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Abstract Book

3rd Edition of Materials Science and Nanoscience Webinar

September 17-18, 2021 | GMT 07:00 – 15:00

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KEYNOTE FORUM

DAY 1

3rd EDITION OF

MATERIALS SCIENCE

AND NANOSCIENCE WEBINAR

SEPTEMBER

17-18, 2021

GMT 07:00 – 15:00

V-Mat2021

D. V. Louzguine[a,b]

[a]Advanced Institute for Materials Research (WPI-AIMR), Tohoku University, Aoba-Ku, Sendai 980-8577, Japan.

[b]MathAM-OIL, National Institute of Advanced Industrial Science and Technology (AIST), Sendai 980-8577, Japan.

Atomic Structure of Bulk Metallic Glasses/Liquids Studied by Synchrotron-Radiation X-Ray Diffraction, Scanning Tunneling Microscopy and ab-Initio Molecular Dynamics Simulation

Structural changes in a Zr-Cu-Ni-Al bulk glass-forming, relatively "strong", liquid alloy on cooling from above the equilibrium liquidus temperature studied by synchrotron radiation X-ray diffraction and first-principles molecular dynamics (MD) simulation are compared with those of a "fragile" Pd-Cu-Ni-P one. According to the results chemical ordering forming Zr-Cu,Ni, Zr-Al and Zr-Zr atomic pairs takes place in the Zr-Cu-Ni-Al supercooled liquid alloy on cooling. However, here the change in the Zr-Cu,Ni peak area to other peaks area ratio is smaller than in case of the Pd-Cu-Ni-P alloy (Cu,Ni-P to other peaks ratio) in accordance with a lower fragility index of the Zr-Cu-Ni-Al melt [1]. It indicates that fragility is a sign of instability of short and medium range order in fragile liquids. We also studied the atomic structure of a Ni-Nb bulk metallic glass by means of ultra high vacuum scanning tunneling microscopy (STM) in local areas of nanometer scale size, and report the direct atomic structure observation supported by MD simulation used to understand the observed structural and electronic features [2]. More recent research results on the subject will also be discussed.

[1] D.V. Louzguine-Luzgin, K. Georgarakis, J. Andrieux, L. Hennet, T. Morishita, K. Nishio, R.V. Belosludov, Intermetallics, 122 (2020) 106795.

[2] R.V. Belosludov, A.I. Oreshkin, S.I. Oreshkin, D.A. Muzychenko, H. Kato, D.V. Louzguine-Luzgin, Journal of Alloys and Compounds, 816 (2020) 152680.

Biography

Prof. Dr. Eng. degree obtained at Tohoku University, Japan. From 2007 until present: Professor, Principal Investigator, WPI Advanced Institute for Materials Research, Tohoku University, Japan. 2018-Present: Concurrent, Principal Investigator, MathAM-OIL, National Institute of Advanced Industrial Science and Technology, Sendai 980-8577, Japan. 2005-2007: Associate Professor, Institute for Materials Research, Tohoku University, Japan. 1998-2005: Research Associate, Institute for Materials Research, Tohoku University, Japan.

Brian Cantor

Department of Materials, University of Oxford; and Brunel Centre for Advanced Solidification Technology, Brunel University London.

Multicomponent High-Entropy Cantor Alloys

All human advances have depended on making new materials, and all materials are alloys, i.e. mixtures of several different starting materials or components. So the history of the human race has been the continued invention of new materials by discovering new alloys. Recently a new way of doing this, by manufacturing multicomponent high-entropy alloys, has shown that the total number of possible materials is enormous, even more than the number of atoms in the galaxy, so we have lots of wonderful new materials yet to find. And multicomponent phase space contains a surprisingly large number of extended solid solutions. The first group of these which was discovered are called Cantor alloys, an enormous composition range with a single-phase fcc structure, based loosely on the original equiatomic five-component Cantor alloy CrMnFeCoNi. This talk will discuss the previous history of alloying, the discovery of multicomponent alloys, the structure of multicomponent phase space, the fundamental thermodynamics of multicomponent solid solutions such as the Cantor alloys, the complexity of local atomic configurations in such materials, the effect of this on properties such as atomic diffusion, dislocation slip, and the resulting outstanding mechanical properties and potential applications.

Biography

Brian Cantor is an Emeritus Professor in the Department of Materials at the University of Oxford and a Research Professor in the Brunel Centre for Advanced Solidification Technology at Brunel University. He was previously Vice-Chancellor of the University of York and of Bradford University, Head of Mathematical and Physical Sciences at the University of Oxford, and a research scientist and engineer at General Electric Research Labs in the USA. He also worked briefly at Banaras Hindu University, Washington State, Northeastern, IISc Bangalore and the Kobe Institute. He founded and built up the World Technology Universities Network, the UK National Science Learning Centre, the Hull-York Medical School, and Oxford's Begbroke Science Park. He was a long-standing consultant for Alcan, NASA and Rolls-Royce, and editor of Progress in Materials Science. He invented the new field of multicomponent high-entropy alloys and discovered the so-called Cantor alloys.

Aharon Gedanken

Department of Chemistry and the BINA center, Bar-Ilan University, Ramat-Gan, Israel, 5290002

Sonochemical Coatings: From the laboratory to the market

Three products originating from my laboratory have reached the International market. They are 1) Prophecy and anti-aging cream based on sonochemically produced Hyaluronic Nanoparticles (NPs), 2) Sono Mask an antibacterial and antiviral mask in which the coating is done sonochemically, and 3) An antibacterial and antiviral filter for the air-conditioning car system.

Number 2 and 3 involve the sonochemical coating technique which deposits metal oxide NPs on the substrate. The substrate in the case of the mask is a textile and a polymer in the filter's case. The reason for the antibacterial effect of the metal oxide NPs will be outlined.

The lecture will introduce the advantages of the sonochemical method and explain why it is considered the best coating technique at least for textile coatings. Two modes of coating will be presented the *in-situ*, and the "throwing stones".

Biography

Emeritus Prof. Aharon Gedanken obtained his M. Sc. from Bar-Ilan University, and his Ph. D. degree from Tel Aviv University, Israel. After his postdoctoral research at USC in Los Angeles, he returned to Bar-Ilan in 1975 as a senior faculty. He was a visiting scientist at AT&T Bell Laboratories in 1980-8l, 1984, and 1987-88, and at NIDDK, NIH in the summers of 1989, 1990 and 1991. In 1994 he switched his research interest from Spectroscopy to Nanotechnology. His special synthetic methods of nanomaterials include: Sonochemistry, Microwave Superheating, Sonoelectrochemistry, and Reactions under Autogenic Pressure at Elevated Temperatures (RAPET). Since 2004 he is mostly focused on the applications of nanomaterials. Gedanken has published more than 782 per-reviewed manuscripts in international journals, and has applied for 38 Patents. His H-Index is 113. Gedanken has served as the Department chairman as well as the Dean of the Faculty of Exact Sciences at Bar-Ilan University. He is on the editorial boards of 7 international journals. He leads a group of 12 research people. He was a partner in five EC FP7 projects one of them, SONO, was coordinated by him. This project was announced by the EC as a "Success Story". He was the Israeli representative to the NMP (Nano, Materials, and Processes) committee of EC in FP7. He was awarded the prize of the Israel Vacuum Society (deals with Nanotechnology) and the Israel Chemical Society for excellence in Research.

Yair Ein-Eli [a, b]

[a]Department of Materials Science and Engineering and [b]Nancy & Stephen Grand Technion Energy Program (GTEP), Technion- Israel Institute of Technology Haifa 3200003 Israel. E-mail id: eineli@technion.ac.il

Metal-free and flexible Li-ion batteries based on CNT tissues

Electrochemical systems hold a great promise as the solution for the vast demand for high energy density in both portable (from small handheld electronic to large mobile systems as EV) and stationary devices. Pressure is imposed on researchers to develop new systems, as the need for more "juice" in mobile device increase, as technology is rapidly evolving. In this talk, we will describe a possible transition from copper and aluminum current collectors into carbon nano tube (CNT) tissues. Such transition may substantially reduce the overall weight of the battery, and at the same time would allow more volume in the cells to be subsequently loaded with the active electrode materials. We will describe the processes needed for implementing CNT tissues in Li-ion batteries, as well as overcoming the massive irreversible capacity associated with the buildup of the solid electrolyte interphase (SEI) onto both the graphite and the CNT surfaces. Copper electroplating onto the CNT fabric predominately at top surface of the tissue will be discussed as well.

Biography

Prof. Yair Ein-Eli graduated from Bar-Ilan University (1995) and he joined (2001) the Department of Materials Engineering at the Technion-Israel Institute of Technology, after serving 3 years as the VP of R&D of Electric Fuel Ltd. (Israel). Before that (1995-1998), he was a post-doctoral fellow at Covalent Assoc. Inc. (MA, USA). Current research projects of Yair in the field of power sources involve advanced materials for Li-ion batteries, alkaline batteries, metal-air cells and fuel cells. He is also engaged in research and development of electroplating methods, as well as **corrosion inhibitors studies.** He has published more than 180 papers in reputed journals and has been serving as an Editor of the Journal of Solid State Electrochemistry.

Tayebeh Ameri

Institute for Materials and Processes, Chemical Engineering, University of Edinburgh, Sanderson Building, Robert Stevenson Road, EH9 3FB, Edinburgh, UK. E-mail id: tayebeh.ameri@ed.ac.uk

Advanced Printed Semiconductors for Highly Efficient and Stable Photovoltaics

WE study advanced functional materials for solar power and energy application. This includes development of emerging printed organic, hybrid, and perovskite photovoltaics. The aim of our work is to understand the fundamentals and improve the performance, stability and manufacturing processes of these technologies to provide cheaper/more effective solutions for issues of key importance of society: particularly solutions to the climate emergency.

The unique selling points of organic photovoltaics (OPVs), such as excellent light harvesting capability, freedom of form, colour and transparency, environmental friendliness, easy scalability and lower manufacturing costs based on roll-to-roll printing methods, position this technology for the mobile power market, and this most properly reflects the state of the art in commercialization. An important milestone towards OPV commercialization has been surpassed by reaching a power conversion efficiency (PCE) of over 17%. To overcome the absorption and thickness limitations, the concept of ternary near IR sensitization of organic solar cells has been explored in the last decade. As one of the pioneer research groups in development of "Ternary Organic Solar Cells", we demonstrated the potentiality of this concept and comprehensively investigated various prototype organic ternary systems with a central focus on the fundamental complexity of microstructure and charge transport mechanisms. Importantly, we realized the key issues that result in modified recombination mechanisms and consequently improved fill factor and open circuit voltage in high efficiency ternary/ multicomponent solar cells. Ternary Solar Cells are nowadays a leading strategy in organic photovoltaic technology with the potential to further address the challenges of global energy demand and climate emergency.

Additionally, hybrid systems, a combination of the unique properties of both organic and inorganic semiconductors, are of significant interest to develop printed hybrid electronic devices for use in modern applications. We focused particularly on developing a comprehensive understanding, design, and development of printable hybrid ternary solar cell by implementing an appropriate inorganic or hybrid compound in the form of nanoparticles (NPs)/ nanostructures (NSs) into the organic host matrices.

Importantly, organic- inorganic hybrid perovskite photovoltaics (PPVs) have attracted tremendous attention due to rapid progress in terms of PCE in the last few years, from 3.8% to present record values in excess of 25%. However, fundamental problems, such as the toxicity of hybrid lead halide perovskites, hysteresis and structural instability remain to be solved for perovskite solar cells. Indeed, the low-temperature solution-processing of perovskite films inevitably causes formation of a certain amount of defects on the surface and at the grain boundaries, which lead to serious trapping, charge accumulation, and recombination problems as well as stability issue. We pursue the interface engineering and defects passivation by introducing various types of multifunctional conjugated organic compounds. We were successfully able firstly to heal detrimental defects on perovskite film surfaces, which adversely affect the photovoltaic performance and stability of corresponding devices, and secondly to convert excess or unreacted PbI_2, which is also detrimental for long-term stability of solar cell devices, into beneficial complex species for efficient hole transfer at the modified interface.

In this presentation, we will discuss our achieved results in details for various prototype organic, hybrid and perovskite systems with a central focus on the fundamental complexity of microstructure and charge transport mechanisms and their correlation to the device performance and stability.

Akrajas Ali Umar

Institute of Microengineering and Nanoelectronics, Universiti Kebangsaan Malaysia, 43600 UKM Bangi, Selangor, Malaysia, Email id: akrajas@ukm.edu.my

Single-crystalline electron transport layer for enhanced carrier dynamic in perovskite solar cells

The crystallinity of the electron transport layer (ETL) of a perovskite solar cells affects the interfacial charge transfer and charge extraction dynamic during the photoelectrical process. In this talk, the role of ETL crystallinity properties and the extent effect of its surface chemistry and morphology on the photogenerated electron transfer at the interface and transport in the perovskite solar cell device will be discussed. The focused of the discussion will be directed to our recent experience in developing new design of ETL for performance improvement.

Biography

Dr. Akrajas Ali Umar received his PhD in Physics from the National University of Malaysia in 2004 in organic thin film for optical sensing application. He is currently Associate Professor in the Institute of Microengineering and Nanoelectronics (IMEN), the National University of Malaysia since 2011. His research interests are mainly in the field of Nanophysics and Nanomaterial Chemistry with the emphasis for energy conversion application, particularly to investigate the role of atomic composition, surface structure and shape of nanostructures in photoactivity and photoelectrical properties. He served as Kyoto University Venture Business Laboratory Postdoctoral Fellow (2004-2005) and Japan Society for the Promotion of Science (JSPS) Postdoctoral Fellow in Kyoto University, Japan, from 2005-2007. He was a appointed as a World Class Professor in Faculty of Mathematics and Natural Sciences, Universitas Halu Oleo-Indonesia in 2018 and a visiting scientist in the School of Information Science and Technology, Fudan University, Shanghai, China from 2018 to 2019. He has published more than 200 papers.

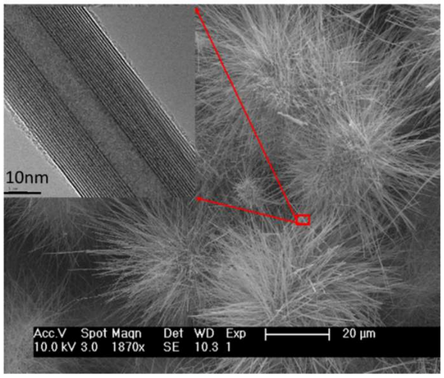
Zak[1]*, S. Ghosh[1] and C. Pallellappa[1], T. Livneh[2], I. Kaplan-Ashiri[3], Y. Zhang[4], V. Bruser[5], A. Di Bartolomeo[6]

[1]HIT-Holon Institute of Technology, Holon, Israel, alzak@hit.ac.il, [2]Nuclear Research Center, Negev, Israel, livneh123@gmail.com ; [3]Weizmann Institute of Science, Israel, ifat.kaplan-ashiri@weizmann.ac.il, [4]Max Planck Institute for Solid State Research, Germany, [5]Leibnitz Institute of Plasma, Germany, brueser@inp-greifswald.de, [6]University of Salerno Italy; adibartolomeo@unisa.it

Synthetic Route Towards Pure Phase of WS2 & MoS2 Inorganic Nanotubes and their Unusual Properties

Inorganic nanotubes (INTs) of WS_2 and MoS_2 demonstrate unique properties due to their nanosize, closed-cage arrangement of the layers into chiral tubes and mechanical strength. An advance in extremely complicated synthesis of INT-MoS_2 by vapor-gas-solid (VGS) reaction of Mo oxides with H_2/H_2S gases and its comparison with the growth mechanism of WS_2 nanotubes will be presented. This multistep process is carried out at elevated temperatures (500-900 °C) in a specially designed quartz reactor. The two main steps of the reaction are the growth of metal (Mo,W) oxide nanowhiskers and their following sulfurization into 5-25 µm long and 20-120 nm width MoS_2/WS_2 nanotubes. Recent discovery of bulk photovoltaic effect (BPVE) in INT-WS_2 will be discussed. The photocurrent in the nanotube-based device was orders of magnitude larger than in other BPVE materials. The BPVE does not require p–n junctions of traditional PVE for generation of electric current, and occurs due to the intrinsic properties of INT-WS_2: small band gap (1.4-2.1 eV), broken inversion symmetry and polar structure. This progress is particularly important for environmentally benign energy harvesting because the efficiency of PVE has been almost reached the theoretical limit. An exponential increase of the resistivity with tensile strain was demonstrated up to a recorded elongation of 16%, thereby making WS_2 NTs suitable for piezoresistive sensor applications. Low temperature CL of single-wall few nm diameter WS_2 nanotubes, produced by high-power plasma irradiation of multiwall WS_2 INTs, demonstrates blue shift, evidencing quantum confinement and strain effect

microscopy images of WS_2 nanotubes for abstract (for the case of need)



Biography

Prof. Alla Zak, is a Head of the Laboratory for Synthesis and Investigation of Nanomaterials and Associate professor in the Faculty of Sciences in the HIT-Holon Institute of Technology, Israel. She is also a Scientific Adviser in the Department of Materials and Interfaces in Weizmann Institute of Science (WIS), Israel. She has completed her Ph.D. study in Weizmann Institute of Science, Israel; served as a Chief Scientist in NanoMaterials, Ltd. company for ~10 years and continue her academic research in HIT from 2012. Alla Zak is an inventor of 3 patents and an author of 67 scientific papers.

Paolino Caputo[1] and Cesare Oliviero Rossi[1]

[1]Department of Chemistry and Chemical Technologies, University of Calabria, Via P. Bucci, Cubo 14/D, Rende (CS), 87036, Italy & UdR INSTM della Calabria

The use of nanomaterials as atmospheric fume-removing additive for bitumen

The eminent issue of environmental pollution has driven research towards finding solutions and developing technologies to alleviate this problem. In the asphalt industry, a lot of research and effort has gone into developing technologies to eliminate or at least reduce the emission of toxic substances which are often released into the environment during several industrial processes most especially asphalt mix production and road paving processes. Of these potential toxic substances, greenhouse gases constitute a major percentage. The gases which pose danger to the environment are the major causes of the current global warming situation and are even more toxic to the road workers who take part in the process of asphalt production and paving. Although additive technologies exist which lower asphalt production and paving temperatures in such a way that the emission of toxic fumes is reduced, there is still a need to eliminate the emission of these substances in order to safeguard the environment and guarantee a safer future for the human populace. This study seeks to evaluate the performances of 2 types of silica-based nanoparticle additives in eliminating bitumen's fume emission into the atmosphere during asphalt production and paving processes. These mesoporous silica-based additives have different porosities and they function by trapping the volatile substances in bitumen thus preventing their release at high temperatures. Gas chromatography-mass spectrometry (GC-MS) and thermogravimetric (TGA) techniques were used to quantify and characterize the emitted fumes while Dynamic Shear Rheology (DSR) was used to analyse the rheological properties of the bitumen and the possible sedimentation issues that could occur after the addition of the additives.

Biography

Caputo Paolino obtained his PhD in Life Science and Technology from the University of Calabria, Italy. He is currently a post-doc researcher in the department of Chemistry and Chemical Technologies at the University of Calabria. His research focuses on physical chemistry with a main focus on bitumen characterization and food based industrial materials and compounds. He has over 35 publications with over 400 citations. He serves as a reviewer for several reputable physical chemistry journals. He is also one of the inventors of the Anti-smoke Patent (release date: October 31, 2018; number 102016000041219)

Mohammad Asadi

Chemical and Biological Engineering Department, Illinois Institute of Technology, Chicago, IL 60616, US

Advanced Materials for a Carbon-Neutral Future

One of the greatest scientific and engineering challenges of the 21st century is to develop sustainable energy technologies to fulfil our current energy needs that mainly depend on fossil fuels with severe environmental impacts. Among various emerging technologies, energy conversion and storage systems have shown tremendous potential to be the alternative of fossil fuels due to their ability to harvest renewable energy, e.g., solar and wind in the form of chemical bonds. In general, energy can be stored or converted into chemical bonds through photo/electrochemical process, e.g., batteries, carbon dioxide reduction reaction (CO_2RR), oxygen reduction reaction (ORR), oxygen and hydrogen evolution reactions (OER and HER) and utilized as the main energy source in the form of electricity or fuels. Despite the rapid development a real activity improvement for clean energy technologies requires novel and advanced materials with unique properties (e.g., electronic, structural, and physical properties) that are currently a bottleneck.

My research goal is to develop cost-effective and energy-efficient sustainable energy technologies to replace fossil fuels. In this presentation, I will discuss some of our recent advancements in developing sustainable energy technologies by performing cutting-edge fundamental research in the various aspects of advanced materials development and photo/electrocatalysis science along with leading innovation in the area of device fabrication.

Reference:

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Biography

Dr. Asadi joined the Chemical Engineering Department at Illinois Institute of Technology (IIT) as Assistant Professor in 2017. Previously, he was a research associate at the University of Illinois at Chicago (UIC). Asadi completed his Ph.D. in Mechanical Engineering at UIC and received his Master of Science Degree in Chemical Engineering from Sharif University of Technology. He spent seven years of working experience in the oil and gas industry before joining UIC. He has authored and co-authored 20 peer-reviewed publications in journals such as Science, Nature, Advanced Materials, Advanced Energy Materials, ACS Nano, and Nature Communications, and has 10 U.S. patents and four patent applications. He has more than 3000 citations (h-index 15) in the area of advanced functional materials, catalysis science, electrochemical energy storage, and energy conversion systems.

You Qiang

[1]Department of Physics, University of Idaho, Moscow, ID 83844-0903, USA.
[2]Center of Advanced Energy Study, Idaho National Laboratory, Idaho Falls, ID, USA.

Advanced Radiation Nanodetector For Nuclear Energy Application

Nano-Nuclear Technology (NNT) deals with applications of engineered-nanomaterials for the improvement of performance and safety of the future generation nuclear reactors. This talk is focused on the fundamental understanding of fast responses in-situ and ex-situ on nanostructure evolution, magnetic and electrical property changing of nanocluster-assembled materials under irradiations by use of He^{+}, heavy ion beam and e-beam. The investigations of highly radiation sensitivity and super-stability up to 800 ºC were performed on nanosensors of Fe-based core-shell nanocluster films. The investigation results show that the core-shell nanoparticles are excellent candidates for the nuclear radiation detection and radiation environment applications. The investigation is leading for the development of highly sensitive new type of radiation detector and monitor in nuclear energy applications.

Biography

Dr. Qiang is professor of physics and the Nuclear Engineering at UI, US. He is the current chairman of Idaho Academy of Science and Engineering, and the director of Nanophysics and Nanomaterials Laboratory. He received his MS degree 1985 at the Harbin Institute of Technology, China, and PhD degree 1997 at the University of Freiburg, Germany. His research focuses on magnetism and magnetic nanomaterials, and applies magnetic nanomaterials in nuclear energy, environmental and biomedical fields. Presently Dr. Qiang's research interests are a) magnetic separation nanotechnology for spent nuclear fuel recycling; b) Nano-Nuclear Technology of radiation detection and c) Iron-based magnetic nanoparticles for cancer treatment and environmental remediation.

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Yunming Wang, Dan Chen

State Key Laboratory of Material Processing and Die & Mould Technology, Huazhong University of Science and Technology, Wuhan, 430074, China, E-mail id: wang653@hust.edu.cn

Fabrication of Polymer Optical Device Combined with Selective Visible-Light Transmission and Zero-Birefringence

Photonic crystals are an advanced quantum and nonlinear optics tool for multi-crystal photonic devices, which exhibit excellent potential that may prove useful for micro- and nanophotonic systems. Although exciting progress has been witnessed in recent decades, the excessive dependence on visible light reflection and poor mechanical properties make it impressible to transparent precision optical equipment directly. Moreover, traditional self-assembly methods for photonic crystals (PCs) limited in poor mechanical properties and microstructure defect makes it hard to be directly applied to structural color devices, whose performance strongly relies on mechanical properties and microstructure of PCs. Here, we report a convenient monolithic approach that transparent/iridescent 3D photonic crystal devices with outstanding mechanical properties were assembled by monodisperse nanosphere powder in a high elastic state. Based on Bragg's law, we subtly regulate the optical band gap beyond visible light by controlling the size of the photonic crystal nanospheres. These polymer transparent optical devices have some excellent performance characteristics including high transparency (89%), visible light selective transmission (400-800 nm) and excellent mechanical properties (hardness reaches 0.32 GPa). These properties enable 3D photonic crystal devices to be applied not only in transparent precision optical components such as the lens of spectacle, microscope, telescope and endoscope, industrial camera and astronaut helmet, but also in anti-counterfeiting, optical displays and pattern printing. The innovative method opens a new route for the rapid and simple fabrication of nanoparticle structure, directly promotes the industrialization of 3D photonic crystal devices.

Biography

Yunming Wang has completed his PhD in 2013 from Dalian University of Technology and postdoctoral studies from University of Wisconsin-Madison. He is currently an associate professor at Huazhong University of Science and Technology. He has published more than 32 papers in reputed journals and has been serving as an editorial board member of repute.

Jufan Zhang[1], Gang Shen[1], Fengzhou Fang[1,2]

[1]Centre of Micro/Nano Manufacturing Technology (MNMT-Dublin), School of Mechanical & Materials Engineering, University College Dublin, Dublin, Ireland.
[2]State Key Laboratory of Precision Measuring Technology and Instruments, Laboratory of Micro/Nano Manufacturing Technology (MNMT), Tianjin University, Tianjin, China.

Development of textured artificial joints

Current commercial artificial joints have a relatively short in-vivo lifespan, saying around 15-20 year, which makes it a major concern when more younger patients are taking the total joint replacement operations. The tribological performance of artificial joints directly influence the lifespan in effective service. So improving the tribological performance is one of the most effective way to extend the lifespan. Surface texturing functions well in reducing the friction and wear of artificial joints. Working mechanisms of surface texturing in bioimplants were comprehensively studied. It was confirmed that the extra lifting pressure provided by hydrodynamic effect was less than 1% of the ambient pressure. The capacity to trap particles and second lubrication effect were found to be the main working mechanisms. A new surface texturing design was proposed for improving the tribological performance of bioimplants. Experimental results suggest that triangle pattern with 200 μm side length, 8-10 μm depth, 10% area density and square-distribution mode performs most effectively and showed a 50% reduction in coefficient of friction and 44.9% reduction in wear rate than that of only polished samples.

Biography

Dr. Jufan Zhang has completed his PhD and postdoctoral studies from Harbin Institute of Technology, China. Currently he is the assistant professor in University College Dublin, Ireland. He has published more than 40 papers and 5 patents. He has been serving as the editorial board member and/or reviewer of several international journals. He is the member of International Academy of Engineering and Technology (AET), the member of International Society for Nanomanufacturing (ISNM). He is the chair of organizing committee or member of program committee of several international conferences.

Chengchen Guo

[1]School of Engineering, Westlake University, Hangzhou, Zhejiang, China, E-mail id: guochengchen@westlake.edu.cn

Translating Silk from Textiles to Functional Materials

Silks spun by the arthropods are "ancient" materials historically utilized for fabricating high-quality textiles. Silks are natural protein-based biomaterials with unique physical and biological properties, including outstanding mechanical properties and biocompatibility. Due to this, since the late 1990s, considerable efforts have been made to extend the applications of silks into biomedical fields by taking advantages of the biocompatibility and enzymatic degradability of silk-based materials. Toward these needs, silk-based materials, including natural and recombinant silks, have been fabricated into a variety of functional biomaterials for tissue engineering, drug delivery, and biomedical devices. In this presentation, some important advances in characterization, processing, and translation of silk-based materials will be discussed.

Biography

Prof. Chengchen Guo has completed his PhD from Arizona State University, USA and postdoctoral studies from Tufts University, USA. He is the leader of Functional Biomaterials Lab at Westlake University. He has published more than 40 papers in high-impact journals including Nature Materials, Nature Reviews Materials, Advanced Functional Materials.

Mariana C. F. Costa[1,2]

[1]Department of Materials Science and Engineering, Faculty of Engineering, National University of Singapore (NUS), Singapore.
[2]Centre for Advanced 2D Materials (CA2DM), National University of Singapore (NUS), Singapore.

2D electrolytes: theory, synthesis, and characterization

We have demonstrated theoretically and experimentally a group of functional materials that shares the properties of two-dimensional (2D) materials and electrolytes, called 2D electrolytes. 2D electrolytes have the ability to dissociate in aqueous-based solvents and change their morphology in response to their surroundings. Particularly, the arrangement from 2D flat sheets to 1D-scrolled arrangements and more complex structures in liquid media is mainly determined by external factors, such as pH, temperature and ionic concentration. The interplay between Coulomb forces, elastic energy and van der Waals interactions are key to understand the different morphological configurations. Several examples of 2D electrolytes have been synthesized, using graphene and its derivatives (graphene oxide – GO, and reduced graphene oxide, rGO) and lithium-intercalated molybdenum disulphide (Li_xMoS_2), and a number of different characterization techniques together with a theoretical framework are presented. Since these materials show stimuli-responsive behavior to

Biography

Mariana Costa is a Materials Science Engineer currently working at the National University of Singapore (NUS) at the Centre of Advanced 2D Materials (CA2DM) and at the Department of Materials Science and Engineering (MSE) under the guidance of Prof. Kostantin Novoselov. Her research is focused on the development of new functional intelligent materials (FIMs) and micro and nano-electronic devices based on those.

Francesca Risplendi[1]*, Mattia Salomone[1], Michele Re Fiorentin[2] and Giancarlo Cicero[1]

[1]Department of Applied Science and Technology, Politecnico of Torino, Torino 10129, Italy.
[2]Center for Sustainable Future Technologies, Istituto Italiano di Tecnologia, Torino 10144, Italy.

Point Defects in two-dimensional Indium Selenide as Tunable Photon Sources: a Theoretical Study

The importance of photonic technologies is steadily growing in our daily lives. In this field a new frontier of research is the development of non-classical light sources, like, for example, sources that produce streams of photons with controllable quantum correlations. With this respect a central building blocks are single-photon emitters (SPEs). Unlike classical light sources, SPEs are fundamental quantum devices for many scalable and leading technologies, such as quantum information, precision metrology and imaging. The ability to tailor and control quantum emitters, to realize efficient and scalable architectures, depends on site-selective defect engineering. In this work we predicted the electronic properties of an InSe monolayer and its applicability as SPE when impurity defects are introduced in the structure. In this work, we analyze the energetic and electronic properties of InSe monolayer with point defects, to assess its applicability as SPEs. The presence of deep defect states within the InSe bandgap is verified when considering substitutional defects with atoms belonging to group IV and V. In particular, the substitution of an Se atom with Ge appears particularly promising when studied within the GW approximation and by solving the Bethe-Salpeter equation. Direct transitions between the valence band maximum and the defect state are responsible for the absorption and spontaneous emission processes, so that the latter results in a strongly peaked spectrum in the near infrared. These properties, together with a high localization of the involved electronic states appear encouraging in the quest for novel SPE materials.

Biography

Dr Risplendi earned her master's degree in Physics Engineering (2010) and her doctoral degree in Electronic Devices from Politecnico of Torino (2014); She carried out postdoctoral research at Massachusetts Institute of Technology (2014-2015) and at Politecnico of Torino (2016-2017). She is currently employed as a researcher at Department of Applied Science and Technology of the Politecnico of Torino. Her research activities have been mainly devoted to the theoretical investigation of nanostructured materials, surfaces, and interfaces. Her research interests span from the simulation of chemical reactivity in photo- and electrocatalysis to the study of excited states in nanostructures for optoelectronic devices.

Poster Presentation

Edgar Paredes-Sotelo [a*], Carlos Emiliano Buelna García [a*], Eduardo Robles Chaparro [c*], César Castillo Quevedo [d*], José Luis Cabellos [b*]

[a]Polymers and Materials Research Department, University of Sonora, Hermosillo, Sonora, Mexico.
[b]Research Department in Physics, University of Sonora, Hermosillo, Sonora, Mexico.
[c]Department of Chemical Biological Sciences, University of Sonora, Hermosillo, Sonora, Mexico.
[d]Department of Fundamentals of Knowledge, North University Center, University of Guadalajara, Colotlán, Jalisco, Mexico.

First principles study of optical and electronic properties of hybrid perovskites for use of solar cells

In this work a theoretical-computational study of the optical and electronic properties[1] of hybrid perovskites with stoichiometry of $CH_3NH_3PbX_3$ (where X = I, Cl, Br) are presented. These materials are considered exceptionally suitable for the construction of solar cells due to their optical and electronic properties which been vastly explored. The calculations were carried out under the scheme of the density functional theory (DFT) as implemented in the Quantum ESPRESSO program.[2] DFT was used together with the Perdew – Burke – Ernzerhof functional, plane waves and the pseudopotential approximation. As results and, for the orthorhombic, tetragonal, and cubic phases of the perovskites[3] $CH_3NH_3PbX_3$, the optical properties are presented, such as the dielectric function, refractive index, and reflectivity, and for the electronic properties, the band structure and the total and projected density of states are presented. The results for each perovskite were compared between its own phases and with the reported results of its experimental counterpart, to determine which structure performs best as a light-absorbing layer in a solar cell. The calculated optical and electronic properties are shown in good agreement with the experimental ones, as well as the effect that the geometric structure of perovskite has on the optical properties.

Biography

Edgar Paredes Sotelo is currently obtaining his master's degree at the Polymers and Materials Research Department of the University of Sonora. He has a total of 2 papers in the reputed journal of Organic Electronics and he is preparing to start his PhD.

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17-18, 2021

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Jianyong Ouyang

Department of Materials Science and Engineering, National University of Singapore, Singapore.

Email id: mseoj@nus.edu.sg

Application of Conducting Polymers for Flexible Electronics

Intrinsically conducting polymers are very interesting materials and can have application in many areas. Recent progress in conducting polymers demonstrated their new important application in important areas such as wearable bioelectrodes for biopotential monitoring. In particular,poly(3,4-ethylenedioxythiophene):poly(styrenesulfonate) (Chemical structure shown in Figure 1 has gained great attention due to its solution processability, high conductivity, good biocompatibility, good thermal stability, and high transparency in visible range.[1] However, it has very limited stretchability due to the rigid backbone. Here, I will present several novel methods to significantly enhance the mechanical stretchability of PEDOT:PSS.[2-6] PEDOT:PSS films with a stretchability of >60% and conductivity of >1000 S/cm are obtained.

I will also present some of our works in developing intrinsically conducting polymers as conformal bioelectrodes.[7] It is important to continuously monitor the biopotential of patients. Nevertheless, the biopotential signal is sensitive to the contact between the bioelectrodes and skin surface. Although stretchable electrodes can follow the muscle movement, their contact to skin can be affected and this can generate motion artifacts. Here, we will present our work to develop stretchable and adhesive intrinsically conducting polymers. They can always form conformal contact to skin and thus give rise to high-quality signals even during body movement. They can be thus used for long-term health monitoring.

Biography

Prof. Jianyong Ouyang received his PhD, master and bachelor degrees from the Institute for Molecular Science in Japan, the Institute of Chemistry of the Chinese Academy of Science, and the Tsinghua university in Beijing, respectively. He worked as an assistant professor at the Japanese Advanced Institute of Science and Technology and a postdoctoral researcher at the University of California, Los Angeles (UCLA) before joining the National University of Singapore (NUS) as an assistant professor in 2006. He was promoted to associate professor in 2012. His research interests include flexible electronics and energy materials and devices. He invented the first polymer-nanoparticle resistive memory, the first hybrid ionic/electronic thermoelectric converter and the first adhesive intrinsically conducting polymers in the world, and continuously reported world-record conductivities and thermoelectric properties of solution-processable intrinsically conductive polymers and world-record thermoelectric properties of ionic conductors.

Michihisa Koyama

[1]Research Initiative for Supra-Materials, Shinshu University, Nagano, Japan.
E-mail id: koyama_michihisa@shinshu-u.ac.jp
[2]Open Innovation Institute, Kyoto University, Kyoto, Japan. E-mail id: koyama.michihisa.5k@kyoto-u.ac.jp

Stability and Catalytic Properties of Multinary Alloy Nanoparticles based on Real System Structure Models

The challenges in theoretical catalysis are the prediction of materials with long-term stability and the prediction of activity that arises from the heterogeneous structure of real systems. The author believes that a real system approach incorporating a large-scale real-system structure model,which requires a large computational cost, is much important than conventional approaches using a small-scale model that simplifies the real system catalyst. The author and coworkers have been challenging the first-principles calculations of real system alloy nanoparticles based on parallel-computing.

Specifically, nanoparticles used in various catalytic processes are known to exhibit properties different from those of the bulk. The author and coworkers have previously clarified the origin of the thermodynamic stability different from that of the bulk by first-principles calculations of the real system structure. Furthermore, the adsorption properties of NO and O on metal nanoparticle models of various real structures have been clarified and generalized descriptors with physical meanings that can describe the adsorption properties have been proposed.

It goes without saying that it is important to conduct research and development based on the thermodynamic stability of materials as well as on the physical understanding behind the activity, in order to discover active materials and make them implemented in our society. In this presentation, the author will introduce the details of the recent work on alloy nanoparticles and the prospects.

Acknowledgements: Part of the work is financially supported by JSPS KAKENHI (20H0562301, 21H01739). Parallel-computing is conducted by using MASAMUNE-IMR of Tohoku University.

Biography

Michihisa Koyama received his Ph.D. from the University of Tokyo in 2002. After serving as Assistant Professor at Tohoku University and Professor at Kyushu University, he is now serving as Professor at Shinshu University, Program-Specific Professor at Kyoto University. Dr. Koyama has authored and co-authored more than 300 review articles, book chapters, and peer reviewed articles. His research activities cover the wide aspects of energy from materials to systems, further to future energy vision. He was awarded The Young Scientists' Prize, The Commendation for Science and Technology by the Minister of Education, Culture, Sports, Science and Technology in 2014.

Guan-Hao Peng, Ping-Yuan Lo, Wei-Hua Li , Shun-Jen Cheng*

Department of Electrophysics, National Yang Ming Chiao Tung University, Hsinchu 300, Taiwan.

Optical Signatures of Momentum-Forbidden Dark Excitons in Transition Metal Dichalcogenide Monolayers

Atomically thin transition-metal dichalcogenide monolayers (TMD-MLs) such as MoS_2 and WSe_2 monolayers, have recently drawn a broad attention because of the exceptional spin-, valley-, and excitonic propertyes. Because of dramatically enhanced Coulomb interactions in low dimensionality, photo-excited electron-hole pairs in TMD-MLs incident by light form tightly bound excitons that are featured with intriguing valley- and spin-related excitonic fine structures, consisting of the states of bright exciton (BX), spin-forbidden (SF) and various momentum-forbidden (MF) dark exciton (DXs) as well. In particular, despite of violating the momentum selection rules, the MF-DXs in TMD-MLs are recently realized to be essential in various optical and dynamical phenomena but not extensively explored yet so far. In this work, we present a comprehensive theoretical investigation of the full excitonic fine structures of WSe_2-MLs by solving the density-functional-theory (DFT)-based Bethe-Salpeter equation (BSE) with the full consideration of both electron-hole direct and exchange Coulomb interactions. Accordingly, we reveal the optical signatures of the optically inactive MF-DX in temperature-dependent photo-luminescence, in excellent agreement with the existing experimental data. Further, under the guidance of symmetry analysis, we show that the MF-DXs with specific finite momenta inherently possess superiorly high degree of valley and optical polarizations and optically accessible by spatially structured laser beam with optical orbital angular momenta. Those findings shed light on the prospect of the valley-based photonics with the utilization of those long-lived, optically accessible and superiorly valley-polarized MF-DXs.

Biography

Shun-Jen Cheng received his PhD from the University of Würzburg, Germany, in 2001. From 2002-2003, he carried out his postdoctoral studies at National Research Council, Ottawa, Canada. In 2003, he joined as a faculty member the Department of Electrophysics at National Chiao Tung University, which was renamed National Yang Ming Chiao Tung University (NYCU) in 2021. He is currently a full professor at NYCU. His research interest is in the general condensed matter theory, ranged from the fundamental band theories of solids, many-body physics, to exciton physics and light-matter interactions in low dimensional materials.

Wen Lei

Department of Electrical, Electronic and Computer Engineering, The University of Western Australia, 35 Stirling Highway, Crawley 6009, WA, Australia.

Heteroepitaxial integration of II-VI semiconductors on III-V substrates – epitaxial growth with large lattice mismatch

In the last decades, significant attention was devoted to the hetero epitaxial growths with large lattice mismatch, such as III-V and II-VI semiconductors on Si. The aim is to lower the production cost, increase the wafer size, enhance the system robustness, as well as achieve monolithic integration of electronic and photonic devices. The serious challenge for these growths is the large lattice mismatch and thus high density of threading dislocation generated in the epilayers, which significantly deteriorate the ultimate device performance. Thus, it is essential to reduce and control the dislocation density below a certain critical level to meet the requirements such as device yield and device performance. In this work, we will introduce our recent work on hetero-epitaxy of high quality, strategically important II-VI HgCdTe/CdTe semiconductors on III-V GaAs and GaSb substrates – material systems with a large lattice mismatch of 14.4% and 6.1%, respectively. We will discuss various experimental approaches/techniques to control the generation and propagation of dislocations, and as a result, to reduce the dislocation density in the HgCdTe/CdTe epilayers. By applying these novel approaches/techniques, high quality CdTe and HgCdTe semiconductors have been achieved on GaAs and GaSb substrates. Typically, dislocation density in the CdTe epilayers grown on GaAs and GaSb at UWA is an order of magnitude lower than those reported in current industry and literatures, which meets the dislocation density requirement for making high performance infrared detectors. More importantly, these strategies/techniques can be extended to other material systems, benefiting the development of semiconductor industry.

Biography

Dr. Wen Lei is a Professor in Electrical Engineering at the University of Western Australia. His main research interests include semiconductor thin materials and optoelectronic devices, and low-dimensional semiconductors and electronic devices. He has published 2 patents and more than 120 high profile papers in top journals like Phys. Rev. Lett., Appl. Phys. Rev., Nano Lett., etc. He is/was also an editorial board member for three international scientific journals, a guest editor for five international scientific journals, and a regular reviewer for various international prestigious journals.

Hsing-Yu Tuan*
[1]Department of Chemical Engineering, National Tsing Hua University, Hsinchu, Taiwan.
E-mail id: hytuan@che.nthu.edu.tw

High-Performance Potassium-Ion Battery Materials

Due to the rarity of lithium (0.0017 wt% in the earth's crust), it is doubtful that lithium-ion batteries (LIBs) will meet the enormous demand for applications such as electric vehicles and grid-scale storage. Potassium-ion batteries (PIBs) may replace LIBs as energy storage systems due to multiple unique attr-ibutes, such as low cost, abundant resource availability (approximately 2.09 wt%, ranking seventh in the crust), and low reduction potential [K^+/K (-2.94 V versus a standard hydrogen electrode); Li^+/Li (-3.04 V); Na^+/Na (-2.71 V)].The emerging high-tech and novel applications require foldable and bendable batteries with high volumetric and gravimetric energy density that can adapt to any electronic devices. High theoretical specific capacity materials for PIB anodes, including Bi, Sb, P, and Se are potential replacement of commercial graphite anodes, but they suffer from dramatic volume changes (~400%) resulted from insertion/extraction of potassium ions during charge/discharge process, which ultimately causes pulverization of active materials and leads to short battery cycle life. In this talk, I will discuss how to alleviate the volume expansion problems of these high-capacity materials by nanostructurization and use them as high-performance potassium ion battery anodes.[1-5] For example, the Figure 1 shows how we effectively activate red phosphorus as an anode for potassium-ion batteries with a record﹣high specific energy density.

Keywords: battery, anode, potassium, nanomaterials, electrode

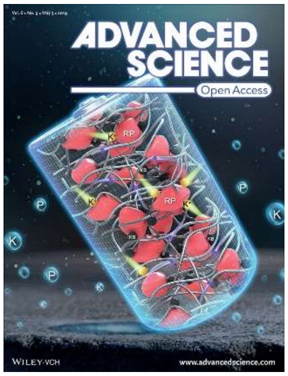


Fig. 1. Activatedred phosphorus as an anode for potassium-ion batteries with a record﹣high specific energy density

1. Kuan-Ting Chen, Yi-Chun Yang, Lian-Ming Lyu, Ming-Yen Lu, and Hsing-Yu Tuan ***Nano Energy*** *2021*, **88, 106233**
2. Yi-Yen Hsieh, Kuan-Ting Chen, and Hsing-Yu Tuan ***Chemical engineering journal*** *2021*, **420, 130451**

   Kuan-Ting Chen, Shaokun Chong, Lingling Yuan, Yi-Chun Yang, Hsing-Yu Tuan ***Energy Storage Materials*** *2021*, **39**

Hua Li

School of Mechanical and Aerospace Engineering Nanyang Technological University, 50 Nanyang Avenue, Singapore 639798. E-mail id: lihua@ntu.edu.sg

A Multiphysics Modelling of Magnetic-Sensitive Hydrogels

A multiphysics model is presented for simulation of the responsive behaviour of the magnetic-sensitive hydrogel, with the effects of magneto-chemo-mechanical-coupled fields. In this work, the magnetic susceptibility for magnetization of the general magnetic hydrogel is defined as a function of finite deformation, instead of a constant for an ideal magnetic hydrogel. The present constitutive equations, formulated by the second law of thermodynamics, account for the effects of the chemical potential, the externally applied magnetic field, and the finite deformation. In particular, a novel free energy density is proposed with consideration of the magnetic effect associated with finite deformation, instead of volume fraction. After examination with published experimental data, it is confirmed that the present model can capture well the responsive behaviour of the magnetic hydrogel, including the deformation and its instability and hysteresis under a uniform or non-uniform magnetic field. The parameter studies are then presented for influences of the magnetic and geometric properties, including the magnetic intensity, shear modulus, and volume fraction of the magnetic particles, on the behaviour of the magnetic hydrogel, for a deeper insight into the fundamental mechanism of the magnetic hydrogels.

Biography

Dr. Li received his B.Sc and M.Eng degrees in Engineering Mechanics from Wuhan University of Technology, P.R.C., in 1982 and 1987, respectively. He obtained his Ph.D degree in Mechanical Engineering from the National University of Singapore in 1999. From 2000 to 2001, Dr. Li was a Postdoctoral Associate at the Beckman Institute for Advanced Science and Technology, University of Illinois at Urbana-Champaign. He has so far published more than 180 papers in reputed journals and 4 monograph books.

Chao Qian, Renkai Tan, Wenjing Ye

Department of Mechanical and Aerospace Engineering, Hong Kong University of Science and Technology.

An adaptive artificial neural network-based deep generative design method for architectured materials

Architectured materials, also known as mechanical metamaterials, are artificial materials with their properties determined by the structures of their building blocks. Conventional design approaches rely on physical intuition or high-dimensional simulations. They often cannot produce the optimal design soluteons and/or are too computationally intensive to be applied as practical design tools. In this talk, an efficient, adaptive artificial neural network-based generative design method is presented. This method uses a generative adversarial network to generate design candidates and thus the number of design variables is greatly reduced. To speed up the evaluation of the objective function, a convolutional neural network is constructed as the surrogate model for function evaluation. The inverse design is carried out using the genetic algorithm in conjunction with two neural networks. A novel adaptive learning and optimization strategy is proposed, which allows the design space to be effectively explored for the search for optimal solutions. As such, optimal design solutions can be obtained with minimum number of training data. The performance of the method is demonstrated on the design of architectured composite materials with high toughness, high stiffness composite that close to theoretical upper bounds and prescribed bulk and shear moduli. In all cases, excellent results are obtained.

Biography

Professor Ye is a full professor in the Department of Mechanical and Aerospace Engineering at Hong Kong University of Science and Technology. She has completed her PhD from Cornell University, USA and postdoctoral studies from Massachusetts Institute of Technology, USA. Prof. Ye is the author and co-author of four book chapters, 74 peer reviewed journal articles and 62 conference publication on various topics. She is an associate editor of Computer Modeling in Engineering and Science, a member of the editorial board of several internal journals such as Engineering Analysis with Boundary Elements, Scientific Reports and International Journal of Computational Methods

Tianbao Ma

[1]State Key Laboratory of Tribology, Tsinghua University, Beijing, China, E-mail id: mtb@mail.tsinghua.edu.cn

Interlayer superlubricity between two-dimensional materials

How to achieve sustainable superlubricity under high contact pressure with environmental insensitivity and long wearlife, has been key challenges towards possible applications of the 2D materials. I'll firstly present theoretical calculations of interlayer friction between 2D materials. By a quasi-static interlayer scanning using density functional theory (DFT) calculations, the potential energy corrugation ΔE and friction for interlayer sliding for 2D materials can be acquired. We found a close connection between potential energy corrugation ΔE and sliding induced interfacial electron density variation $\Delta\rho$. During the interlayer sliding process between MoS2 layers, the interfacial electron density distribution changed significantly. For graphene/MoS2 heterostructure, however, electron density distribution does not vary during the sliding process. So superlubricity of 2D heterostructure was proposed due to the almost invariable interfacial electron density during sliding. Then experimental study of interlayer friction between 2D materials has been conducted by using atomic force microscopy (AFM). We have proposed two means to realize robust superlubricity under high local contact pressure: First, to fabricate graphite wrapped tip (GWT) to form single-crystalline 2D heterostructure sliding interface; Second, to prepare graphene-coated microsphere (GMS) to form multi-asperity contact with random crystalline orientation of graphene. The lowest friction coefficient measured in the experiments was about 4×10^{-5}.

Biography

Tianbao Ma has completed his PhD from Tsinghua University, China. He is the vice director of State Key Laboratory of Tribology, Tsinghua University. He has published more than 80 papers in journals such as Nature Communications, Nano Letters, ACS Nano, Advanced Functional Materials etc. He has been serving as Young Scientists Committee of the journal "Science China Technological Sciences".

Sahrim Ahmad

School Of Applied Physics Faculty Of Science And Technology Universiti Kebangsaan Malaysia 43650 Ukm, Bangi Selangor, Malaysia.

Magnetic And Conducting Thermoplastic Rubber Based Nanocomposites For Microwave Absorption Application

The main objectives of our research work are to produce conducting and magnetic hybrid thermoplastic rubber nanocomposites. Our recent work is to prepare thermoplastic blend with polyaniline (PANI) nano-composites filled with the hybrid fillers of graphene nanoplatelet (GNP) and magnetite (Fe_3O_4), nickle zink ferrite nanoparticles using melt blending method. Thermoplastic rubber were prepared by mixing 40wt% of linear low density polyethylene (LLDPE) with 50 wt% of natural rubber (NR) and liquid natural rubber (LNR) as compatibilizer (10 wt%). In the first stage, the effects of processing parameters which are processing temperature, rotation speed, processing time and the content of PANI (1-5 wt%) on mechanical, thermal, electrical conductivity and physical properties were investigated. The mechanical test results showed the optimum processing parameter was obtained at 130 °C with 30 rpm for 13 min. The mechanical properties of sample increased with addition of PANI into the blend and the highest tensile strength were obtained at 3 wt% of PANI with improvement of 42 % as compared with thermoplastic matrix. In the second stage our work is to study the effect of GNP (1 – 5 wt%) in TPNR/PANI/GNP nanocomposites on mechanical, thermal, electrical conductivity, physical and magnetic properties. TPNR/PANI samples filled with GNP showed an increase of 54 % in tensile strength.TGA results showed good improvement in thermal stability especially with addition of small composition of GNP. In the third stage is to study the effect of magnetite nanoparticles (Fe_3O_4) addition on magnetic properties in TPNR/PANI blend . The addition of Fe_3O_4, nanoparticles in the nanocomposites the thermal stability also increased significantly which was obtained from TGA thermogram . The addition of Fe_3O_4 nanoparticles also showed good increment in magnetic properties and thermal stability.

Biography

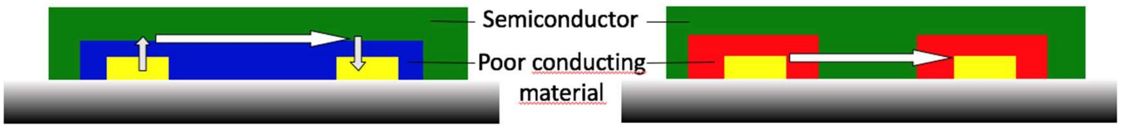
Professor Dr Sahrim Ahmad obtained his PhD from University of Loughborough, United Kingdom in 1988. He is an expert in the field of magnetic, nanocomposites and advanced materials. He has completed more than 50 research projects and consultancy work as a leader and co-researcher. His work on novel radar absorbing materials (RAM) subjected to transverse electromagnetic (TEM) has been successfully developed. His team managed to produce products that offered proper characteristics for handling, flexibility and lightweight, meeting requirement for various applications. He has published more than 200 papers in various journals and supervised more than 50 PhD students. Dr Sahrim was former Dean of Faculty Science of Technology and Editor In Chief of Journal Sains Malaysiana (ISI/WOS} .

Marcel Bouvet, Rita Meunier-Prest, Abhishek Kumar

Institut de Chimie Moléculaire de l'Université de Bourgogne, CNRS UMR 6302, Université Bourgogne Franche-Comté, Dijon, France, E-mail id : marcel.bouvet@u-bourgogne.fr

From Molecular Material – Based Heterojunctions to Ambipolar Gas Sensors

In ambipolar materials, negative and positive charge carriers participate equality to the conduction process. They have been the object of numerous studies in organic electronics, but were introduced only very recently in conductometric transducers for gas sensing. In this work, we report on the electrical properties of molecular materials and on different types of heterojunctions as well. We will show the key role of the energy barrier in the performances of gas sensors and the interest of ambipolar materials for gas sensing. The tuning of heterojunctions' performances by electrografting of an organic layer on the electrodes will also be discussed. The heterojunctions favorably compete other conductometric transducers for the detection of ammonia, with a limit of detection as good as 140 ppb, at RT and in a broad range of relative humidity.



Schematic view of two types of molecular material-based heterojunctions used as gas sensors

1) M. Mateos et al. ACS Applied Materials&Interfaces, 10, 19974, **2018**; Sens. Actuators B Chem., 299, 126968, **2019** ; ACS Sensors, 4, 740, **2019**; 2) G. Bengasi et al. Adv. Electron. Mater., 6, 2000812, **2020** ; 3) G. Loma Kikobo et al. J. Mater. Chem. C, **9**, 5008, **2021** ; 4) M. Bouvet, et al. Ambipolar materials for gas sensing, in Ambipolar Materials and Devices, ed. Y. Zhou, S.-T. Han, RSC, **2021**.

Biography

Prof. Marcel Bouvet prepared his PhD at the ESPCI (Paris) in 1992, on electrical properties of phthalocyanines. He has been working at the ESPCI, but also at UPMC (Paris) and at the University of Connecticut (USA). He got a Full Professor position at the University of Burgundy (Dijon, France), in 2008, where he is currently the head of the team Electrochemistry, Molecular Materials and Devices (EMMD) in the ICMUB. His research interests are in the field of molecular materials, conductometric transducers, electrochemistry and chemical sensors. He has published more than 100 papers and 9 book chapters.

Chen Yang

[1]Department of Electrical and Computer Engineering, Boston University, Boston, MA, U.S.A.
E-mail id: cheyang@bu.edu
[2]Department of Chemistry, Boston University, Boston, MA, U.S.A.

Photoacoustic Neural Interface for Modulation

Neuromodulation at high precision poses great significance in advancing fundamental knowledge in the field of neuroscience and offering novel clinical treatments. Here we reported our research on developing the photoacoustic neural interface based on highly efficient photoacoustic materials, such as carbon nanotubes and PDMS, and applying them in neural stimulation in vitro, in vivo and for neural regeneration. Specifically, four different platform technologies with either implantable and noninvasive potentials will be discussed, including fiber based photoacoustic emitters, nanocomposite based photoacoustic films, photoacoustic nanotransducers and optic-driven focus ultrasound based on photoacoustic lenses. Our technology employs an optoacoustic process, in which pulsed light is delivered into an absorbing layer, generating a localized acoustic wave at ultrasonic frequency. High spatial resolution of sub-millimeter up to single neuron and sub-cellular structures, such as axons and dendrites have been achieved. Single acoustic pulse of sub-microsecond converted from a single laser pulse of 3 ns is shown as the shortest acoustic stimuli so far for successful neuron activation. Direct stimulation of brain target, electrophysiology recording and behavior responses have been demonstrated in vivo. Promoted outgrowth of neural tissue upon photoacoustic stimulation has been shown. Our work demonstrated that photoacoustic stimulation is a high precision and non-genetic neural stimulation and offering various neural interface with a non-invasive potential.

Biography

Prof. Yang graduated obtained her doctoral degree in Chemistry from Harvard University in 2006. She joined Purdue University as an Assistant Professor in 2007 and was promoted to Associate Professor in 2013. She is currently an Associate Professor in Department of Electrical and Computer Engineering and Department of Chemistry and Associate Chair in Department of ECE at Boston University. Prof. Yang's research interest is focusing on nano materials with applications in nanoscale devices and biological applications. Her research has been published in high profile journals, including *Science* and *Nature*. She was a NSF Career Awardee in 2008.

Rui He

Department of Electrical and Computer Engineering, Texas Tech University, Lubbock, Texas, USA,
E-mail id: rui.he@ttu.edu

Raman Spectroscopy of Spin Waves and Magnetism-Induced Phonons in van der Waals Magnet CrI_3

Van der Waals (or 2D) materials with intrinsic ferromagnetism have attracted massive interest because of their potential applications in data storage and spintronics devices. Atomic layers of chromium triiodide (CrI_3) are one of such 2D ferromagnetic (FM) materials that have been demonstrated to realize long range FM order in its monolayer limit. In this talk, I will present our recent Raman spectroscopy studies of magnons (spin waves) and magnetism-induced phonons in bulk and thin layers of CrI_3. Using magnetic field- and temperature-dependent ultralow frequency Raman spectroscopy, we reveal a novel mixed state of layered antiferromagnetism (AFM) and FM in 3D CrI_3 bulk crystals where the layered AFM survives in the surface layers and the FM appears in deeper bulk layers. In thin layers (1-4 layers) of CrI_3, we use a combination of polarized Raman spectroscopy experiment and magnetism-phonon coupling calculation to study the rich magneto-Raman effect. Our results explain why a van der Waals magnet may show different magnetic behaviors in its layered and bulk forms and reveal the spin-phonon coupling physics in its atomic layers.

Biography

Dr. He obtained her B.S. from Fudan University in China in 1999. She received her Ph.D. from Columbia University in 2006. After graduated from Columbia, she joined the Hong Kong University of Science and Technology as a postdoc. In 2009 she returned to Columbia University and worked as a postdoc. She joined the Physics Department at the University of Northern Iowa as an assistant professor in August 2011 and then joined the ECE Department at Texas Tech University as an associate professor in July 2017. Her research interests focus on Raman studies of nanostructures, especially 2D materials and their heterostructures.

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M. Romanini[1,2], L. Mañosa[1], P. Lloveras[2], J. Ll. Tamarit[2], A. Planes[1], K. Gurpinar[3], B. Emre[4], O. Atakol[3], M. Shatruk[5], Y. Wang[5,6]

[1]Dept. Física de la Matèria Condensada, Universitat de Barcelona, Spain.
[2]Grup de Caracterització de Materials, Dept. Physics, Universitat Politècnica de Catalunya, Spain.
[3]Dept. Chemistry, Ankara University, Ankara, Turkey.
[4]Dept. Physics, Ankara University, Ankara, Turkey.
[5]Dept. Chemistry and Biochemistry, Florida State University, Florida, United States.
[6]School of Materials Science and Engineering, University of Science and Technology Beijing, Beijing, People's Republic of China.

Barocaloric Effect in a Novel Spin-Crossover Compound

The search for materials with giant caloric effects is a hot topic in materials science, owing to the potential of such systems as environment-friendly replacement of current refrigeration technologies which raise serious environmental concerns [1-4]. Recently, a giant barocaloric effect has been reported in a spin cros-crossover (SCO) compound [5]. In SCO compounds, the spin state of a metal ion (typically, Fe^{2+}) interconverts between two magnetic states (low-spin, LS, and high-spin, HS) by a redistribution of *d*-electrons among two non-equivalent sets of orbitals. The HS-LS phase transition is accompanied by a change in the crystal structure and can be induced by a variety of external stimuli such as temperature and pressure changes or light irradiation [6,7].
For their successful implementation in Brayton cycles for solid-state refrigeration, SCO compounds must display a large barocaloric effect (large latent heat of the HS-LS transition) and at the same time a negligible thermal hysteresis.

We have synthesized a novel SCO compound (Fe3(bntrz)6(tcnset)6 (bntrz=benziltriazole and tcnset=tetracy-anothioalkylpropenide) [8]) which exhibits abrupt spin-state switching at 318 K with negligible thermal hysteresis and large entropy change of ~ 80 J kg^{-1} K^{-1}. Under an applied pressure of 2.6 kbar, the transition temperature increases to 383 K, while maintaining the non-hysteretic character of the transition [9]. Such behavior leads to a remarkably large and reversible barocaloric effect in the Bryton cycle, characterized by entropy change of 120 J kg^{-1} K^{-1} and temperature change of 35 K, among the highest reversible values reported for any caloric material so far.

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Biography

Dr. Michela Romanini obtained her PhD from the Universitat Politècnica de Catalunya (UPC), Spain. After her PhD she worked as postdoctoral researcher at the Barcelona Center for Multiscale Science and Engineering (UPC) and later at the Universitat de Barcelona, Spain, in the group of prof. Lluis Mañosa. She is currently a postdoctoral researcher at the UPC in the Group of Characterization of Materials where she carries out research projects on molecular glass formers and on multicaloric effects in solid-state materials. She is author of 39 papers in reputed journals.

Vipin Amoli

Department of Sciences & Humanities Rajiv Gandhi Institute of Petroleum Technology (RGIPT) Jais, Amethi, Uttar Pradesh, India. E-mail id: vamoli@rgipt.ac.in

Visco-Poroelastic Iontronic Polymer Pumps for Low-powered Wearable Electrochromic Devices

Electrochromic devices (ECDs) exhibit reversible color change on the application of voltage. Due to their high color contrast and low voltage operation, ECDs have been explored for diverse applications including smart glasses, mirrors and displays. A typical ECD consists of an electrochromic active material and an electrolyte layer sandwiched between two transparent electrodes. Recently, the use of mechanically robust ionic polymers as solid-state electrolytes has led to the fabrication of flexible and durable ECDs for prospective applications in adaptive camouflage technologies and wearable display applications. Despite considerable efforts most of the flexible ECDs developed so far struggle to maintain desirable functioning in wearable applications. In this talk, I present visco-poroelastic iontronic polymer pump-based multicolor wearable electrochromic devices (MCWECD) with excellent cyclic coloration/bleaching stability (35,000 s), fast response (~1.75 s), and high durability even under repeated cycles of compressive forces and tensile strains. The electrochromic polymers such as P3HT (poly(3-hexylthiophene-2,5-diyl)), MEH-PPV (poly[2- methoxy-5-(2-ethylhexyl-oxy)-1,4-phenylenevinylene]), and P4a (green color polymer) are used to create purple, orange, and green colors, respectively. Iontronic polymer pump is composed of 1-Ethyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide ($[EMIM^+][TFSI^-]$) ion pairs incorporated in thermoplastic polyurethane (TPU) that served as a deformable and transparent solid-state electrolyte enabling low-voltage (±3 V) functioning. The excellent stability/durability and low voltage functioning of MCECD realized the integration of MCECD with flexible printed circuit board for demonstrating the human adaptive camouflage applications. The presented work opens new avenues for next-generation wearable optoelectronics devices.

Biography

Dr. Vipin Amoli has completed his PhD in Physics from Academy of Scientific & Innovative Research (AcSIR), India and postdoctoral studies from Soongsil University and Hanyang University, South Korea. He is working as Assistant Professor in the Department of Sciences & Humanities, at Rajiv Gandhi Institute of Petroleum Technology (RGIPT), India. His research interests are in the fields of Flexible/Wearable Sensors, Flexible Electrochromic Devices, Solar Energy Devices and Nanotechnology. He has published 4 patents and 17 research papers in the prestigious journals including Nature Communications, Advanced Functional Materials and Nano Energy.

Giuliana Grasso[1], Anil Chandra[1], Riccardo Rizzo[1], Carlo Crescenzi[2], Börje Sellergren[3], and Loretta L. del Mercato[1]

[1]Institute of Nanotechnology – NANOTEC, Consiglio Nazionale delle Ricerche (CNR), c/o Campus Ecotekne, via Monteroni, Lecce, 73100, Italy.
[2]Department of Pharmacy, University of Salerno, Via Giovanni Paolo II, 132 – 84084 Fisciano (SA), Italy.
[3]Biofilm Research Centre for Biointerfaces, Department of Biomedical Sciences, Malmö University, Per Albin Hanssons väg, 35 - SE 20506 Malmö, Sweden.

Detection of Biomarkers Involved in Neurodegenerative Diseases and Study of Tumour Microenvironment (TME) Employing Innovative Smart Sensing Tools

Nowadays, there is a constant need of adequate tools for studying important biomarkers that could not be detected in complex matrices, being obstacles for the development of effective diagnostic tools and treatments. Sphingosine 1-Phosphate (S1P)[1], a physiological metabolite of sphingosine pathway, has been recognized as a relevant biomarker for neurodegenerative diseases, and its analogue FTY-720 (Fingolimod, Gilenya™, Novartis)[2] has been approved by FDA for the treatment of relapsing-remitting multiple sclerosis. Focusing on these targets, we have developed the synthesis of fluorescent sensory core-shell molecularly imprinted polymer (MIP) particles[3], responsive to near physiological levels of S1P and the S1P-receptor antagonist FTY720-P in spiked *H. Serum* samples.

On the other hand, cancer represents one of the major health challenges worldwide. The acidification of the tumour microenvironment (TME) is a prominent environmental driver of cancer progression.[4] Within this context, we developed efficient optical ratiometric microparticles suitable to detect intra- or extracellular pH changes in *in vitro* cell cultures.[5] By means of time-lapse confocal microscopy we were able to generate spatially resolved maps of pH across the 3D cultures of human mesenchymal stem cells.[6] More recently, we developed a novel methodology to successfully couple the ratiometric dye pyranine with silica microparticles. The resulting pH-sensing microparticles show superior pH sensitivity and good biocompatibility, two key properties for their applications as pH-sensors in living systems.[7] The research leading to these results received partial funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation program (grant No. 759959, ERC-StG “INTERCELLMED”).

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Biography

Giuliana Grasso has completed her PhD in "Drug Discovery and Development" within a collaboration born between Salerno University (UNISA), Italy, and Malmö University (MAU), Sweden, acquiring skills in Analytical Chemistry, with particular focus on synthesis and evaluation of innovative micro-shaped materials and fluorescent nano-sensors by MIP (Molecularly Imprinted Polymers) technology for identification and separation of biomarkers, pharmaceuticals, and biocompounds. She started her postdoctoral studies at the Institute of Nanotechnology (NANOTEC-CNR), Italy, centered on the development of new nano-patterned platforms for quantifying metabolic changes in mediated drug resistance in pancreatic cancer and metastatic melanoma within the ERC-INTERCELLMED- and the AIRC-funded projects.

Seongwoo Woo[1]

[1]Department of Mechanical Engineering, College of Electrical and Mechanical Engineering, Addis Ababa Science & Technology University, Ethiopia.

Improving the Fatigue of Newly Designed Mechanical System Subjected to Repeated Impact Loading

To Improving the fatigue of newly designed mechanical system subjected to repeated loading, this paper develops parametric accelerated life testing (ALT) as a systematic reliability method to produce the reliability quantitative (RQ) specifications—mission cycle—for recognizing missing design defects in mechanical products as applying the accelerated load. Parametric ALT is a way to enhance the prediction of fatigue failure for mechanical systems subjected to repeated impact loading. It incorporates: (1) A parametric ALT plan formed on the system BX lifetime, (2) a fatigue failure and design, (3) customized ALTs with design alternatives, and (4) an assessment of whether the last design(s) of the system fulfills the objective BX lifetime. A BX life concept with a generalized life-stress model and a sample size equation are suggested. A domestic refrigerator hinge kit system (HKS), which was a newly designed mechanical product, was used to illustrate the methodology. The HKS was subjected to repeated impact loading resulting in failure of the HKS in the field. To conduct ALTs, a force and momentum balance was utilized on the HKS. A straightforward impact loading of the HKS in closing the refrigerator door was examined. At the first ALT, the housing of the HKS failed. As an action plan, the hinge kit housing was modified by attaching inside supporting ribs to the HKS to provide sufficient mechanical strength against its loading. At the second ALT, the torsional shaft in the HKS made with austenitic ductile iron (18 wt% Ni) failed. The cracked torsional shaft for the 2nd ALTs came from its insufficient rounding, which failed due to repeated stress. As an action plan, to have sufficient material strength for the repetitive impact loads, the torsional shaft was reshaped to give it more rounding from R0.5 mm to R2.0 mm. After these modifications, there were no problems at the third ALT. The lifetime of the HKS in the domestic refrigerator was assured to be B1 life 10 years.

Biography

Dr. Woo has a BS and MS in Mechanical Engineering, and he has obtained PhD in Mechanical Engineering from Texas A&M. He major in energy system such as HVAC and its heat transfer, optimal design and control of refrigerator, reliability design of mechanical components, and failure Analysis of thermal components in marketplace using the non-destructive such as SEM & XRAY. Especially, he developed parametric accelerated life testing (ALT) as new reliability methodology. If there is design fault in the mechanical system that is subjected to repetitive stress, it will fail in its lifetime. Engineer should find the design faults by parametric ALT before product launches. In 1992–1997 he worked in Agency for Defense Development, Chinhae, South Korea, where he has researcher in charge of Development of Naval weapon System. In 2000-2010 he had been working as a Senior Reliability Engineer in Side-by-Side Refrigerator Division, Digital Appliance, SAMSUNG Electronics, where he focused on enhancing the life of refrigerator as using parametric the accelerating life testing. He has published more than 120 research articles, 10 book chapters and edited three books in the field of mechanical engineering. He has published more than 25 papers in reputed journals and has been serving as an editorial board member of Journal of Modern Industry and Manufacturing (JMIM, ISSN 2788-8096).

Danica M. Bajić[1], Bojana Fidanovski[1], Igor Radisavljević[1], Marica Bogosavljević[1], Ljubica Totovski[1], Dušica B. Stojanović[2]

[1]Military Technical Institute, Belgrade, Serbia, Email id: simic_danica@yahoo.com

[2]University of Belgrade, Faculty of Technology and Metallurgy, Belgrade, Serbia.

WS2 nanostructures as thermo-mechanical reinforcement of composite materials for advanced applications

As one of transition metal dichalogenides, tungsten disulphide (WS_2) is well known for its solid lubricating behavior, but besides this feature, it exhibits extraordinary thermal stability and mechanical resistance. The outstanding mechanical strength of WS_2 is most pronounced when it comes in form of multi-layer hollow nanoparticles and nanotubes: inorganic fullerene-like nanoparticles and inorganic nanotubes, denoted as IF-WS_2 and INT-WS_2, respectively. These structures have extraordinary shock resistance properties, pressure and heat resistance, that can be exploited for a variety of applications. They have been studied as reinforcing fillers of various polymers, but they might be also added as reinforcement of matrix in more complex composites, like CFRPs. Our research aimed to examine their reinforcing effect on laminated composites based on aramid fabric and poly(vinyl butyral), PVB, intended for demanding applications: in personal protection equipment, ballistic protection, sports equipment, automotive, nautical and aircraft engineering. WS_2 nanostructures have been incorporated in PVB by temporary dissolving in ethanol, by ultrasonication and intensive mechanical mixing. After impregnation of aramid fabrics ethanol would evaporate, and layers of aramid with thermoplastic binder PVB would be integrated by hot pressing. SEM analysis confirms the uniform distribution of WS_2 nanostructures in the prepared composite material. DSC analysis reveals the effect of WS_2 addition on thermal resistance of the new material, while PVB/aramid mechanical resistance was examined using DMA, impact test and tensile test. IF- WS_2 has imported higher thermal resistance and ductility improvement, while INT-WS_2 has significantly improved tensile and impact strength of the composite.

Biography

Dr. Danica Bajić has completed her academic and PhD studies at University of Belgrade, at the Faculty of Technology and Metallurgy. She is at position of a project leader at the Military Technical Institute and at position of assistant professor at Military academy, University of Defense, Belgrade. She is engaged in research in the field of nanotechnology and of energetic materials. She has published more than 60 papers in journals and conferences.

Jyoti Ahlawat and Mahesh Narayan*

[1]Chemistry and Biochemistry, University of Texas at El Paso, El Paso, TX, USA. E-mail id: mnarayan@utep.edu

Graphene Quantum Dots mitigates paraquat-induced oxidative stress in neuronal cells

IN recent years, Graphene Quantum Dots (GQDs) have gained enormous attention worldwide owing to their mesmerizing properties, such as small size, bioimaging, ease of synthesis, low toxicity, and resistance to photobleaching. In this work, we have investigated the potential of GQDs in serving as a neuroprotectant by mitigating the oxidative stress induced by paraquat in SH-SY5Y cells. Here, we synthesize GQDs from small molecules such as glucose using the hydrothermal method and test their prophylactic activity using paraquat as an insult inside the cells. Our preliminary results illustrate the prophylactic efficacy of our as-synthesized GQDs against paraquat-induced cell insult.

Biography

Jyoti Ahlawat is a Ph.D. Research Associate (NIH sponsored FYRIS program) and Dr. Keelung Hong Chemistry Graduate Research Fellow at the University of Texas at El Paso, USA. Her research focus involves developing materials and testing them invitro to develop therapeutics against the gravest of human diseases such as Alzheimer's (AD) and Parkinson's disease (PD). She has published more than 15 papers in reputed journals. She graduated from the University of Delhi with a bachelor's degree in Zoology in 2012 and a Master's degree in Biotechnology from the Indian Institute of Technology, Roorkee, in 2015 with cum laude. She is a recipient of the title "Rising Star in Nanoscience and Nanotechnology" at the 10th IEE International Conference on nanomaterials and applications (IEEE-NAP 2020). She has also won Best presentation awards at the 26th Annual BioEnvironmental Polymer Society (BEPS-2019), Graduate Expo (2018), and 8th International conference on smart materials, structure, and systems (ISSS-2017). In addition, she has also received various travel awards (2018-2020) and four research awards (2019-2021), and graduate scholarships (2019-2020).