'NIL NOCERE' - DO NO HARM

A Hippocratic Oath, modeled on the medical oath, was proposed for corrosionists:

**HIPPOCRATIC OATH REVISED FOR CORROSIONISTS**

I swear to fulfill, to the best of my ability and judgment, this covenant:

I will respect the hard-won scientific gains of those corrosionists in whose steps I walk, and gladly share such knowledge as is mine with those who are to follow.

I will apply, for the benefit of humanity, all measures [that] are required, avoiding those twin traps of over-treatment and therapeutic nihilism.

I will remember that there is art to corrosion control and durability as well as science, and that warmth, sympathy, and understanding may outweigh an engineering solution.

I will not be ashamed to say "I know not, nor will I fail to call on my colleagues when the skills of another are needed.

I will adhere to the highest standards of professionalism, confidentiality, and advice in dealing with all stakeholders involved in a project. I will remember that I do not treat just a corroding structure whose durability may affect societal, environmental, and economic stability . My responsibilities must include these broader related issues, if I am to adequately perform my job.

I will prevent corrosion and subsequent failure whenever I can, for prevention is preferable to cure.

I will remember that I remain a member of society, with special obligations to all my fellow human beings.

If I do not violate this oath, may I enjoy life and art, respected while I live and be remembered with affection thereafter. May I always act so as to preserve the finest traditions of my profession and may I long experience the joy of helping those who seek my counsel.

The key papers are:

Northwood, D.O., Faldu, N.

Corrosion: The circular materials economy and design for sustainability
(2020) *Corrosion and Prevention 2019*, .

Abstract
Ursula Franklin (1992) contended that in order to make both socially responsible decisions, and to develop and use “redemptive technologies”, which turn harmful practices into less harmful ones, a community needs three sets of (accountancy and bookkeeping) books. The first is the “dollars-and-cents” book. The second book is related to people and social impacts. The third book is” environmental accounting”, which addresses the health and viability of nature, as well as the built environment. This paper will examine corrosion through these three cost lenses and show how both a 'Design for Sustainability' and a 'Circular Materials Economy' approach can be used to address the “costs” challenges. Optimization is a commonly used tool in the development of high-performance structures and materials but has traditionally had only purely economic objectives and is not “optimal” in terms of sustainability or circularity. However, the coupling of sustainability metrics with optimization leads to a consideration of all three of Franklin's “accounting books”. Further, through consideration of the Circular (Materials) Economy, we can, for instance, either develop sustainable coatings or choose a concrete mix that both meet societal and environmental drivers and maintain and/or extend performance in more extreme environments. Developments such as additive manufacturing can also bring advantages to the circular economy and can potentially improve the sustainability of manufacturing. Whilst these approaches are not fully “redemptive”, they fit what Robert Muir-Wood (2016) describes as “predictive technologies” in his book, “The Cure for Catastrophe”. However, as stressed by Muir-Wood, even if we utilize these “predictive/redemptive” technologies, information AND action must come together in order to produce sustainable solutions

Northwood, D.O.

Corrosion and society
(2019) *Corrosion and Materials*, 44 (1), pp. 50-55. Cited 1 time.

Northwood, D.O.

Corrosion and society
(2018) *Corrosion and Prevention 2018*, . Cited 1 time.

Abstract
It has long been well known that corrosion can seriously damage your wealth. Various studies over the past 50 or so years have shown that the economic impact worldwide of corrosion represents about 3.5% of the GDP. This percentage GDP lost to corrosion has remained constant despite the development of new materials and corrosion prevention methods, and constant reminders that awareness of corrosion is essential to reduce the cost burden of corrosion. Probing further into these costs, it is estimated that 25 to 35 percent of those costs are preventable using known methods. With the global cost of corrosion estimated to be 2.5 trillion USD these “preventable” costs could potentially be up to $875 billion. Is this acceptable? What if anything are we doing “wrong”? The “costs” so far examined are the financial costs but corrosion costs society in three ways: financially; wasteful of natural resources; causes considerable inconvenience to human beings, including loss of life. The last two are considered to be 'social implications'. These 'social implications' have, in part, been addressed by making society more aware of corrosion. Corrosion, and its associated costs, both financial and social, is a complex, often called “wicked”, problem. Problem solving should be solution, rather than problem (i.e., corrosion), focused and involves not only financial and materials/engineering considerations, but also social, political and ethical considerations. As encouraged by Nick Birbilis, “Let's keep corrosion in mind as we design not only new structures and components, but in the designing a more sustainable future”. Sustainability is, after all, design for the purpose of enriching human life.

# Non-invasive Load Monitoring of Induction Motor Drives using Magnetic Flux Sensors

**by Wenping Cao, Member EUAS**

Short Biography

***Wenping Cao*** *(M'05-SM'11) received the B.Eng in electrical engineering from Beijing Jiaotong University, Beijing, China, in 1991, and the Ph.D. degree in electrical machines and drives from the University of Nottingham, Nottingham, U.K., in 2004. He is currently Chair Professor of Electrical Power Engineering at Aston University, Birmingham, U.K., and also a Visiting Professor at School of Electrical Engineering and Automation, Anhui University, P. R. China.*

*Prof. Cao is presently the Chairman for the Industrial Electronics Society, IEEE UK and Ireland Section, and also a "*Royal Society Wolfson *Research* Merit Award" holder, U.K. *He was a semi-finalist at the "Annual MIT-CHIEF Business Plan Contest", U.S.A., in 2015; the "Dragon's Den Competition Award" winner from Queen's University Belfast, U.K., in 2014, the "Innovator of the Year Award" winner from Newcastle University, U.K., in 2013.*

*He received the "Best Paper Awards" from the IET International Conference on Renewable Power Generation (RPG)* ***in 2019 and*** *the 9th International Symposium on Linear Drives for Industry Applications (LDIA) in 2013.*

*His research interests include fault analysis and condition monitoring of electrical machines and power electronics.*

## Research Publications

### Non-Invasive Load Monitoring of Induction Motor Drives Using Magnetic Flux Sensors.

*IET Power Electronics*, Vol. 10, Issue 2, pp. 189-195, 2017.

Z. Liu, G. Tian, W. Cao, X. Dai, B. Shaw, R. Lambert

### Abstract

Existing load monitoring methods for induction machines are generally effective, but suffer from sensitivity problems at low speeds and non-linearity problems at high supply

frequencies. This paper proposes a new non-invasive load monitoring method based on giant magnetoresistance (GMR) flux sensors to trace stray flux leaking from induction motors. Finite element analysis (FEA) is applied to analyse stray flux features of test machines. Contrary to the conventional methods of measuring stator and/or rotor voltage and current, the proposed method measures the dynamic magnetic field at specific locations and provides time-spectrum features (e.g. spectrograms), response time load and stator/rotor characteristics. Three induction motors with different starting loading profiles are tested at two separate test benches and their results are analysed in the time-frequency domain. Their steady features and dynamic load response time through spectrograms under variable loads are extracted to correlate with load variations based on spectrogram information. In addition, the transient stray flux spectrogram and time information are more effective for load monitoring than steady state information from numerical and experimental studies. The proposed method is proven to be a low-cost and non-invasive method for induction machine load monitoring.

## Assessment of an Electric Vehicle Powertrain Model Based on Real-World Driving and Charging Cycles.

*Vehicular Technology*, Vol. 68, Issue 2, pp. 1178-1187, Feb. 2019

G. Du, W. Cao, S. Hu, Z. Lin, T. Yuan

### Abstract

An analytical model for an electric vehicle (EV) powertrain has been developed in this paper to study the vehicular dynamics, based on a *Nissan Leaf* EV. The electrical components of the powertrain include a battery pack, a battery management system (BMS), a DC/DC converter, a DC/AC inverter, a permanent magnet synchronous motor (PMSM), and a control system while the mechanical system consists of power transmissions, axial shaft and vehicle wheels. The driving performance of the EV is studied through the real-world driving tests and simulation tests in Matlab/Simulink. In the analytical model, the vehicular dynamics is evaluated against changes in the vehicle velocity and acceleration, state of charge (SOC) of the battery, and the motor output power. Finally, a number of EVs are introduced in the system to optimize the power dispatch. The greenhouse gas emissions of EVs are analyzed under various driving and charging conditions, and compared with conventional internal combustion engine (ICE) vehicles. For a given driving cycle, Nissan Leaf can reduce $CO_2$ emissions by 70%, depending on its duty cycle and the way electricity is supplied.

## In Situ Diagnostics and Prognostics of Solder Fatigue in IGBT Modules for Electric Vehicle Drives.

*IEEE Transactions on Power Electronics*, Vol. 30, Issue 3, pp. 1535-1543, Mar. 2015.

B. Ji, X. Song, W. Cao, V. Pickert, Y. Hu, J. Mackersie, and G. Pierce

**Abstract**

This paper proposes an *in-situ* D&P technology to monitor the health condition of IGBTs used in EVs with a focus on the IGBTs' solder layer fatigue. IGBTs' thermal impedance and the junction temperature can be used as health indicators for through-life condition monitoring where the terminal characteristics are measured and the devices' internal temperature-sensitive parameters are employed as temperature sensors to estimate the junction temperature. An auxiliary power supply unit, which can be converted from the battery's 12V DC supply, provides power to the in-situ test circuits and condition monitoring data can be stored in the on-board data-logger for further offline analysis. The proposed method is experimentally validated on the developed test circuitry and also compared with finite-element thermo-electrical simulation. The test results from thermal cycling are also compared with acoustic microscope and thermal images. The developed circuitry is proved to be effective to detect solder fatigue while each IGBT in the converter can be examined sequentially during red-light stopping or services. The D&P circuitry can utilize existing on-board hardware and be embedded in the IGBT's gate drive unit (GDU).

## Overview of Electric Motor Technologies used for more Electric Aircraft (MEA).

*IEEE Transactions on Industrial Electronics,* Vol. 59, Issue 9, pp. 3523-3531, Sep. 2012.

W. Cao, B.C. Mecrow, G.J. Atkinson J.W. Bennett, D.J. Atkinson

**Abstract**

This paper presents an overview of motor drive technologies used for safety-critical aerospace applications, with a particular focus placed on the choice of candidate machines and their drive topologies. Aircraft applications demand high reliability, high availability, and high power density while aiming to reduce weight, complexity, fuel consumption, operational costs and environmental impact. New electric driven systems can meet these requirements and also provide significant technical and economic improvements over conventional mechanical, hydraulic or pneumatic systems. Fault-tolerant motor drives can be achieved by partitioning and redundancy through the use of multi-channel three-phase systems or multiple single-phase modules. Analytical methods are adopted to compare caged induction, reluctance and PM motor technologies and their relative merits. The analysis suggests that the dual (or triple) three-phase PMAC motor drive may be a favored choice for general aerospace applications, striking a balance between necessary redundancy and undue complexity, while maintaining a balanced operation following a failure. The modular single-phase approach offers a good compromise between size and complexity but suffers from high total harmonic distortion of the supply and high torque ripple when faulted. For each specific aircraft application, a parametrical optimization of the suitable motor configuration is needed through a coupled electromagnetic and thermal analysis, and should be verified by finite-element analysis.