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Abstract Book

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Plenary Presentations

E-Mobility with Hydrogen and Fuel Cells-challenges for Materials

Thomas von Unwerth

Chemnitz University of Technology, Faculty of Mechanical Engineering, Department Advanced Powertrains), Germany

Abstract

Starting with the drivers for electromobility and the need for emission free powertrains, battery and fuel cell electric mobility concepts regarding several parameters like energy and power density, and other usability factors are compared. While battery driven vehicles seem to be preferred because of higher efficiencies and easier in design, consisting mainly of a battery and an e-drive, the tide might turn when looking also at other important technical and economical parameters like power, safety, lifecycle and costs.

Additionally, materials play an important role in the overall powertrain design, for hydrogen fuel cells as well as for batteries. Challenges are starting with availability of raw materials like lithium or platinum, head through issues with selection of materials for components affecting safety and lifetime and lead to recycling issues. To get an impression on the state of the art and the potential next development steps for materials in hydrogen fuel cell powertrains and their components, different examples for e.g. MEAs, bipolar plates or hydrogen storage vessels are presented and evaluated concerning the given numbers and aims for series production of mobile fuel cell applications.

These main aims and topics like durability, RCS, certification and reduced costs will be addressed in the new German Hydrogen Innovation Centre (HIC) at Chemnitz, Germany.

Biography:

Thomas von Unwerth is Professor for Advanced Powertrains and Director at Institute for automotive research at TU Chemnitz. His research work is on hydrogen and fuel cell systems for automotive applications as well as on series manufacturing technologies. He joined TUC in 2010 from Volkswagen AG, Wolfsburg, where he was responsible for fuel cell systems and later for fuel cell fleet at Shanghai Volkswagen, China. Also founder and CTO of FCP Fuel Cell Powertrain GmbH, Germany. He is chairman of the hydrogen fuel cell cluster 'HZwo' in Saxony and scientific director of the german national hydrogen innovation centre Chemnitz (HIC).

A New Semiconductor: Boron Arsenide

Zhifeng Ren

Department of Physics and Texas Center for Superconductivity at the University of Houston (TcSUH), University of Houston, Houston, TX, USA

Abstract

Semiconductors are crucial to the society. A good semiconductor should have a wide band gap, high carrier mobility in both electrons and holes, high thermal conductivity, well matched

coefficient of thermal expansion, etc. Unfortunately, such a semiconductor did not exist before not long ago. Boron arsenide (BAs) seems to have all these good properties. It has a bandgap of 2.1 eV, carrier mobility above 1400 cm2 s-1 V-1 for both the electrons and holes, isotropic thermal conductivity higher than 1,300 W m-1 K-1 at room temperature, etc. In this presentation, I will present what we have learned and what need to be done on this special material in order to realize the promising applications.

Biography

Zhifeng Ren is an M. D. Anderson Chair Professor at the Department of Physics and the Director of the Texas Center for Superconductivity at the University of Houston (TcSUH). He received his BS in 1984 from Sichuan Instotute of Technolgy, MS in 1987 from Huazhong University of Science and Technology, and PhD in 1990 from the Institute of Physics, Chinese Academy of Sciences. His research focuses on thermoelectrics with high ZT, boron arsenide single crystals for high thermal conductivity and carrier mobility, nanomaterials for enhanced oil recovery, good catalysts for water splitting for H2 generation, heated filters for catching and killing SARS-CoV-2 causing COVID-19 pandemic, carbon nanotubes, solar absorbers, flexible transparent conductors, superconductors, etc.

Low-D Syntheses by Numbers: Atoms, Lattice, Chemical Kinetics

Boris I. Yakobson

Rice University, Houston, TX

Abstract Not Available!!!

Keynote Presentation

3D and 4D Printing of High Performance and Nanostructured Polymers

Rigoberto C Advincula, University of Tennessee, Knoxville, TN

Abstract Not Available!!!

Plasmonic Metals and Semiconductors for Solar Fuel Generation

Nianqiang Wu, University of Massachusetts Amherst, Amherst, MA

Abstract Not Available!!!

Electron-phonon, Exciton, and Trion Interactions in Two-dimensional Materials

Vasili Perebeinos

Electrical Engineering Department, University at Buffalo, Buffalo, NY

Abstract:

Atomically thin two-dimensional materials are direct bandgap semiconductors with a rich interplay of the valley and spin degrees of freedom, which offer the potential for such technologies. A strong Coulomb interaction leads to tightly bound electron-hole pairs or excitons and two-electron one-hole quasiparticles or trions. We solve the two-particle and three-particle problems for the

wavefunctions for excitons and trions in the basis set of the model Hamiltonian for single particles [1]. The calculated linear absorptions [2], photoluminescence spectra [3], and polariton spectra [4] as a function of doping and temperature explain the experimental data in 2D monolayers. The strong-electron phonon interactions in boron nitride substrate offer the potential of using graphene as a quantum phonon sensor down to a single phonon level [5] via remote electron-phonon scattering [6]. This material is based upon work supported by the Air Force Office of Scientific Research under award number FA9550-22-1-0312.

Biography:

Vasili Perebeinos is a Professor of the Electrical Engineering Department at the University of Buffalo. During his research career, he became a Fellow of the American Physical Society. He received the highly competitive IBM Research Technical Accomplishment" award three times and the best paper award by the IBM Materials Research Council. Perebeinos's research interests are in theory and simulations of advanced materials and nanostructures for electronics and optoelectronics, specifically novel 2D materials, and 1D carbon nanotubes. He is the author or co-author of over 100 journal articles cited over 16,500 times (h-index 54 – google scholar).

Realizing the Lowest Bandgap and Exciton Binding Energy in the 2D Single Layer Lead Halide Family of Compounds

Dipankar Das Sarma

Indian Institute of Science, India

Abstract Not Available!!!

Oral Presentation

Large Polycrystalline Diamonds: Equipment, Fabrication and Applications

Oleg A. Voronov

Diamond Materials, Inc., USA

Abstract:

The modern technology advances allow us to create the large polycrystalline diamonds and diamond composites. Diamond components can be synthesized near-net shape as pure or doped carbon using high pressure-high temperature techniques. The high pressure-high temperature equipment of our design is applicable for the research in very wide pressure and temperature ranges. The advantages of this design are the ability to achieve pressures close to the value of anvil's hardness in a relatively large volume and the possibility of rapid turnaround in industrial manufacturing. High pressure application in fabrication process minimizes porosity, excluding its detrimental effect on mechanical properties of polycrystalline structures and composites. The same equipment can be used for the research in the field of pressure-assisted sintering of powders, single crystals growth, pressure-assisted oligomerization, polymerization, decomposition of organic compounds, other chemical reactions, for the fabrication of carboncarbon composites and new carbon materials. We have developed a new type of monolithic carbon material called "Diamonite", a fullerene-derived carbon, which is neither graphite-like nor diamond-like. It is almost as hard as diamond, and as thermally stable as graphite. The high pressure sintered polycrystalline diamonds and diamond-carbide-metal composites can be used for bearing and rock drill-bit applications. Our experiments show that well-polished diamond materials have low friction coefficients and experience negligible wear, even in dust or sand. The high hardness,

lightweight and high-surface finish make diamond materials and Diamonite also suitable for both mechanical and electronic aerospace applications.

Biography:

Voronov is co-founder and President of Diamond Materials, Inc. (DMI). While working for DMI, he invented a High Pressure-High Temperature Apparatus for generating static high pressure and high temperature in relatively large volume, method for rapid transformation of graphite into diamond, discovered and developed a new line of carbon materials, diamond-based and ceramic-metal composites. He was elected to the Head position of the Department for Carbon Materials at the Academy of Sciences of U.S.S.R., the Vereshchagin Institute, and has more than 100 scientific publications (in Russian and English), author's certificates of invention.

The Central Role of Isostatically Rigid Local Structures in Determining Topological Phases and Melt Dynamics of Network Glasses

Punit Boolchand*
Vamshi Gogi
Aaron Welton

Department of Electrical Engineering and Computer Science, University of Cincinnati, Cincinnati, Ohio

Abstract

Network glasses of chalcogenides and modified oxides are made up of short-range covalent and longer-range ionic forces which serve as mechanical constraints in assembling networks. In these glasses one observes1 two sharply defined elastic phase transitions, a rigidity- and a stress-transition, which separates composition space into three Topological phases, Flexible, Intermediate and Stressed-rigid. Calorimetric measurements1 using Modulated-DSC have proved to be remarkably useful to measure the glass Enthalpy of relaxation at Tg, ΔHnr (<r>), which displays a square-well variation with the term near vanishing across the Intermediate Phase (IP). Here <r> represents the mean coordination number of a network. IP are composed of isostatically rigid local structures (ISRLSs), in which the count of constraints/atom, nc, due to nn bond-stretching and nnn bond-bending interactions equals 3 in 3D networks. The observation of ΔHnr term is fully consistent with it representing the open degrees of freedom/atom in general. MDSC also permits one to measure the melt fragility index at T > Tg, which generally display a Gaussian-like global minimum of m = 15 centered in the IP. These features are widely observed1 in many families of chalcogenide glasses such as GexSe100-x, AsxS100-x, GexAsx(or P)Se100-2x, GexS100-x. In modified oxide glasses such as (Na2O)x(B2O3)100-x and (Na2O)x(P2O5)100-x glasses1, trends in ΔHnr (<r>) and m(<r>), each show a square-well like variation across the IP range largely because of extended nature of the ISRLSs occur as rings or chains. Ref1. P. Boolchand and M. Micoulaut. Complimentary pdf copy of eBOOK available at https://www.frontiersin.org/research-topics/9016/topology-of-disordered-networks-and-their-applications

Biography:

Punit Boolchand is a materials scientist, a professor in the Department of Electrical Engineering and Computing Systems (EECS) in the College of Engineering and Applied Science (CEAS) at the University of Cincinnati (UC), where he is director of the Solid State Physics and Electronic Materials Laboratory[1] He discovered the Intermediate Phase: an elastically percolative network glass distinguished from traditional (clustered) liquid–gas spinodals by strong non-local long-range interactions. The IP characterizes space-filling, nearly stress-free and non-aging, critically self-organized non-equilibrium glassy networks (such as window glass, ineluctably complex high-temperature superconductors, microelectronic Si/SiO2 high-k dielectric interfaces, and protein folding).

Chemically Recyclable Crosslinked Polydiene Elastomers based on Thiol-Disulfide Exchange Reactions

Kailong Jin*
Saleh Alfarhan

Arizona State University, Tempe, AZ, USA

Abstract:

Crosslinked polydiene elastomers, e.g., polybutadiene and polyisoprene, are widely used synthetic rubbers because of their robust network structures and excellent thermomechanical properties. However, these elastomeric networks cannot be recycled/reprocessed and are often discarded after their service life in landfills or incinerated at elevated temperatures. While the introduction of dynamic covalent chemistry has allowed researchers to develop crosslinked elastomers that can be reprocessed under certain external stimuli, closed-loop chemical recycling of crosslinked polydiene elastomers is yet to be demonstrated. Herein we report a chemically recyclable polydiene elastomer formed by photoinitiated thiol-ene click reactions between commercially available building blocks. Specifically, liquid polysulfides containing photoreactive thiol end groups and internal dynamic disulfide bonds were chosen to undergo crosslinking reactions with the carbon-carbon double bonds (i.e., ene groups) in polydienes such as polybutadiene and polyisoprene. The disulfide bonds within the resulting crosslinked polydiene elastomers permit these networks to undergo base-catalyzed thiol-disulfide exchange reactions with the starting liquid polysulfides, which can eventually decrosslink or degrade completely into photoreactive thiol oligomers. Next generation of crosslinking reactions between these chemically recycled thiol oligomers and polydienes were repeated under similar conditions and at identical chemical compositions as the first generation, resulting in crosslinked polydiene elastomers with nearly identical thermomechanical properties. Overall, this study demonstrates a scalable approach for fabricating chemically recyclable crosslinked polydiene elastomers that can retain material properties after multiple recycling times.

Biography:

Kailong Jin is an assistant professor in chemical engineering in the School for Engineering of Matter, Transport and Energy (SEMTE) at Arizona State University, where he began in 2020. Kailong Jin earned his Ph.D. in chemical engineering from Northwestern University under the direction of Professor John Torkelson. Then, he worked as a postdoctoral researcher with Professors Frank Bates and Christopher Ellison in the Department of Chemical Engineering and Materials Science at the University of Minnesota. His research broadly seeks to design, synthesize, engineer, and characterize polymeric materials that can help address technological issues in energy, the environment, and sustainability.

Effect of Oxides Formed on Steel Surface after Cavitation Treatment on Corrosion Resistance

Masataka Ijiri*

Tokyo Metropolitan University, Japan

Abstract

Rust in rust-prone steel is promoted in water by corrosive factors. Therefore, to prevent the formation of rust, it is necessary to eliminate various corrosive factors before plating or other rust prevention measures. In this study, we investigated improvement of the corrosion resistance of steel surfaces by mechanochemical-multifunction cavitation (MC-MFC) with a sodium hypochlorite solution and MFC in water. The compounds formed on the steel surface after MFC and MC-MFC were α-FeOOH and β-FeOOH. Furthermore, red rust was less likely to occur on the surface after

MC-MFC; therefore, it was concluded that the amount of β-FeOOH was relatively high. A combined cycle test was conducted to confirm the rust prevention property. Based on these results, MC-MFC is considered to be effective for suppressing rust. Nevertheless, it is difficult to completely prevent the occurrence of red rust over long periods of time. However, as a treatment prior to plating, MC-MFC may improve the adhesion strength of the protective film by removing impurities or forming compounds on the surface. In future studies, we plan to investigate the long-term improvement effect of MC-MFC processing on plated surfaces.

Biography:

Masataka Ijiri obtained a Bachelors Degree in engineering, a Masters Degree in mechanical and systems engineering, and a Ph.D. Degree in engineering at Okayama University. He is a specialist in materials engineering for titanium alloys. After obtaining a doctoral degree, he was a postdoctoral researcher at Sanyo-Onoda city University and studied cavitation processing technology. Currently he is working as an assistant professor at the Department of Mechanical Systems Engineering, Tokyo Metropolitan University.

Loading Path and the Effect of Specimen Geometry on the Facture Behaviour of Metallic Alloys

Madhav Baral*

Department of Mechanical and Aerospace Engineering, University of Kentucky, Paducah, KY, USA

Abstract

Ductile fracture is one of the basic mechanisms of material failure, that terminates the useful life of a product or makes its manufacturing impractical. Thus, establishing the fracture envelope of a material is of interest for both component and process design. Recent studies have highlighted the dependence of the fracture locus on the specimen geometry, the through-thickness gradients, and non-proportional loading. In this talk, the effect of specimen geometry and the resultant non-proportional path on the fracture locus of different aluminum and steel alloys will be presented. First, the fracture behavior of flat specimens using conventional notched tension

and central hole specimens, as well as the proposed novel specimen designs will be shown. The improved specimen designs exhibit stress states that develop at the neighborhood of the fracture initiation point to remain proportional throughout the loading history. Second, the fracture behavior of the tubular specimens loaded under axial force and internal pressure along different stress paths will be shown. The ability to control the force/pressure ratio in the tubular tests enables probing the fracture behavior under proportional loading. The fracture behavior of these metallic alloys is investigated through a combined experimental-numerical approach utilizing a series of specialized experiments followed by corresponding finite element analyses.

Biography:

Madhav Baral is an assistant professor in the Department of Mechanical and Aerospace Engineering at the University of Kentucky. Dr. Baral's research interests include plasticity, constitutive modeling, ductile fracture, experimental and numerical methods, sheet metal and tube forming, material characterization, manufacturing processes, and acoustic emissions.

Optical Properties for Y_2O_2S and Er Doped Y_2O_2S

Nicholas Dimakis*
Eric Baldemar Rodriguez Jr.
Kofi Nketia Ackaah-Gyasi

Madhab Pokhrel

University of Texas Rio Grande Valley, Edinburg, USA

Abstract

Density functional theory (DFT) and simulated x-ray near edge (XANES) spectra are used to analyze changes in the electronic and optical properties of Y2O2S due to doping with Er atoms. Y2O2S is a wide band semiconductor and serves as a phosphorescent host for doping with Eu, Er, Mg, and Ti atoms. Absorption experiments show Y2O2S:Er+3 light emissions in the visible and near infrared, which are not related to light emissions from the host Y2O2S. These Er emissions correspond to Er f–f intraband transitions. We generate Y2O2S:Er+3 supercells are various Er concentrations, where we calculate optical properties using the independent particle approximation. These calculations on the Y2O2S:Er+3 reveal transitions in the energy region of the bandgap, which are absent in the host spectrum. We assign these to Er f–f intraband transitions in the visible and near infrared, by applying a rigid energy shift. Reflectivity calculations show that the lowest peak in energy in the bandgap region is of reduced light transmission, in agreement with experiments, which measured small near infrared Er emission. XANES is proportional to the imaginary part frequency-dependent dielectric function, and it provides information about transitions from core and valence states to unfilled and partially filled bound states and to the continuum. XANES calculations at the Er M5-edge reveal a pre-edge broad shoulder in the proximity of the Er 4f band, which supports f–f intraband transitions, in agreement with DFT and experiments.

Biography:

Nikolaos (Nicholas) Dimakis is a Full Professor and Department Chair for Physics and Astronomy at the University of Texas Rio Grande Valley. He graduated with a Ph.D. in Physics from Illinois Institute of Technology (IIT) in Chicago and worked at the IIT collaborative access team at the Advanced Photon Source for several years before joining UT Pan-American as Assistant Professor in 2004. His research is on computational material science applicable to a variety of materials such as platinum-based alloys, heterostructures, and pyrochlores. He has about 52 peer-reviewed publications and participated in externally funded grants of about $8M.

AI-assisted Design of Low-carbon Cost-effective Concrete Toward Carbon Neutrality

Yi Bao*
Weina Meng

Department of Civil, Environmental and Ocean Engineering, Stevens Institute of Technology, Hoboken, NJ

Abstract

As the most used construction material in the world, concrete plays critical roles in the carbon emissions of civil infrastructure and the protection of the environment, since the production, construction, and demolition of concrete involve substantial carbon emissions and generates a large amount of waste. It is prudent to convert waste into valuable concrete to reduce the cost and carbon footprint of concrete while improving the properties of concrete and minimizing the landfill. This research develops an AI-assisted approach to intelligently design low-carbon cost-effective concrete with various types of wastes. The presented approach is built on a prediction-optimization framework that is composed of machine learning and multi-objective optimization modules. The proposed AI-assisted design approach is able to predict concrete properties based on the concrete design variables including the physicochemical information of raw ingredients and optimize the concrete mixture design to minimize the material cost and carbon footprint. The AI design model is able to update by learning from new documents and thus improve its capabilities of designing new concrete. The proposed approach has been implemented into

designing ultra-high-performance concrete with low material cost and low carbon footprint while having superior flowability, mechanical properties, and durability. This research will advance the capabilities of designing new materials efficiently and effectively.

Biography:

Yi Bao is an Assistant Professor in Civil Engineering at Stevens Institute of Technology. Prior to joining Stevens, Dr. Bao was a Postdoc at the University of Michigan - Ann Arbor and served as a Guest Researcher at National Institute of Standards and Technology (NIST). Currently, Dr. Bao directs the Smart Infrastructure Laboratory at Stevens Institute of Technology.

Significance of Non-uniform Heat Source on the Carreau Bio-nanomaterial Emhd Flow: Modified Buongiorno Approach for Biomedical Applications

Alphonsa Mathew*
Sujesh Areekara
A S Sabu

Department of Mathematics, St. Thomas' College (Autonomous), India

Abstract

Owing to its applications in the field of theranostics, cancer therapy, target drug delivery and treatment of cardiovascular diseases, the main goal of the present study is to elucidate the effect of non-uniform heat source and external electro-magnetic fields on the Carreau bionanomaterial flow. The flow over a stretching cylinder has been devised using the modified Buongiorno model. A comparative analysis between the Carreau nanomaterial and Carreau-gold bio-nanomaterial is also presented. Only the shear-thinning nature of the Carreau nanomaterial is considered for its similarity with the human blood. Using apposite similarity transformation, the modeled flow equations are treated numerical using the finite-difference based bvp5c numerical scheme. The findings are explored using contour-shaped graphs. The heat source and radiation parameter induces a supplement energy that increases the thermal field which is biologically relevant in the field of cancer therapy and theranostics.

Graphical Abstract:

A steady two-dimensional hydromagnetic blood-based Carreau gold nanomaterial flow over a stretching cylinder with r = E_o fixed at origin, E_o is analysed (see Figure 1). The cylinder is elongated along the E_o-direction with E_o. A uniform magnetic field (of strength E_o) and a uniform electric field (of strength E_o) are administered normal to the flow direction. The induced magnetic field was neglected due to the small magnetic Reynolds number. The nanomaterial has been modeled using the modified Buongiorno model. Effects like passive control of nanoparticles, convective heating, thermal radiation, chemical reaction and second-order hydrodynamic slip are also incorporated that improves the practicality of the current model.

Biography:

Alphonsa Mathew, Assistant professor working in department of Mathematics St. Thomas College (Autonomous), Thrissur since 2010. My area of expertise include Newtonian and nonnewtonian fluids, Magnetohydrodynamics, Nano Fluids, Blood Flow, Heat and mass transfer, and Bioconvection. I have published 39 research papers in International Journals of High impact factor. My h-index is 10. I have also received the young Scientist Award in 2017.

Mid-infrared Emitting Self-doped Colloidal Quantum Dots

Kwang Seob Jeong[1,2*]

[1] Institute for Basic Science (IBS), Korea University, Republic of Korea
[2] Department of Chemistry, Korea University, Republic of Korea

Abstract

Mid-IR active materials have been of great interest due to their increasing demands in various research fields, including telecommunications, biosensing, gas sensing, and unmanned vehicles. Colloidal quantum dots, intensively studied in the visible range, can also be promising materials to realize the efficient mid-IR emitter due to their tunable and selectable electronic energies. Especially self-doped quantum dots, where excess carriers occupy the lowest quantized energy states of the conduction band, is a new approach to exploit the mid-IR energy. In this talk, I will focus on the optical and electrical properties of the self-doped mid-IR nanomaterials.

Biography:

Kwang Seob Jeong obtained his B.S. in chemistry at Korea University and Ph.D. in chemistry at the Pennsylvania State University in 2013. He worked at the University of Chicago as a JFI post-doctoral scholar before joining the chemistry department at Korea University in 2015. His research focuses on finding new electronic transitions of low-dimensional nanomaterials and infrared optoelectronics. He was nominated as 2018 emerging investigators by the Chemical Communications of Royal Society of Chemistry (RSC), won the POSCO TJ Park Science Fellow in 2019, and received the Korean Chemical Society (KCS)-Wiley Young Chemist Award in 2021.

Modified 2D-graphitic like Carbon Nitride Nano Sheets for the Degradation of Volatile Organic Carbons under Visible-light Irradiation

Rengaraj Selvaraj*
Said Al Mamari

Department of Chemistry, College of Science, Sultan Qaboos University, Muscat, Oman

Abstract

The photocatalytic oxidation method can be used to remove effectively volatile organic compounds and has the ability to degrade even at low concentrations. In the present work we have developed hollow TiO2/g-C3N4 nanocomposite using solvothermal method. Two-dimensional g-C3N4 nanosheets were coupled with TiO2 hollow spheres at different ratios to investigate the charge-carrier interactions with the aim of enhancing the photocatalytic properties of the nanocomposite. This coupling was systematically examined by various advanced analytical techniques such as scanning electron microscopy, transmission electron microscopy, energy-dispersive X-ray spectroscopy, X-ray diffraction, photoluminescence, X-ray photoelectron spectroscopy, and UV diffuse reflectance spectroscopy. The prepared nanocomposite was applied for the photodegradation of various volatile organic carbons methyl tetra-butyl ether and toluene present in aqueous solution. Elemental analysis and X-ray diffraction revealed a high-purity sample, while the UV diffuse reflectance spectroscopy demonstrated the presence of a well-defined anatase crystal phase for the TiO2 hollow sphere; and the photoluminescence measurements showed an enhancement in visible-light absorbance, with a good reduction in the electron-hole recombination rate. The performance of the nanocomposites in the photocatalytic degradation of MTBE and toluene under irradiation with visible-light was evaluated. The 20/80 % TiO2/g-C3N4 nanocomposite materials showed highest photocatalytic activity for toluene and methyl tetra-butyl ether, achieving a degradation of more than 90 %; this is attributed to the interaction between the two surfaces in the TiO2/g-C3N4 nanocomposite, resulting in a higher performance than the individual components.

Biography:

RENGARAJ Selvaraj., Ph.D., FRSC, is a Professor of Analytical and Environmental Chemistry in the Sultan Qaboos University, Muscat, Oman with responsibility for teaching, research and consultancy in the field of Analytical and Applied Environmental Chemistry. Prof. Rengaraj graduated from Anna University, Madras, India with a PhD in Chemistry in 1999. He has 30 years of research experience in Materials, Environmental Science and Engineering, particularly in the area of Environmental Nanotechnology, wastewater treatment, water quality analysis, and solid waste management. He has published more than 90 research articles in reputed National, International Journals, and Proceedings (h-index 33) and has been serving as an editorial board member of two International Journals.

The Effect of Antimony Additions on the Microstructure and Performance of Automotive Zn-Al-Mg Steel Coatings

Daniel Britton[1*]
David Penney[1]
Amar Malla[1]
Shahin Mehraban[2]
James Sullivan[1]
Matthew Goldsworthy[1]
Richard Johnston[2]
Tom Dunlop[2]
Clive Challinor[3]

[1]Materials Research Centre, Swansea University, UK
[2]College of Engineering, Swansea University, UK
[3]TATA Steel UK

Abstract

It is estimated that one metric tonne of steel turns to rust every ninety seconds [1]. Traditional galvanizing provides a solution to this by utilising a thin coating of almost pure zinc as a sacrificial anode, corroding in preference to the steel substrate. Additions of 1-2wt.% Al and Mg have brought about improvements in processability of these coatings, as well as greater protection in harsh coastal environments. Additionally, increased performance means coatings can be almost halved in thickness, leading to savings in weight and materials [2]. Despite these benefits, the brittle MgZn2 binary eutectic phase that forms in these alloys can cause the coating to crack during automotive body panel pressing, causing a range of surface finish defects. Therefore, a strategy to mitigate the cracking issues but retain the corrosion benefits afforded by the Mg additions is investigated here. Additions of 0-2wt.% Sb were added to Zn-Mg-Al alloy and fast cooled from 800oC, resulting in the formation of Mg3Sb2 needle intermetallics which tie up Mg and reduce the volume fraction of the brittle MgZn2 phase. This improves the coating's ductility, helping to reduce or eliminate defects. Scanning Vibrating Electrode Technique showed an addition of 1wt.% antimony resulted in a 45% improvement in corrosion-induced metal loss, whilst Linear Polarisation Resistance found increasing this addition further led to a rise in the kinetics of corrosion. Open-Circuit Potential testing revealed mixed results regarding the effect of antimony on thermodynamic potential.

Biography:

Daniel completed his undergraduate degree in materials science and engineering from Swansea University, UK, in 2019. He is now studying for his Engineering Doctorate (EngD), titled 'Development of Zn-Mg-Al Coated Steels for Automotive Applications'. Being situated close to the UK's Port Talbot steelworks, Swansea University has numerous links with industry and a strong research background in metallurgy, manufacturing, and steel production. This is complemented by the Coatings and Corrosion research group, which consists of post-graduate and post-doctoral researchers alike.

Soft Materials: From Fundamentals to Applications

Lenore L. Dai

Arizona State University, USA

Abstract

Soft materials are ubiquitous in natural and industrial processes. In this presentation, we will elaborate on three groups of lesser explored soft materials: Pickering emulsions, mechanophore incorporated polymers, and ionic liquid-based electrolytes. Conventional emulsions use organic surfactants as stabilizers. Although solid particle stabilized emulsions (Pickering emulsions) are often encountered in crude oil recovery, oil separation, cosmetic preparation, and wastewater treatment, this phenomenon is not well-understood. Here we report the fundamentals and applications of Pickering emulsions, including the self-assembly and diffusion of solid particles at liquid-liquid interfaces and the subsequent polymerization to synthesize composite particles. In addition, we will present the design and optimization of mechanophore incorporated polymers for self-sensing applications and ionic liquid-based electrolytes for space exploration.

Biography:

Lenore Dai is a Professor of Chemical Engineering and the Vice Dean of Faculty Administration in the Fulton Schools of Engineering at Arizona State University. She was the Director of the School for Engineering of Matter, Transport and Energy at ASU from 2016 to 2022, overseeing aerospace engineering, chemical engineering, materials science & engineering, mechanical engineering, etc. She holds a Ph.D. in Materials Science and Engineering from the University of Illinois.

Comparison of Air Void Structures of High-performance Concretes Remixed by Cellular Sprayed Method

Kyong-Ku YUN[1*]
Seunghak CHOI[1]
Taeho HA[1]
Changseok SONG[1]
Seungyeon HAN[2]

[1]Kangwon National University, S. Korea
[2]Korea Institute of Civil Engineering and Building Technology, S. Korea

Abstract

The air void structure in concrete directly affects both the fresh-state workability and the freeze-thaw durability of high-performance concretes. In order to effectively study the air void structures, the air volume, spacing, and size distribution of the air bubbles must be quantified by valid test methods.

A very simple and economic method for remixing an ordinary Portland cement concrete (OPC) into a high-performance concrete (HPC) at a job site was developed, which is called 'cellular sprayed concrete'. The method of cellular sprayed concrete enables remixing OPC into HPC incorporating silica fume, powdered polymer or latex at a job site.

This paper compares and describes the air void structures of high-performance concretes: ordinary high performance concrete (HPC) using silica fume, latex modified concrete(LMC) for bridge deck overlay and top lift concrete of two-lift concrete pavement(2LCP). The test methods adopted for measuring air void structure includes pressure method and image analysis method.

Biography

Kyong-Ku YUN is a professor at Kangwon National University in S. Korea. He received his Ph.D. degree from Michigan State University in 1995. His research area includes concrete materials, shotcrete, concrete pavement and bridge repair and rehabilitation. He had served as a president of Korean Society of Road Engineers (KSRE) from 2018 to 2019. He is a member of The National Academy of Engineering of Korea (NAEK) since 2019.

Oxide Reduction for Pore Formation in Metals and Alloys: Current Understanding and Future Directions

Julian Tse Lop Kun
Braden Jones
Mark Atwater*

Mechanical Engineering, Liberty University, Lynchburg, VA

Abstract

Porous metals produced by oxide reduction have been investigated in numerous metals and alloys, through different processing protocol, and for various properties. This process, known as additive expansion by the reduction of oxides (AERO), produces pores throughout metal particles by the reduction of oxide dispersions. This results in micron and nanoscale open porosity throughout the material volume. It has been demonstrated in forms ranging from micron-scale powder to millimeter-scale spheres, to solid, centimeter-scale rods. The unique aspect of this process is that it is not only a standalone technique, but it can be readily integrated into other powder metal "foaming" processes to increase the overall porosity, such as additive manufacturing or space holder and scaffolding techniques. Even entirely nanoporous structures can be made at low temperatures in a rapid, scalable, and environmentally friendly way, which has been demonstrated in samples ranging from micron to centimeter dimensions (i.e., truly "bulk" nanoporous metals). These porous materials display unusually high strength due to their nanoscale to ultra-fine-grained microstructure, and they have been characterized by a wide variety of techniques, including X-ray CT, FIB tomography, and in-situ tensile testing. The outcomes of this work indicate that there are significant opportunities in mechanical and functional applications. The process-property-performance relationships of these materials in the context of other solid-state foaming methods and lightweight alloys, as well as their synergy in hybrid foaming materials, will be discussed.

Biography:

Since completing his PhD in materials science from North Carolina State University, Mark Atwater has extended his dissertation work in mechanical alloying and nanostructured materials to include various structural and functional applications. His current projects include the NSF CAREER grant supporting this porous metal work as well as surface nanocrystallization for strength-ductility optimization. He is an Associate Professor of Mechanical Engineering at Liberty University. Other ongoing research interests include catalysis of carbon nanofibers and applications thereof, metal additive manufacturing, and in-situ mechanical testing within the SEM.

Influences of Heat Treatment and Marine Temperature on Corrosion Behavior of Selective Concentrated Complex Alloy (CCA)

Marcelo Paredes

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Abstract

Usually, failure of engineering materials operating in aqueous environments is catastrophic and difficult to predict due to the complexity of the electrochemical corrosion processes taking place. More recently, Complex Concentrated Alloys (CCAs) have shifted current design paradigms for metallic bulk materials manufacturing. Over the last two decades, CCAs have exhibited unprecedented structural and functional properties compared to their counterpart standard alloys. Moreover, environmentally resistant properties are not the exception, especially for corrosive environments in the form of bulk material or coating. As regards corrosion processes, understanding how the passive film forms during material dissolution and how it is constituted in terms of composition and structure is paramount to designing better Corrosion Resistant Alloys (CRAs) based on this new metallurgical philosophy. This work presents the results of a comprehensive study on a specific HEA base alloy, where different compositional and microstructural gradients material libraries were investigated in marine environments at different temperatures. Further heat treatment to enhance strain hardening and promote grain refinement yields better corrosion resistance characteristics compared to the as-received configuration. Advanced research tools such as XRD, SEM, EDS, and EBSD are employed to probe microstructural changes due to heat treatment, whereas the corrosion characteristics are measured by potentiodynamic, potentiostatic, and EIS experiments. Moreover, the composition of the passive film was studied via XPS and SIMS. The results show that by decreasing the grain size, the localized corrosion resistance of the material increases.

Acoustic Metamaterials for HVAC Noise Control

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Golakoti Pavan[1]

Indian Institute of Technology Roorkee, India.

Abstract

Acoustic metamaterials have been trending for over a decade. Research shows that these materials can manipulate sound waves extraordinarily and can be effective for noise control in frequencies lower than 1000 Hz; where the traditional materials are ineffective. The ability of acoustic metamaterials to absorb low frequency noise within low volume and low weight paves the way for their applications in many HVAC household appliances. This paper presents various case studies of development and application of space coiling (labyrinthine) metamaterials for noise control in commercial HVAC appliances. The developed metamaterials have been found to achieve a significant noise reduction of up to 6 decibels in the test appliances; within the weight and space constraints of the appliance. Additive manufacturing was used to fabricate the metamaterial prototypes, and the effect of manufacturing process parameters on the material performance has been investigated. The paper closes with the discussion of the practical challenges faced in development and application of the acoustic metamaterials.

Biography:

Sneha Singh is presently an Assistant Professor in the Indian Institute of Technology Roorkee, India. She completed her Ph.D. in 2016 from the University of Warwick (UK), and her B.Tech. in 2011 from the Indian Institute of Technology Kharagpur. She specializes in the area of Acoustics, Noise Control, and Metamaterials. In a short career span, she has published 12 International journal papers, and filed 5 Patents. She is a recipient of the Young Professional Award from the International Institute of Noise Control Engineering (I-INCE) and was selected among the "Top 20 Young Women Leaders in India in the year 2022" by the British Council.

Formation of Bismuth Oxide Nanostructures *via* Laser Ablation in Water

Cory J. Trout[1,2]
Julianne C. Griepenburg[1,3]
Sean M. O'Malley[1,3*]

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[2] Rutgers University - Newark, Department of Applied Physics, Newark, USA
[3] Rutgers University - Camden, Center for Integrative and Computational Biology, USA

Abstract

Bismuth oxide nanomaterials have gained attention due to their electronic and optical properties making them suitable candidates for electrochemical and biomedical applications. In this study, we show that various bismuth oxide nanostructures can be synthesized via the pulsed laser ablation in liquids method by altering the concentration of dissolved gasses from ambient conditions. Structure and composition were studied using a combination of x-ray diffraction, Raman spectroscopy, and FTIR spectroscopy, while morphology was investigated by atomic force microscopy and transmission electron microscopy. Findings indicate that pressure, dissolved gases, and laser fluence are deterministic factors in the final structure and composition of the resulting colloids. The various phases range from spherical metallic bismuth nanoparticles to monoclinic bismuth oxide nanowires, and orthorhombic bismuth carbonate oxide nanosheets. These results point to the production of free radicals during the ablation event, in combination with longer time-scale oxidation processes, playing a significant role in overall composition and morphology.

Biography:

Sean M. O'Malley is Associate Professor and Chair of the Department of Physics at Rutgers University - Camden. He is also serves as Lead Champion for the Sustainability Cluster on campus. O'Malley has over 10 years of research experience in the area of laser materials interactions with particle focus on pulsed laser ablation in liquids (PLAL) and nanoparticle plasmonic excitation. He often collaborates with biomaterial investigators to bring about photo-stimulated material systems.

Interaction of Photons and High Energy Ions with Highly Ordered Low Dimensional Semiconductors

Oomman K. Varghese[1,2*]
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Abstract

Highly ordered nanostructures are known for displaying scientifically intriguing properties. Nevertheless, discovering a spectrum of novel properties through experimental studies requires

significant efforts, time and resources. Numerical simulations using appropriate scientific models can help identify the unique properties and conditions necessary for revealing them. Experiments can then be designed for a narrow range of conditions. In a recent work, we demonstrated using simulations that highly ordered titania nanotubes could steer ions with energy in the mega electron-volt (MeV) range through the pores. The process is called ion channeling. The nanotube geometry would enable focusing and bending of high-energy ion beams, which are processes normally requiring very strong magnets. We revealed also that the geometric features and dimensions of this material could modulate the propagation of photons though it. This ability could be used for designing the components of efficient solar devices such as solar cells. This presentation would provide the details of these studies.

Biography:

Oomman K. Varghese received Ph.D. from Indian Institute of Technology Delhi (IITD). He is an Associate Professor and Chairman of the Graduate Program in the Department of Physics, University of Houston, USA. His group develops nanoscale materials and investigates unique properties for solar energy conversion and medical applications. In 2011, Thomson Reuters ranked him 9th among 'World's Top 100 Materials Scientists' in the previous decade. From 2014 to 2016 he received the title 'Highly Cited Researcher' and had his name listed in Thomson Reuters' World's Most Influential Scientific Minds. He is among the top 2% of the scientists in the world per the Stanford University Report, 2020.

Investigation of Various Nonthermal Plasma Reactor Configurations for Silver Nanoparticle Synthesis

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Ndeddy Aka Robinson junior
Sarah Wu

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Abstract

This work investigated the effect of nonthermal plasma reactor configurations on the synthesis of silver nanoparticles (AgNPs). Three reactor configurations: (i) coaxial dielectric barrier discharge (DBD), (ii) like-free ground DBD, and (iii) corona plasma, were studied to synthesize AgNPs. To make this work simple, cost-effective, and eco-friendly, no reducing agent was used but to get stable particles, inexpensive and environmentally friendly sucrose was used as a capping agent. The formation AgNPs was found to be dependent on various parameters, including the applied voltage, gas flow rate, treatment time, nozzle distance from the solution surface, concentration of silver nitrate, and concentration of sucrose. The formation of the AgNPs and the stability test were done using UV-Vis spectroscopy. The surface morphology and particle size distribution were studied using transmission electron microscopy (TEM). The nanoparticles (NPs) synthesized by coaxial DBD and corona plasma were spherical in shape with a wide particle size distribution (PSD), and their average size was 6.2 nm and 9.6 nm, respectively. On the other hand, the NPs synthesized by like-free ground DBD were mostly spherical, along with a few hexagon and triangular shapes. With like-free ground DBD, the PSD was found to be narrow, and the average particle size was 20 nm which is bigger compared to NPs synthesized by coaxial DBD and corona plasma.

Biography:

Md. Mokter Hossain was born in Dhaka, Bangladesh, in 1986. He received a B.S. and M.S. degree in Electrical and Electronics Engineering in 2009 and 2014, respectively. Mr Hossain received his PhD degree in Energy and Chemical Engineering from the Faculty of Applied Energy System, Jeju National University, Jeju, South Korea, in 2019. Since 2022, he has been a Postdoc Fellow with the

Department of Chemical and Biological Engineering at the University of Idaho, USA. His current research interests include atmospheric pressure plasma and its various applications, such as thin film, catalyst preparation, nanoparticle synthesis, VOC removal, wastewater treatment etc.

Silica@ferrite Nanostructures for Synergistic Radiation and Hypoxia Therapy

Stefanie Klein*

Friedrich-Alexander University Erlangen-Nuremberg

Abstract

Aggressive growth of tumor cells leads to the development of a disorganized blood vessel network. This inadequate vasculature causes heterogeneity of solid tumors in oxygen, pH, glucose distribution, etc. In particular, oxygen is rapidly metabolized and the diffusion depth is extremely limited. The imbalance between oxygen supply and consumption in solid tumors is responsible for areas with mild (hypoxia) and severe (anoxia) oxygen deficiency. Especially hypoxia is strongly associated with radio-resistance but can also cause chemo-resistance.

To adapt to hypoxic conditions, cancer cells induce distinct changes in gene expression. This hypoxia-response program is controlled by oxygen-regulated transcription factors among which hypoxia-inducible factor 1 (HIF-1) is essential. Anticancer drug acriflavine is an inhibitor of HIF-1. This inhibition controls the adaption of cancer cells to hypoxia and increases their radio-sensitivity.

Mesoporous and non-mesoporous silica@ferrite nanostructures were loaded with acriflavine. The X-ray irradiation of the loaded nanostructures triggered not only the release of acriflavine inside cells, but also initiated an energy transfer from the nanostructures to surface adsorbed oxygen to generate singlet oxygen. The drug loaded mesoporous nanostructures showed an initial drug release before irradiation and a second one upon X-ray irradiation. The drug was primarily released upon irradiation in case of the non-mesoporous nanostructures. However, the drug loading capacity was less efficient for the non-mesoporous nanostructures. Both drug-loaded nanostructures proved to be very efficient in irradiated breast cancer tumor spheroids. In contrast, the damage towards non-tumorigenic breast spheroids was very limited because of the small number of nanostructures that entered these spheroids.

Biography:

Stefanie Klein actually works as a senior scientist at the Department of Chemistry and Pharmacy, Physical Chemistry I, University Erlangen-Nuremberg. During her PhD thesis, she optimized the application of silicon quantum dots as a transfecting agent for ABCB1-siRNA. During her post-doctoral research in La Plata, Argentina and Lubljana, Slovenia amine-terminated ultra-small and iron doped silicon nanoparticles for radiation therapy were developed. Her current research focused on ferrite, mesoporous silica ferrite and noble metal iron oxide nanoparticles to be used as synergistically X-ray dose enhancers and drug carriers in multimodal cancer therapy.

Investigating the Mechanics of Ti/TiB Interfaces at Multiple Scales

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Abstract

Titanium/titanium boride (Ti/TiB) composites are interesting technological materials with

prospective applications in the aerospace, automotive, and biomedical industries. However, not much has been studied about the failure mechanisms of these composites. This study thoroughly investigates the adhesion and strength of two well-known Ti/TiB interface variants formed during the production of Ti/TiB composites above and below 910 °C, respectively. The studies were carried out at room temperature using different theoretical methods at multiple scales, including density functional theory (DFT), molecular dynamics (MD), cohesive zone modeling (CZM), and the finite element method (FEM). First, we employed DFT to investigate the interfacial adhesion and strength and identify weak crystallographic planes. Then, MD simulations were utilized to study the misfit dislocation networks and derive interfacial CZMs for FEM modeling and simulation of composites. Our FEM simulations showed that the Ti/TiB interface has sufficient strength to transfer the shear load from Ti to TiB without debonding. The results have confirmed the same phenomenon observed in some experimental studies and interpreted this phenomenon from a multiscale point of view.

Biography:

Xiao is an associate professor in the Department of Mechanical Engineering at The University of Iowa. He graduated from Northwestern University with a Ph.D. degree in mechanical engineering. His original expertise lies in computational nanomechanics and materials science, especially multiscale modeling and simulations. Recently, he has extended his efforts to artificial intelligence (AI) and its applications in science and engineering problem-solving. His group's current research interests include machine-learning enhanced numerical modeling of composite materials, reinforcement learning for robotics and control, AI-powered design of reservoir systems for flood mitigation, data analytics of greenhouse gases emission, and quantum computing.

Multi-functional Cross-linked Carbon Nanotube/Hydrogel Nanocomposites for Sustainable Agriculture

Yunxiang Gao*

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Abstract

Low fertilizer utilization rate and frequent drought are two major challenges in the agricultural industry. Hydrogels with high water absorption capacity have been explored as novel materials for soil water retention to alleviate the impact of drought. However, hydrogels have low mechanical strength, and their swelling is dramatically suppressed in soil matrix, greatly inhibiting their effectiveness in water retention in soil. This project funded by the United States Department of Agriculture focuses on embedding cross-linked carbon nanotubes (XCNT) as nano-skeletons in hydrogels to significantly increase the mechanical strength of hydrogels and maximize their swelling spaces in the soil for multiple wetting-drying cycles. Simultaneously, the XCNT-hydrogel nanocomposite will function as a slow-releasing fertilizer. Urea is used as a model fertilizer to investigate the fertilizer loading capacity and releasing kinetics of the hydrogel nanocomposite. The XCNT-strengthened composites can also be modified for carbon capture and sequestration applications.

Biography:

Yunxiang Gao is an Assistant Professor of Chemistry at Prairie View A & M University in Prairie View, TX. He obtained his Ph. D. in Physical Chemistry from Ohio University in 2010. Gao's current research interests include composites, soft matter, and nanomaterials for sustainable agricultural and environmental applications, liquid crystalline elastomers (LCEs) for actuation and tissue engineering applications, as well as the mechanical properties of materials.

Design of Conductive PLA Composite *via* Secondary Polymer-induced Particle Aggregation

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Kyung Hyun Ahn

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Abstract

The performance of polymer composites is significantly determined by particle percolation formation. Particle dispersion is manipulated through the addition of secondary polymer with high affinity to particles in a composite and analyzed corresponding changes with electrical conductivity and mechanical moduli via scaling theory. A ternary composite of PLA, poly(caprolactone) (PCL) and carbon black (CB) exhibits the PCL-induced CB aggregation when the amount of the PCL is comparable to that of particles. Also, depending on mixing protocol, PLA/PCL/CB ternary composite further expand percolation structure, from CB aggregation in the form of a high aspect ratio and large aggregates to that with a high-order structure. Interestingly, when thermoplastic polyurethane (TPU) that has a higher affinity to CB than that of PCL is used as a secondary polymer, the composite forms noticeably larger-sized CB aggregates than those in PCL-added composite. Particle percolation of such a high-order structure improves the performance of composite like high storage modulus, high young's modulus, high dielectric loss, and negative-positive switching of dielectric constant at high frequency (~ 100 Hz). The secondary polymer-induced aggregation enhances the electrical percolation with a lower percolation threshold. The addition of secondary polymer makes the aggregates well dispersed, leading to a brittle-ductile transition and significant enhancement of ductility of PLA.

Biography:

Joung-Sook Hong is currently research professor in the institute of chemical processes at Seoul National University, Korea. She received Ph.D. degree from Seoul National University in 2005. Dr. Hong had been working as a post-doctoral research fellow at Korea University and University of Queensland, Australia between 2006 and 2008, and working at Samsung Cheil Industry from 2008 to 2009. After then, Dr. Hong moved to academia, worked as assistant professor in Department of Chemical Engineering at Soongsil University till 2015. Her research interests are particle dispersion in emulsion and blend composite and interfacial rheology of particulate interfacial layer.

Sustained Release of Curcumin Prodrug with Calcium Ions from Biomimetic Calcium Phosphate Bone Substitute Suppresses Osteosarcoma and Promotes Osteogenesis

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[2]Department of Biomedical Engineering, School of Materials Science and Engineering, South China University of Technology, Guangzhou, China

Abstract

Introduction: Osteosarcoma (OS) is the most common primary malignancy of bone. Standard OS treatment with surgery and chemotherapy has limitations in therapeutic outcome and side

effects. Biomimetic calcium phosphate (BioCaP) is bioactive material used as drug delivery carriers and bone substitute. Curcumin is an anticancer remedy with extensive biological functions but limited by poor solubility and bioavailability. Aim: to synthesize a soluble polyethylene glycol (PEG)-modified curcumin prodrug (mcur) incorporated BioCaP (mcur@BioCaP), and explore its crystal physiochemical property, drug release, the osteogenesis and anticancer efficacy. Materials and methods: mcur@BioCaP were synthesized at different mcur concentration through a well-established biomimetic mineralization method. The mcur@BioCaP crystal structure, morphology and crystalline phase was explored via scanning electron microscope and selected area (electron) diffraction. The subsequent anticancer, osteogenesis and anti-fibrosis efficacy were investigated in 143B OS cells, MC3T3-E1 pre-osteoblasts and L929 fibroblasts, respectively. Results: The mcur@BioCaP has a modified crystal size and shape and was homologous synthesized in a dose-dependent manner. The release of mcur from mcur@BioCaPs was pH-responsive, which sustained over at least 6 weeks and the mcur release was 2-fold higher in pH 6.5 than pH 7.4. Mcur@ BioCaPs significantly inhibited OS cells and fibroblasts viabilities rather than normal OB cells and promoted osteogenic differentiation. These biological effects of mcur@BioCaPs depended on the amount of released mcur and in synergy with effective Ca2+ release. Conclusion: mcur@BioCaP provides a multi-functional strategy for OS management with the function of bone regeneration, anticancer and anti-fibrosis.

Biography:

Yuelian Liu is an Associate Professor at the department of Oral Cells Biology, Academic Centre for Dentistry Amsterdam (ACTA), VU University and University of Amsterdam in the Netherlands. She received PhD degree in the Faculty of Medicine, University of Leiden, the Netherlands in 2003. She is a medical doctor by training and has obtained more than 20 international research grants and authored and co-authored more than 60 papers. She got more than 8 million Euro grants for her research projects and lectured nationally and internationally in the fields of biomaterials, bone tissue engineering as well as in biomedical technology.

Multiphoton Lithography of Organic Semiconductor Devices for 3D Printing of Flexible Electronic Circuits, Biosensors, and Bioelectronics

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Anto Sam Crosslee Louis Sam Titus
Sheereen Majd
Chandra Mohan

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Abstract

In recent years, 3D printing of electronics have received growing attention due to their potential applications in emerging fields such as nanoelectronics and nanophotonics. Multiphoton lithography (MPL) is considered the state-of-the-art amongst the microfabrication techniques with true 3D fabrication capability owing to its excellent level of spatial and temporal control. Here we introduce a homogenous and transparent photosensitive resin doped with an organic semiconductor material (OS) compatible with MPL process to fabricate variety of 3D OS composite microstructures (OSCMs) and microelectronic devices. Inclusion of 0.5 wt% OS in the resin enhanced the electrical conductivity of the composite polymer about 10 orders of magnitude and compared to other MPL-based methods, the resultant OSCMs offered high specific electrical conductivity. As a model protein, laminin was incorporated into these OSCMs without a significant loss of activity. The OSCMs were biocompatible and supported cell adhesion and growth. Glucose oxidase encapsulated OSCMs offered a highly sensitive glucose sensing platform with nearly

10-fold higher sensitivity compared to previous glucose biosensors. In addition, this biosensor exhibited excellent specificity and high reproducibility. Overall, these results demonstrate the great potential of these novel MPL-fabricated OSCM devices for a range of applications from flexible bioelectronics/biosensors, to nanoelectronics and organ-on-a-chip devices.

Biography:

Mohammad Reza Abidian is currently an Associate Professor at University of Houston in the Departments of Biomedical Engineering. He directs the laboratory Advanced Regenerative Biomaterials and Therapeutics for Neural Interfaces, which investigates at the interface of biomaterials and electronic devices to develop the next-generation of neural interfaces. His lab utilizes interdisciplinary material-based approaches, to develop micro/nano-scale technologies with the goal of triggered delivery of drugs and biomolecules to the nervous system, neurochemical sensing, neural recording, and neural tissue engineering. His research has been featured several times on the cover of frontier journals including Advanced Materials and Advanced Functional Materials. Prof. Abidian has received many awards and honors including Materials Research Society Silver Award, the University of Michigan Rackham Pre-Doctoral Fellowship, College of Engineering Student Distinguished Achievement Award, and Plenary Speaker in US-Turkey Advanced Study Institute on Healthcare Challenges. Prof. Abidian received his B.S. in Mechanical Engineering and M.S. in Biomedical Engineering from Amirkabir University of Technology (Tehran Polytechnic) and his Ph.D. in Biomedical Engineering from University of Michigan. He completed his postdoctoral training in the Center for Neural Communication Technology and Plastic Surgery Department at the University of Michigan.

Photothermal Effect and Cytotoxicity of CuS Nanoflowers Deposited over Folic Acid Conjugated Nanographene Oxide

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Abstract

Herein, we present the rational synthesis of a multimode photothermal agent, NGO-FACuS, for advancing photothermal therapy for cancer. The hierarchical architecture created in NGO-FA-CuS was attained by covalent conjugation of folic acid (FA) to nanographene oxide (NGO) through amide bonding, followed by hydrothermal assisted deposition of CuS nanoflowers. In this approach, instead of mere mixing or deposition, FA was covalently bonded to NGO, which permitted them to retain their intrinsic properties after binding and allowed them to access the resulting hybrid nanostructure. In this specifically designed photothermal agent, NGO-FA-CuS, each component has the explicit task of quencher, cancer cell-targeting moiety, and photothermal transduction agent for NGO, FA, and CuS, respectively. Prior to the grafting of FA molecules and deposition of CuS nanoflowers, sulfonic acid groups were introduced to NGO to render their stability under physiological conditions. By irradiation to a 980 nm laser, NGO-FA-CuS was able to attain the temperature of 63.1 °C within 5 min, which is far beyond the survival level of temperature for cancer cells. Therefore, the resulting temperature recorded for NGO-FA-CuS was sufficient to induce hyperthermia in cancer cells to cause their death. In contact with cancer cells,NGO-FA-CuS can lead to the rapid increase in temperature of their nucleus, destroy the genetic substances, and ultimately lead to exhaustive apoptosis under illumination to nearinfrared (NIR) laser. The

excellent photothermal efficiency of 46.2% under illumination to 980 nm laser and outstanding cytotoxicity against HeLa, SKOV3, and KB cells was attained with NGO-FA-CuS. Moreover, NGO-FA-CuS persists with exceptional photo-stability without photocorrosiveness. The photothermal effect of NGO-FA-CuS was dependent on the concentration and power density of the laser source. It was found that cytotoxicity over cancer cells was enhanced with an increase in the concentration of NGO-FA-CuS and incubation period.

Potential use of Carbon Nanotubes in Nanovaccine Development

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Abstract

Carbon nanotubes (CNTs) are cylindrical nanoparticles composed of single or multiple graphene layers. After purification with acids, CNTs can be functionalized with a diversity of molecules. Per se, CNTs are considered good adjuvants, and several studies have demonstrated that they promote a CD8+ T cell response. In our research group, we have been working on the development of two different types of nanovaccines using functionalized CNTs. In the first case, we functionalized CNTs with an 80 KDa peptide derived from 220 KDa lectin of Entamoeba histolytica (PL220-CNTs), the parasite that causes amoebiasis. In the second case, CNTs were functionalized with a synthetic peptide designed in silico from fucosyl transferase-4 sequence (Fut4-CNTs), an overexpressed enzyme in different types of cancer. The functionalized CNTs were characterized by Raman, FTIR, and HR-TEM. In both cases, functionalized CNTs demonstrated non-significant cytotoxicity on cell lines. Macrophages captured Fut4-CNTs and induced the presence of lysosomes. The immune response detected in BALB/c mice and hamsters immunized with PL220-CNTs showed low titers of antibodies, and the cytokine pattern of mice or hamster splenocytes revealed a Th17 cell response. The efficacy of the vaccination tested in the amebic liver abscess model in hamsters immunized with PL220-CNTs was 100%, which suggests that the immune response elicited by PL220-CNTs in animals protects them against infection. In the case of Fut4-CNTs, studies are on course to demonstrate their efficacy in an immune-competent model of cancer in C57BL/6 mice. These results suggest that CNTs have great potential for the development of nanovaccines.

Biography:

Blanca Estela Sánchez-Ramírez is a Professor at Chemical Sciences College at the Autonomous University of Chihuahua. She obtained her degree and M.Sc. in Immunology at the same institution. She received her Ph.D. in Experimental Pathology at CINVESTAV-IPN México in 1997. She is member of the Mexican National System of Researchers (Level II). Her main interest is toxicology, and research projects focus on i) the design of safety nanomaterials for biomedicine; ii) toxicological analysis in vivo and in vitro; and iii) exposure biomarkers in populations exposed to geological or anthropogenic contaminants such as lead, arsenic, or pesticides.

Plasmon-enhanced Optical Nanostructures Toward Biosensing in Home Care and Resource-limited Community

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Nianqiang Wu

University of Massachusetts Amherst, USA

Abstract

Acute infection diseases, such as Covid-19 and human immunodeficiency virus (HIV) demand rapid diagnosis in point-of-care (POC) settings, such as home, clinics, and resource-limited communities. Colorimetric paper lateral flow strip (PLFS) is one of the common tools for rapid detection. However, it suffers from lower detection sensitivity and lack of efficacy in antiinterfering effects, thus it hardly detects ultralow levels of biomolecules (~ sub-ng/mL to subfg/mL). To mitigate the limitations, we developed plasmon-enhanced optical PLFS for fluorescence and surface-enhanced Raman scattering (SERS) sensing with highly increased detection sensitivity. Plasmon-enhanced nanoparticle probes and nanoarray patterns, with intense local electromagnetic (EM) field and more "hot spots" can modulate optical processes to increase SERS and fluorescence signals. Also, the probe resonance wavelength can be tuned to drop into the biological transparency windows with minimized background noise from biological matrices to highly reduce the interference effect. The plasmon-enhanced SERS and fluorescence PLFSs can ultra-sensitively detect disease biomarker proteins and nucleic acids. With portable Raman and fluorescence reader development, the plasmon-enhanced optical PLFSs show the promise in home care and POC settings for disease diagnostics.

Biography:

Weirui Tan gained her PhD degree in Chemical Engineering from Monash University, Australia. She is now a postdoctoral research associate in Department of Chemical Engineering, University of Massachusetts Amherst, USA. Her research interests involve paper-based microfluidic devices for point-of-care detection of disease biomarkers, plasmon-enhanced nanostructure design, plasmon-enhanced biosensors.

Sustainable Epoxy-based Composite Materials with Bio-binder from Hydrothermal Liquefaction Processing of Microalgae

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[2]Department of Natural Resources and Environmental Design, College of Agriculture and Environmental Sciences, North Carolina Agricultural and Technical State University, Greensboro, NC, USA

Abstract

Epoxy resin, one of the most prevalent thermoset polymer matrices in polymer composite materials, is produced through precursors from the petroleum-based chemical industry. Concerns have been raised about the sustainability of epoxy resin system in recent years. In this research, we prepared a bio-binder from microalgae through hydrothermal liquefaction process where microalgae are directly decomposed in water at moderate temperature and pressure and generate a bio-binder that can be mixed with conventional epoxy resin. It is observed that epoxy/

bio-binder bicomponent system can be cured/solidified following regular epoxy curing cycle. By adding small amount, i.e. 2.5 wt.%, regular hardener/curing agent of epoxy resin, the mechanical performance of the epoxy/bio-binder system after curing can be significantly improved. Upon our research results, we enabled a game-changing epoxy resin system with a considerable proportion from sustainable resources.

Biography:

Lifeng Zhang is currently an associate professor of nanoengineering in North Carolina Agricultural and Technical State University and an adjunct professor in the University of North Carolina at Greensboro. He earned his Ph.D. degree in Fiber and Polymer Science from the University of California at Davis. Dr. Zhang's research interests lie in engineered materials at nanometer scale and environmental sustainability. Dr. Zhang has published over 100 peer-reviewed journal articles and 12 book chapters and received 5 U.S. patents.

20%-Efficient Cd(Se,Te) Solar Cells with Composition and Bandgap Gradient at the Front Interface

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Abstract

Bandgap gradient is a proven approach for improving the open-circuit voltages (VOCs) in Cu(In,Ga)Se2 and Cu(Zn,Sn)Se2 thin-film solar cells, but has not been realized in Cd(Se,Te) thin-film solar cells, a leading thin-film solar cell technology in the photovoltaic market. Recently, we demonstrated the realization of bandgap gradient in Cd(Se,Te) thin-film solar cells by introducing a Cd(O,S,Se,Te) region with the same crystal structure of the absorber region near the front junction.

To form this region via intermixing of multi layers, oxygen management is a key to avoiding the formation of undesirable Cd(S,Se) photo-inactive region at the front interface. The details of oxygen management during the deposition of each layer and post treatment: while both the CdS and CdSe layer depositions and the post CdCl2 treatment should be carried out in the presence of oxygen, the CdTe deposition should be conducted in an oxygen-free atmosphere to avoid over-oxidization to maximize the device performance. Inappropriate oxygen management may lead to low device performance due to the formation of a photo-inactive region and reduced absorber quality.

The introduction of the bandgap gradient with Cd(O,S,Se,Te) at the front interface reduces the hole density in the front junction region and introduces a small spike band alignment between this and absorber regions, effectively suppressing the nonradiative recombination therein and leading to improved VOCs in Cd(Se, Te) solar cells using commercial SnO2 buffers. A champion

device achieves an efficiency of 20.03% with a VOC of 0.863 V.

Biography:

Deng-Bing Li received his B.S. degree in School of materials science and engineering from Nanjing University of technology in China in 2009. He received his Ph.D. degree in Institute of Solid State Physics, Chinese Academy of Sciences in 2014. He worked in Wuhan National Laboratory for Optoelectronics (WNLO) at HUST of China as a postdoc researcher until 2016. After that, he joined Yanfa Yan's group and now works as a research assistant professor at the University of Toledo. His investigation interests focuses on stable and efficient inorganic photovoltaics.

Cellulosic Microfiber Extraction from Ecofriendly Fibers: Structure and Morphological Property Studies

K. Sankaranarayanasamy*
J. Ronald Aseer

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Abstract

In the present scenario, researchers are focusing towards lignocellulosic fiber materials due to their abundant availability in nature. Many researchers disseminated their results of fiber characterization using various chemical treatments. Several research groups are focusing their attention towards lignocellulosic fibers including jute, coir, abaca, banana fiber, etc. They can be a good substitute as they are available in fibrous form at low cost, low density, relatively high tensile, flexural modulus, and biodegradable. The abundance of natural fibers makes it a desirable substitute for synthetic fibers in composite industry. However, hydrophilic nature of these natural fibers reduces the compatibility with the polymers. This incompatibility resulting in poor mechanical properties of the composites. Chemical treatment of natural fibers reduces hydrophilic nature of the fibers which improves adhesion properties and also improves fiber structure and surface morphology. Bahunia racemosa fibers are used as replacement for synthetic fibers in epoxy composites for light weight material applications.

Recently, Bahunia Racemosa (BR) fibers were selected to extract cellulose microfibers through various chemical treatments. The composites reinforced with microfiber are developed by compression molding method with various proportions. Surface properties of the produced fibers are analyzed through microscopic techniques. The reinforcement of microcellulosic fiber extracted from lignocellulosic materials enhance the structural properties. The developed composites could be a feasible alternate for industrial and construction industries.

Nanoplasmonic Material Based Immunoassays for Personalized Immune Therapy

Pengyu Chen*

Materials Engineering, Department of Mechanical Engineering, Auburn University, Alabama, United States

Abstract

The study of immune functional responses is essential to understand the central role of the immune system in providing immunological host defense and its intercommunication with other systems. Cytokines are one of the key biomolecules acting as intercellular mediators and modulators to regulate the diverse functions in the immune response. Rapid and accurate quantification of

cytokine-based immune fingerprints plays a decisive role in effectively treating immune-related diseases especially at point-of-care, where an immediate decision on treatment is needed upon precise determination of individual patient's immune status. Derived from the emerging clinical demands, there is an urgent need for cytokine immunoassays that offers unprecedented sensor performance with high sensitivity, throughput, and multiplexing capability, as well as short turnaround time at low system complexity. In this talk, we will present several novel plasmonic nanomaterial based optofluidic cytokine biosensors for immune functional analysis from whole blood to single-cell level. The multi-scale research both experimentally and theoretically will bridge the gap in fundamental understanding of immune system and enhance the applicability, diagnosis and prediction power for immune diseases. The developed platforms would ultimately gear the biologists and clinicians with capability to real-time monitor the immune status of patients, a transformative achievement that has immense potential towards safe, effective, and personalized immune therapy.

Biography:

Pengyu Chen is currently Hugh and Leoda Francis Endowed Associate Professor in Materials Engineering at Auburn University. He received his B.S. in Materials Science and Engineering from Nanjing University in 2006 and obtained Ph.D. in nanomaterials and biophysics (2012) from Clemson University. He then worked as a research fellow in Mechanical Engineering at the University of Michigan and join Auburn in 2016. He was the recipients of Ginn Faculty Achievement Fellow, NIH Maximizing Investigators' Research Award and NSF CAREER Award. Chen's research focuses on advanced nanomaterial-based biosensors for biomarker detection, single cell secretion imaging, and cellular communication.

Development of Absorbable Bioactive Magnesium Metal Matrix Composite with High Shear Melt Processing for Bone Implants

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Pedram Sotoudeh Bagha[1]
Mehdi Razavi[1,2]

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[2]Department of Material Sciences and Engineering, University of Central Florida, Orlando, FL

Abstract

Absorbable magnesium bioactive composites are a promising new material for bone regeneration, which aims to repair damaged bones and be absorbed by the body fluid. In recent years, high-shear mixing has been demonstrated as an effective method for producing these metal matrix composites. This mixing method allows for the uniform distribution of bioactive ceramic components within the magnesium matrix, resulting in improved mechanical properties and biocompatibility. In this study, magnesium-bioactive ceramic composite was prepared with a novel high-shear mixer. The microstructure, corrosion, mechanical properties, and in vitro tests, including cell viability and osteogenic properties, were investigated. Then, the composite was implanted in the rat's femur to evaluate biocompatibility and osteoinductivity by histological analysis. Combining the benefits of bioceramics and high shear mixing, magnesium composites will show great potential for use in bone repair and regeneration, providing a promising solution for the fixation of bone fractures and treatment of bone-related disorders.

Biography:

Andrés Larraza discovered his passion for biomaterials while completing his undergraduate classwork at Cornell University (BS MSE '18). His intrigue for biomaterials research was refined after participating in cell biomechanics and metallurgical research. He is currently pursuing his Ph.D. in Materials Science and Engineering from the University of Central Florida in collaboration with the Biionix Cluster at the College of Medicine. His research focuses on improving the mechanical and *in situ* properties of magnesium-based composites for bone healing.

Biomaterial Synthesis and Robotic 3D printing in Architecture and Building

HyoungIn Choi*
Hwang Yi

Ajou University, South Korea

Abstract

Hydrogels are great sources of biodegradable building components, and they enable to fabricate ecological building through robotic additive building manufacturing (RABM, 3D printing) process. In this research, we present synthesizing major bio-ink hydrogels (cellulose, agar, gelatin and hyaluronic acid, etc.) with several nature-sourced materials/industrial byproducts for extrusion-based 3D printing work in a building scale. Rheological and mechanical properties of 40 hydrogel mixture samples have been investigated to identify their material characteristics and suitability in building construction. In an RABM environment with a six-axis robotic 3D printing system, we measured shear-thinning effect, material extrudability, workability (flowability), buildability, and interlayer bond strength. As a result of the material experiments, two types of hydrogel composite building applications were developed: (i) bio-brick and (ii) self-growing material design. Our findings suggest that cellulose and collagen mixtures generally show advantageous mechanical properties and those hydrogel-based materials qualify the primary constructability in RABM. Gelatin and hyaluronic acid exhibited promising performance of living cell viability in hydrogel-seed composites.

Biography:

HyoungIn Choi is a graduate researcher at the Architectural Research of Technology and Scientific Design (ARTS) Lab in Ajou University, South Korea. He focuses on biofabrication in Architecture by analyzing bio 3D printing performance.

Novel Silicon-titanium Diboride Micropatterned Substrates for 3D culture of Cancer Cells

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Maram Quttina[1]
Margaret Eisenbrandt[1]
Lewis Francis[2]
Tasneem Bawa-Khalfe[1]
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[2]Swansea University, UK

Abstract

Cell aggregates or spheroids are commonly used in vitro models for studying cancer biology. Unlike 2D models, 3D models allow interactions between cells and ECM and can mimic the in vivo microenvironment. Currently, to study the metastatic phenotype, cancer cells are cultured in conventional 3D systems like hanging-drop, ultra-low adhesion plates (ULP), and embedded matrices. These 3D culturing systems suffer from handling limitations, lack reproducibility in terms of aggregate dimensions and shape, and do not provide direct accessibility to probe surface properties. We have developed a novel micropatterned substrate fabricated with circle patterns of titanium di-boride on silicon (Si-TiB2) and validated it use for in vitro culture of endothelial cells and for culture of 3D aggregates of mesenchymal stem cells. Here, we introduce the novel micropatterned substrate for culturing ovarian cancer cells; the less aggressive OVCAR3 and highly aggressive SKOV3. OVAR3 with an epithelial phenotype failed to form aggregates and grew into monolayers, while SKOV3 with an intermediate epithelial-mesenchymal phenotype formed spheroid-like aggregates on the substrate. Cell viability, proliferation, and phenotypic features were all maintained on the micropatterned substrate, and response of cells to epigenetic drug SAHA was assessed. The Si-TiB2 substrate offers a low-cost, multi-testing platform for in vitro 3D culture, for studying tumorigenic potential of cancer cells and for anti-cancer drug screening.

Biography:

Fatima Merchant received her M.S. and Ph.D. degrees in biomedical engineering from The University of Texas at Austin. She is currently Professor and Chair at the Department of Engineering Technology, University of Houston. She has co-edited a book on Microscope Image Analysis, and authored numerous papers in the area of imaging and tissue engineering. She is on the Editorial Board of the journals Computers in Biology and Medicine, Biomedical Engineering Online, and Frontiers in Bioinformatics-Computational BioImaging. Dr. Merchant directs research at the Computational Biology and Medicine Laboratory that is supported by funding from the National Institutes of Health.

Multi-stimuli Responsive Pt(II) and Ir(III) Complexes

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Abstract

Transition-metal complexes that exhibit absorption and/or emission property changes upon external stimuli are intriguing sensing materials. Due to the possible intermolecular p-p , C-H...p, and/or metal-metal interactions, square-planar Pt(II) complexes and octahedral cationic iridium(III) complexes bearing p-conjugated ligands are emerging as new types of multi-stimuli responsive compounds. Upon formation of aggregates, applying pressure, exposure to organic vapors, altering temperatures, variation of pH, or encountering cations or anions, the intermolecular interactions or electronic structures of these complexes would change. Consequently, the absorption and/or emisssion energies and/or intensities would change, leading to aggregation induced/enhanced emission (AIE/AEE), piezochromic effect, vapochromic effect, or thermochromic effect. These effects have potential applications in imaging, pressure, temperature, or chemical sensing. In this talk, the AIE effect, piezochromic, vapochromic, or thermochromic effects of several Pt(II) and Ir(III) complexes will be reported. The impact of ligand substitutions on the sensing ability of some Pt(II) and Ir(III) complexes toward acid/base or metal cations will be discussed.

Biography:

Wenfang Sun is the Robert Ramsay Chair in the Department of Chemistry and Biochemistry at The University of Alabama (UA). Prior to joining UA, she was the James A. Meier Senior Professor at the North Dakota State University. She obtained her Ph.D. degree from the Institute of Photographic Chemistry, Chinese Academy of Sciences. She has published 145 peer-reviewed journal papers and obtained over $10,000,000 research grants. She received numerous awards including the NSF CAREER Award. Her research program focuses on the organic/organometallic nonlinear optical materials, organic/organometallic light emitting materials, photosensitizers for photodynamic therapy, and optical sensing materials.

The use of Distributed Piezoelectric Sensor for Measuring Dynamic Response of a Cracked Timoshenko Beam to Moving Harmonic Load

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Dang Xuan Trong[2]
Pham Van Kha[2]

[1] Institute of Mechanics, VAST, Vietnam
[2] HCMC Occupational Safety and Health Inspection and Training JSC, Vietnam

Abstract

The present report addresses frequency response analysis of cracked Timoshenko beam bonded with a piezoelectric layer as a distributed sensor under moving harmonic force. Using the double beam model, governing equations of a cracked beam integrated with the piezoelectric layer-sensor are derived with Hamilton's principle and solved by analytical method in the frequency domain. First, changes in the modal parameters such as natural frequencies, mode shapes and so-called modal sensor charge of the integrated beam due to crack are investigated. Then, the beam midspan deflection and sensor output charge acknowledged respectively as mechanical and electrical frequency responses to moving harmonic load are examined versus crack and load parameters. Numerical analysis with the so-called spectral assurance criterion demonstrates that the mechanical and electrical frequency responses are spectrally identical and robustly sensitive to crack. So that the modal sensor charge and spectral assurance criterion that can be obtained from the electrical frequency response measured by a distributed sensor provide novel and promising indicators for crack identification in beam structures using moving harmonic excitation.

Biography:

Nguyen Tien Khiem, Doctor of Science (1992, Kiev, Ukraine), Professor (2006, Vietnam Academy of Science and Technology – VAST), born in 1955, Bac Ninh, Vietnam. He was Director of Institute of Mechanics, VAST (2002-2008) and Chairman of Director Board of the Institute of Mechanics and Environment Engineering , Vietnam Union for Science and Technology Associations (VUSTA) from 2010; President of Vietnam Association for Mechanics from 2017. He published more than 80 research papers on Dynamics of Structures and Structural Health Monitoring, 5 monographies on the fields. His present research field is the application of smart materials for structural health monitoring.

Experimental Investigation of the Mechanical Properties of Aluminum Crumpled Metamaterials

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Abstract

Metamaterials have received considerable attention in recent decades because their mechanical response can be manipulated depending on the design of their structures. In particular, mechanical metamaterials have been shown to possess superior properties such as high strength, high stiffness, and light weight, compared to conventional materials. A typical method used to manufacture metamaterials is 3D printing, which allows the generation of a highly ordered cell structure. Therefore, imperfections in the structure due to the manufacturing process or environmental conditions may affect the expected mechanical response. Recently, crumpled materials have been considered as mechanical metamaterials with low sensitivity to defects because a simple way to manufacture them is through the process of crumpling a sheet (2D geometry) to create a 3D geometry with a random structure. It has been reported that crumpled mechanical metamaterials exhibit peculiar mechanical properties such as low density and high energy absorption, even for certain relative densities a Negative Poisson's Ratio (NPR). However, Poisson's Ratio was estimated using an equation for isotropic solid materials as a function of Young's modulus and shear modulus. Therefore, in this talk we report the findings of an experimental study of the elastic properties of crumpled mechanical metamaterials, with greater emphasis on Poisson's Ratio, supported by the Digital Image Correlation (DIC) technique.

Biography:

Luis A. Alcaraz-Caracheo received his B.Sc. and M.Sc. degrees in mechanical engineering from the Tecnológico Nacional de México en Celaya, México, and Ph.D. degree in mechanical engineering from the Instituto Politécnico Nacional, México. He is currently a full-time professor in the Department of Mechatronics Engineering, Tecnológico Nacional de México en Celaya. He is also a member of the National Network of Researchers in México. His research interests include machine design, metamaterials, crumpled materials, polymeric thin films and finite element simulation.

Development of Smart "Skin-like" Textile Fabric for Personal Comfort and Protection

Jintu Fan*

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Abstract

Acting as a "second skin", clothing plays an indispensable role in providing comfort and protection in the wide range of environmental conditions. However, Comfort and protection are often competing requirements and difficult to improve simultaneously. Moisture management fabrics that promote wicking of sweat away from skin are commercially available, but such fabrics are not repellent to external liquid water. On the other hand, commercially available breathable fabrics, although water repellent, can only allow a moisture vapor transmission rate up to ~460 g/m2 per hour, which is far less than the sweating rate of an average person under moderate exercise (~1000 g/m2 per hour).

By mimicking the exceptional one-way liquid transport property of human skin, we developed a "skin-like" fabric, which enabled continuous one-way liquid flow through spatially distributed channels acting like "sweating glands" yet repels external liquid contaminants. More recently, by grafting a temperature responsive polymer onto the skin-like fabric, we further achieved temperature-responsive regulation of liquid sweat transport and water repellency depending on the surrounding temperature. As the temperature increases, the wettability gradient in the spatially distributed channels (acting like "sweat glands") increases, promoting sweat transport and evaporative heat dissipation. As the temperature decreases, on the other hand, the wettability gradient diminishes, reducing liquid transport and evaporative heat loss, thereby promoting heat retention. During this presentation, the fabrication process. performance and potential applications of the fabric will be reported and discussed in detail.

Biography:

Jintu Fan is currently Lee Family Professor in Textiles Technologies and Chair Professor of Fiber Science and Apparel Engineering at Hong Kong Polytechnic University (PolyU). Prof. Fan holds PhD from Leeds University, UK and BSc from Donghua University, Shanghai, China. He served as Head of Institute of Textiles and Clothing at PolyU from 2018-2022 and Chair of Department of Fiber Science & Apparel Design at Cornell university from 2012-2018. He is honored with some most prestigious awards in the textile field including Warner Memorial Medal, Honorary Fellow of Textile Institute and Distinguished Achievement Award of The Fiber Society.

Application of Graphitic Carbon Nitride Material as Photocatalysts to Organic Redox Reactions

Yingchun Li*
Emily Mcguire
Makobi Chukwuemeka Okolie

Prairie View A&M University, USA

Abstract

Graphitic carbon nitride (g-C3N4) has attracted great attentions of material scientists due to its interesting layered graphite-like structure and expected unique electronic properties for applications in various fields, such as hard material, semiconductor, catalysts and even as disinfectants. Since the discovery of its photocatalytic capability of splitting water under visible light, most research have focused on its activity enhancement. It has been well documented that g-C3N4 based material catalyze degradation of organic pollutants in water under visible light. One kind of such pollutants are azo dyes from fabric-dying industry. The degradation of azo compounds

is usually monitored by color disappearance which is currently attributed to oxidation by oxygen in the air catalyzed by g-C3N4 under visible light. Our experimental results revealed that the initial products in the degradation of azo dyes are amines. The color disappearance in the initial stage of degradation process is due to reducing cleavage of nitrogen-to-nitrogen double bond to amines. The reductant should be the hydrogen gas from the water splitting process catalyzed by g-C3N4 under visible light. Based on this photocatalytic mechanism, we developed an efficient method to reduce azo compounds to amines at room temperature in water under visible light with g-C3N4 as the catalyst. The photocatalytic activity of g-C3N4 in this reduction exhibited great dependence on the temperature at which the catalyst is prepared. The potential application of g-C3N4 as photocatalysts to other organic redox reactions has been actively explored in our research.

Biography

Yingchun Li graduated as Ph.D majored in chemistry from University of Houston in the year of 2000. He has shown expertise in traditional organic synthesis, enzyme inhibitor design and activity assessment, resolution of racemic mixture with enzymes. He is currently an assistant professor in the Department of Chemistry in Prairie View A&M University with research focused on mechanism-based development of photocatalysts for application to organic reactions

Characterization of Carbon Doped Silicon Oxide Thin Films after Etching in CF4 Plasma

Seonhee Jang*
Rajib Chowdhury
Thomas Poche

Department of Mechanical Engineering, University of Louisiana at Lafayette, USA

Abstract

As integrated circuits (ICs) continue to shrink, their performance is limited due to a RC (resistance × capacitance) delay, increased power dissipation, and increased crosstalk in multilevel interconnects. To reduce the resistance, copper (Cu) has replaced aluminum (Al) because the resistivity of Cu (1.68 μΩ·cm) shows a smaller than that of Al (2.65 μΩ·cm). To decrease the capacitance, a low dielectric constant (low-k, k<4.0) thin films have replaced traditional silicon oxide (SiO2, k~4.2) for intermetal dielectric (IMD) layers. For interconnects, the dielectric patterning followed by Cu filling, so-called 'damascene' process is required. The dielectric films should undergo plasma etching and it is important to reduce the plasma induced damage and keep the dielectric properties. In this study, as low-k thin films, carbon doped silicon oxides were prepared by plasma-enhanced chemical vapor deposition (PECVD) of tetrakis (trimethylsilyloxy)silane precursor. The material properties such as refractive index, contact angle, surface roughness, k-value, and hardness/elastic modulus were characterized depending on the deposition plasma powers. The films were then etched in CF4 plasma using an inductively coupled plasma-reactive ion etching (ICP-RIE) method. Surface roughness and hydrophilicity of the film were observed depending on plasma etching conditions. Using Fourier transform infrared (FTIR) spectroscopy and X-ray photoelectron spectroscopy (XPS), the chemical structure and elemental composition of the as-deposited film were compared with those of the film after plasma etching. From current-voltage (I–V) and capacitance-voltage (C–V) characteristics, electrical properties including the k-values and leakage current densities were examined for the electrical stability after plasma etching.

Biography

Seonhee Jang is an assistant professor of the Department of Mechanical Engineering at University of Louisiana at Lafayette. She received her PhD in Materials Science and Engineering from North Carolina State University in 2007. Before she joined University of Louisiana at Lafayette, she worked as a principal researcher at Samsung Electro-Mechanics from 2007 to 2015. Her research focuses on advanced semiconductor materials, processing, and manufacturing, semiconductor packaging, printed/flexible electronics, and plasma processing.

Compartmentalized Systems for *In-situ* Formation of Antibacterial Thiosulfinates

Kašpar Ondřej*
Lucie Mašková
Petra Janská
Eliška Večerníková
Viola Tokárová

Department of Chemical Engineering, University of Chemistry and Technology Prague, Czech Republic

Abstract

Garlic has been well-known for its healing properties since the dawn of humankind. These properties are mainly attributed to the volatile thiosulfinate of typical garlic odor - allicin. Allicin is enzymatically produced from its precursor when the internal cell structure is compromised and, for a limited time, provides an effective form of protection.

Allicin's high instability, which is simultaneously required for its persistent biological activity, has always been considered a critical weakness and prevented further practical use. Controlled in-situ synthesis of such reactive compounds from their precursors near a target site is a feasible way to (re)utilize their full potential. This approach can significantly extend the palette of currently used active compounds in various areas of human life, overcoming the lack of antibiotics in the future and issues associated with their gradual accumulation in the environment. Moreover, the fact that allicin-like compounds (in contrast to other antibiotics) are volatile means that the physical presence of the carrier in the vicinity of the target site is not essential.

In our work, encapsulation techniques such as ionic gelation, spray drying, film casting, and 3D bioprinting were employed to prepare compartmentalized carriers and structured materials where enzyme and substrate(s) are present but physically separated. Additionally, humidity and temperature-controlled triggers were incorporated, allowing allicin in-situ formation only when particular environmental conditions are satisfied. We believe that such a nature-proved sustainable concept can contribute to the reduction of the annually increasing number of bacterial infections caused by multi-drug-resistant bacteria.

Biography:

I am an assistant professor at the University of Chemistry and Technology, Prague (the Department of Chemical Engineering). During my post-doc at McGill University, I investigated the use of biological agents (bacteria, fungi) to solve complex mathematical problems. After two years, I returned to my alma mater and co-founded the Laboratory of Biomimetic Engineering at UCT Prague in 2017. The main topics of our research are biomimetics, mimicking natural antibacterial systems using a wide variety of encapsulation methods, non-enzymatic cell harvesting using hierarchically structured surfaces and microfluidic preparation of bioinspired nanoparticles.

Composite Materials to Combat Antimicrobial Resistance for Cutaneous Application

Viola Tokárová*
Lucie Mašková
Lenka Závišová
Lucie Večerková
Petra Janská
Kašpar Ondřej

Department of Chemical Engineering, University of Chemistry and Technology Prague, Czech Republic

Abstract

Human skin is facing pathogen transmission every day through contact with different surfaces, in the form of aerosols or our surroundings such as contaminated water streams and soils. Infections are common complications of the wound healing process, which are most dangerous in medical facilities (with a higher concentration of MRSA strain) and for elderly people. This problem is getting more and more challenging due to the gradually increased number of resistant microbes to ordinary antibiotics. Therefore, new strategies and materials need to be developed to combat the microbial-resistant crisis.

In this work, we present materials with strong antimicrobial effect and low or no antimicrobial resistance to be developed. One such material in the form of composite polymer thin films and micro-particles is using precursors of antimicrobial agent allicin, inactive alliin and alliinase, that are naturally present in allium plants (such as garlic, leek or onion). The external trigger(s) such as level of humidity, temperature or pH could initiate enzymatic reaction and produce allicin on demand. Allicin is a very effective antimicrobial agent applied to wide range of microbes (bacteria, fungi and viruses). But it's volatile nature and short half-time makes it almost impossible for bacteria to develop resistance to it. We will present materials for skin applications in a form of hand sanitizers with prolonged effect as well as wound healing patches.

Biography:

Viola Tokarova is an Assistant Professor at the Department of Chemical Engineering, University of Chemistry and Technology, Prague. Viola obtained her doctoral degree in 2014 at the same department and then spent two years (2015-2017) at McGill University (Laboratory of biological microfluidics) where she studied microbial behavior in confined spaces with a focus on biocomputations (SSP problems) and biosimulations (traffic problems). Viola together with her colleague Dr. Ondrej Kaspar established the Laboratory of Biomimetic Engineering in 2017, research group aiming to design, syntheses, and characterization of functional materials with a main application being pharma industry.

Uranium-Zirconium Hydride Nuclear Fuel Performance in the Marvel Microreactor

Jordan A. Evans*
Ryan T. Sweet
Dennis D. Keiser
Yasir Arafat

Idaho National Laboratory, USA

Abstract

The Microreactor Applications Research Validation and EvaLuation (MARVEL) project is producing a high temperature, unpressurized, liquid metal-cooled nuclear reactor research and development test bed at the Idaho National Laboratory (INL) to ultimately improve integration of microreactors to end-user applications. This ambitious effort seeks to design, license, construct, test, and operate the reactor within five years. Additionally, the MARVEL reactor will be integrated with the world's first net-zero microgrid at INL in the next two years, in sync with other emission-free technologies like wind and solar power. In this presentation, Dr. Evans will provide an overview of the MARVEL reactor design with a focus on the selected fuel system: 304 stainless steel-clad U-ZrHx. Fuel element thermal stability, hydrogen evolution, and radiation effects will be discussed in detail. Though this fuel system is already commercially available and licensed by the United States Nuclear Regulatory Commission for use in a variety of water-cooled research reactors, fuel

performance analysis in the MARVEL reactor is necessary to show that its behavior under MARVEL conditions is bounded by the current licensing basis. Finally, fuel element performance analysis under the reactor's most severe and unprotected "beyond design basis accident" scenario will be presented whereby the fuel system's thermophysical integrity remains stable and predictable passively, i.e., with extended complete failure of all on-site safety systems and without human intervention.

Biography:

Jordan Evans graduated from Texas A&M University with a B.S. and M.S. in Nuclear Engineering, and Ph.D. in Materials Science and Engineering. Prior to joining Idaho National Laboratory as a nuclear materials scientist, Dr. Evans held the Glenn T. Seaborg Distinguished Postdoctoral Fellowship at Los Alamos National Laboratory. His research interests include nuclear materials science and engineering; design of nuclear fuel, cladding, and materials for use in extreme conditions and advanced nuclear reactor systems; development of high performance textured and nano-strengthened materials; and analysis of nuclear materials through a variety of diffraction, microscopy, spectroscopy, ultrasonic, and probe/indentation techniques.

Liquid Metal and Molten: Their Corrosion and Chemistry

Jinsuo Zhang

Nuclear Engineering Program, Department of Mechanical Engineering, Virginia Tech

Abstract:

Liquid metal and molten salt have broad applications in high-temperature energy systems such energy thermal storage, concentrated solar energy and advanced nuclear energy. The liquid metal (e.g. liquid lead)-cooled fast reactor (LFR) and molten salt reactor are two Gen. IV reactor concepts. Both liquid lead and molten salt are corrosive to most of the structural materials. However, their corrosion mechanisms are different because of their unique chemistries. For example, most of the oxides of steel components are stable in liquid lead but unstable in molten salt. The seminar will discuss their corrosion mechanisms and the corrosion process, and then will analyze the liquid/solid interfacial interactions including material dissolution, oxidation and liquid penetration which results in material corrosion and degradation. The seminar will also discuss how to mitigate the corrosion by controlling the liquid chemistry through active oxygen control for liquid lead, redox potential control for molten salt and salt purification.

Biography:

J. Zhang has been a professor of the Nuclear Engineering program in Virginia Polytechnic Institute and State University (known as Virginia Tech) since January 2017. He was an associate professor at The Ohio State University (OSU) through Sept. 2012 to Dec. 2016. Before that, Prof. Zhang had been a staff scientist of Los Alamos National Laboratory (LANL) through 2004 to 2012, and a postdoc research associate through 2001 to 2004. Prof. Zhang focuses on studies of advanced used nuclear fuel reprocessing, material compatibility and materials corrosion in advanced and current nuclear reactors.

Assessment of Irradiation Hardening based on Microstructure Features

Ghiath Monnet

EDG R&D, MMC, Moret-Loing et Orvanne, France

Abstract

Instead of the widely used empirical predictions of irradiation hardening in low alloy steels, it is shown that the mechanical behavior can be predicted using multiscale modeling of the physical mechanisms involved in plastic deformation: the Hall-Petch effect, the forest strengthening and the lattice friction. The physically based assessment of lattice friction allows for the determination of the flow stress at low and high temperature deformation as a function of strain rate. The model parameters reduce to the microstructure characteristics of the steel: the grain size, the dislocation density, the size and the density of solute clusters forming under neutron irradiation. The stress-strain tensile curves are thus predicted with no adjustable parameters. In the talk, the sensitivity to the different microstructure features is discussed. It is shown that, unlike the grain size, the dislocation density has a significant effect on irradiation hardening. Predictions of the model are compared with many experimental tensile tests, performed under different conditions: different initial yield stress, different temperature and strain rates and different irradiation microstructures. The comparison confirms the close agreement in all the investigated cases.

Examination of Ion Irradiation Induced Defects in 6061 Aluminum Alloy

Ahmad Azzam*
Bénédicte Kapusta

CEA Paris Saclay, France

Abstract

The 6061 alloy is a key material for the manufacturing of the nuclear research reactors (NRR). This material possesses excellent mechanical properties at the operating temperature (between 70-90°C), good corrosion resistance and low neutron absorption. The void swelling due to the rapid neutrons (E>0.1 MeV) is one of the major problemsthat causes a degradation of mechanical properties in the 6061 alloy. This phenomenon has been the subject of very few studies. In this paper, we perform Si ions irradiation to reproduce the irradiation defects in 6061 alloy. Two metallurgical states (oil and water quenched alloy) are investigated. The effect of the cooling rate on the microstructure is firstly studied. The correlation between the microstructure and the swelling behavior is also investigated. A study at a different scale is carried out by transmission electron microscope (TEM) and by atom probe tomography. We show that the microstructure is mainly consisting of needle shaped (β''+L) precipitates and small Guinier-Preston zones GPZ (<5 nm). After irradiation, an evolution of the nano-precipitates composition is observed. The two elements Cr and Zn are found to strongly partition to the nano-precipitates. Also, we highlight that swelling strongly depends on the microstructure. TEM analyses show that nano-recipitates can act as preferential sites for cavities. TEM lamellae prepared by focused ion beam allow us to determine the evolution of swelling as a function of depth. The maximum swelling is about 0,28 ± 0,09 % and 0.14 ± 0.04 % in the oil and water quenched samples respectively. Finally, the threshold value of swelling is estimated at 18 dpa.

Biography:

I have a PhD in material science from the University of Rouen (France). I joined the CEA Paris Saclay in June 2021 as a postdoc researcher. My research works at CEA are focused on studying the irradiation defects in 6061 aluminum alloy that are used in the research reactors. As a microscopist I am in charge to investigate the microstructure and irradiation effects at a different scales and down to atomic scale.

Multiphoton Lithography of Organic Semiconductor Devices for 3D Printing of Flexible Electronic Circuits, Biosensors, and Bioelectronics

Mohammad Reza Abidian*

Omid Dadras-Toussi
Milad Khorrami
Anto Sam Crosslee Louis Sam Titus
Sheereen Majd
Chandra Mohan

Department of Biomedical Engineering, University of Houston, USA

Abstract

In recent years, 3D printing of electronics have received growing attention due to their potential applications in emerging fields such as nanoelectronics and nanophotonics. Multiphoton lithography (MPL) is considered the state-of-the-art amongst the microfabrication techniques with true 3D fabrication capability owing to its excellent level of spatial and temporal control. Here we introduce a homogenous and transparent photosensitive resin doped with an organic semiconductor material (OS) compatible with MPL process to fabricate variety of 3D OS composite microstructures (OSCMs) and microelectronic devices. Inclusion of 0.5 wt% OS in the resin enhanced the electrical conductivity of the composite polymer about 10 orders of magnitude and compared to other MPL-based methods, the resultant OSCMs offered high specific electrical conductivity. As a model protein, laminin was incorporated into these OSCMs without a significant loss of activity. The OSCMs were biocompatible and supported cell adhesion and growth. Glucose oxidase encapsulated OSCMs offered a highly sensitive glucose sensing platform with nearly 10-fold higher sensitivity compared to previous glucose biosensors. In addition, this biosensor exhibited excellent specificity and high reproducibility. Overall, these results demonstrate the great potential of these novel MPL-fabricated OSCM devices for a range of applications from flexible bioelectronics/biosensors, to nanoelectronics and organ-on-a-chip devices.

Biography:

Mohammad Reza Abidian is currently an Associate Professor at University of Houston in the Departments of Biomedical Engineering. He directs the laboratory Advanced Regenerative Biomaterials and Therapeutics for Neural Interfaces, which investigates at the interface of biomaterials and electronic devices to develop the next-generation of neural interfaces. His lab utilizes interdisciplinary material-based approaches, to develop micro/nano-scale technologies with the goal of triggered delivery of drugs and biomolecules to the nervous system, neurochemical sensing, neural recording, and neural tissue engineering. His research has been featured several times on the cover of frontier journals including Advanced Materials and Advanced Functional Materials. Prof. Abidian has received many awards and honors including Materials Research Society Silver Award, the University of Michigan Rackham Pre-Doctoral Fellowship, College of Engineering Student Distinguished Achievement Award, and Plenary Speaker in US-Turkey Advanced Study Institute on Healthcare Challenges. Prof. Abidian received his B.S. in Mechanical Engineering and M.S. in Biomedical Engineering from Amirkabir University of Technology (Tehran Polytechnic) and his Ph.D. in Biomedical Engineering from University of Michigan. He completed his postdoctoral training in the Center for Neural Communication Technology and Plastic Surgery Department at the University of Michigan.

Dielectric Characterization of Multi-phase Cementitious Composites at 10GHz Frequency

Tzuyang Yu*

Department of Civil and Environmental Engineering, University of Massachusetts Lowell, Lowell, Massachusetts, U.S.A.

Abstract

Electromagnetic (EM) properties of construction materials are important for the use of EM

sensors (e.g., microwave, radar) on critical civil infrastructure systems for condition assessment and structural health monitoring (SHM). Among existing construction materials, Portland cement concrete (PCC) is the most widely used engineering material in modern civilizations. PCC is a multi-phase cementitious composite. It is also paramagnetic, making its electrical or dielectric property (dielectric constant and loss factor) essential for the use of EM sensors in civil engineering. In this talk, a non-contact synthetic aperture radar (SAR) method is presented for the dielectric characterization of PCC in the microwave frequency range. A 10GHz carrier frequency, non-contact SAR sensor was used on PCC samples containing various level of moisture for remotely extracting dielectric constant of the samples. A range of 0.4~0.6 for the water-to-cement (w/c) ratio was considered in the design of PCC samples. Various moisture levels inside PCC samples, ranging from complete saturation to oven-dried, were created and used in this investigation. From our experimental data, it was found that the remotely collected SAR images of PCC samples can reveal the effective dielectric constant of multi-phase cementitious composites like PCC. The non-contact feature also allows engineers to deal with rough surface condition of samples, saving time and effort in sample preparation.

Biography:

Tzuyang Yu is a full professor (Ph.D., MIT) in Structural Engineering in the Department of Civil and Environmental Engineering at the University of Massachusetts Lowell. He specializes in structural materials and remote electromagnetic imaging of concrete structures. His research has been sponsored by NIST, AFRL, NSF, DOE, U.S.DOT, UMass S&T Office, AFFOA, and NextFlex. His research is currently supported by the U.S.DOT through the University Transportation Center Transportation Infrastructure Durability Center since 2018, and the NSF CPS program. He is an author of two books, three book chapters, and more than 100 journal and conference papers.

Machine Learning Approach for Studying Brittle Fracture in Polycrystalline Graphene

Alireza Tabarraei*
Mohan Elapolou

University of North Carolina at Charlotte, U.S.A.

Abstract

Graphene is a two-dimensional material with exceptional mechanical properties, including high strength, stiffness, and toughness. However, graphene is susceptibility to brittle fracture. Polycrystalline graphene, in which the material consists of multiple crystals with different orientations, exhibits even more complex fracture behavior due to the interaction between the grains. Studying the fracture properties of polycrystalline graphene is crucial for understanding its mechanical behavior and improving its practical applications. Moreover, the fracture behavior of polycrystalline graphene can provide insights into the fundamental mechanisms governing fracture in two-dimensional materials. As graphene is a prototype of two-dimensional materials, its fracture behavior can shed light on the fracture behavior of other two-dimensional materials with potential applications in electronics, energy, and other fields.

Molecular dynamics simulations have been widely used to study the fracture of materials, including graphene. However, these simulations are computationally expensive and time-consuming. In recent years, machine learning (ML) has emerged as a powerful tool to accelerate materials simulations. This study presents a machine learning approach for predicting brittle fracture in polycrystalline graphene under tensile loading. The proposed model employs a combination of convolutional neural network, bidirectional recurrent neural network, and fully connected layer to process both spatial and sequential features. The spatial features are grain orientations and location of grain boundaries whereas sequential features are associated with the crack growth. Molecular dynamics modeling is used to obtain the fracture process in pre-cracked polycrystalline

graphene sheet subjected to tensile loading. The data from molecular dynamic simulations along with novel image-processing techniques are used to prepare the data set required to train and test the proposed model. Crack growth obtained from the machine learning model shows close agreement with the molecular dynamic simulations. The proposed machine learning model predicts crack growth instantaneously avoiding the computational costs associated with molecular dynamics simulations.

Biography:

Tabarraei is an Associate professor at the University of North Carolina at Charlotte. He serves as the Director of Multiscale Material Modeling Lab at the Department of Mechanical Engineering and Engineering Science. With a Ph.D. in Structural Mechanics from UC Davis and postdoctoral experience at Northwestern University, Dr. Tabarraei's research focuses on unraveling the mechanical response of materials and structures through multiscale computational modeling and simulations. Utilizing cutting-edge tools such as molecular dynamics, finite elements, and machine learning, he has published over 60 articles in top journals and conference proceedings.

Direct Inverse Analysis of Machine Learning Model for Molecular, Material, and Process Designs

Hiromasa Kaneko*

Department of Applied Chemistry, Meiji University, Japan

Abstract

In molecular, material, and process designs, it is important to perform inverse analysis of mathematical models constructed with machine learning using target values of the properties and activities. While many approaches actually employ a pseudo-inverse analysis, Gaussian mixture regression (GMR) can achieve direct inverse analysis. Although Bayesian optimization (BO) is an effective tool, BO merely selects a candidate from a limited number of samples, and the samples do not necessarily contain the optimal solution. Furthermore, because upper and lower limits are set for explanatory variables x, it is not possible to obtain solutions that go beyond these limits. To solve these issues, direct inverse analysis of the GMR model was proposed because GMR models can estimate x values directly based on the target values of objective variables y (Chemom. Intell. Lab. Syst. (2021) 104226). The proposed method could allow the target y value to be achieved with a dramatically smaller number of experiments than by BO, especially when the number of x-variables was large. Furthermore, the proposed direct inverse analysis was applied to time-series data analysis and process design and could design both the batch time and the process variable profiles (x) to ensure that the endpoints (y), such as the product quality and the material properties, possess the target values following a batch process (Comput. Chem. Eng. (2022) 108072).

Application of Graphitic Carbon Nitride Material as Photocatalysts to Organic Redox Reactions

Yingchun Li[1*]
Emily Mcguire[2]
Makobi Chukwuemeka Okolie[3]

Prairie View A&M University, USA

Abstract

Graphitic carbon nitride (g-C3N4) has attracted great attentions of material scientists due

to its interesting, layered graphite-like structure and expected unique electronic properties for applications in various fields, such as hard material, semiconductor, catalysts and even as disinfectants. Since the discovery of its photocatalytic capability of splitting water under visible light, most research have focused on its activity enhancement. It has been well documented that g-C3N4 based material catalyze degradation of organic pollutants in water under visible light. One kind of such pollutants are azo dyes from fabric-dying industry. The degradation of azo compounds is usually monitored by color disappearance which is currently attributed to oxidation by oxygen in the air catalyzed by g-C3N4 under visible light. Our experimental results revealed that the initial products in the degradation of azo dyes are amines. The color disappearance in the initial stage of degradation process is due to reducing cleavage of nitrogen-to-nitrogen double bond to amines. The reductant should be the hydrogen gas from the water splitting process catalyzed by g-C3N4 under visible light. Based on this photocatalytic mechanism, we developed an efficient method to reduce azo compounds to amines at room temperature in water under visible light with g-C3N4 as the catalyst. The photocatalytic activity of g-C3N4 in this reduction exhibited great dependence on the temperature at which the catalyst is prepared. The potential application of g-C3N4 as photocatalysts to other organic redox reactions has been actively explored in our research.

Biography

Yingchun Li graduated as Ph.D majored in chemistry from University of Houston in the year of 2000. He has shown expertise in traditional organic synthesis, enzyme inhibitor design and activity assessment, resolution of racemic mixture with enzymes. He is currently an assistant professor in the Department of Chemistry in Prairie View A&M University with research focused on mechanism-based development of photocatalysts for application to organic reactions.

Effects of Graphene Oxide on Catalytic Activities of Nano-scaled Co and Ni Promoted MoS_2 Catalysts in the HDS of Dibenzothiophene

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Daniel Ramirez[1]
Veronica Padillia[2]
Ramiro Gonzalez[2]
Mataz Alcoutlabi[2]

[1]Department of Chemistry the University of Texas Rio Grande Valley, University Blvd Brownsville TX, USA
[2]Department of Mechanical Engineering, the University of Texas Rio Grande Valley, University Dr. Edinburg TX, USA

Abstract

The hydrodesulphurization (HDS) reaction is used in fuel processing to remove sulfur from crude oil. The research in this field has recently focused on unsupported Ni and Co-promoted MoS2 for the HDS reaction. In the present work, graphene oxide (GO) supported NiMoS2 and CoMoS2 catalysts were prepared and used for the HDS reaction of DBT in decahydronaphthalene. The effects of carbon-based supports on the catalytic activity and possibly on the HDS mechanism of Co and Ni promoted MoS2 was investigated The catalysts were synthesized as pure Ni, Co promoted MoS2 or with 4, 17 and 34 mmol supported on GO. The synthesized catalysts were characterized using SEM, XPS, BET (surface area and porosity), as well as XRD. The catalysts' ability to remove DBT from solution was followed by using GC-MS while the reaction products were identified as tetrahydro-dibenzothiophene, biphenyl, and cyclohexyl benzyl. The reaction was observed to follow zero order kinetics for both Ni and Co based catalysts. Intriguingly, the catalytic activity of NiMoS2 was enhanced after being supported on GO; while the catalytic activity of CoMoS2 was decreased after supporting on GO. The highest rate constant values observed for both NiMoS2 and CoMoS2 were both the same, i.e., 7.9 x10-6 molL-1s-1. The catalytic mechanisms

for both the Co and Ni promoted MoS2 catalyst will be discussed in detail.

Biography:

Jason G. Parsons is a full professor in the Department of Chemistry at the University of Texas Rio Grande Valley. His Primary research interests are in the areas of inorganic-nanomaterials, hybrid nanomaterials, and their applications in catalysis and environmental processes. His recent research focuses have been on the synthesis of graphene-oxide supported transition metal sulfide and transition metal oxide nanomaterials for applications in photocatalysis, high temperature/ pressure catalysis, and in electrocatalysis.

Symmetry-enabled Data-driven Design of Quantum Defects in 2D Materials

Qimin Yan

Northeastern University, USA

Abstract

Being atomically thin and amenable to external controls, two-dimensional (2D) materials offer a new paradigm for the realization of patterned qubit fabrication and operation at room temperature for quantum information sciences and technologies. In this talk, as an example of quantum material design by local bonding symmetry, I will discuss how data-driven material science can be combined with symmetry-based physical principles to guide the search for quantum defects in 2D materials for quantum information processing and quantum computing. In our initial work, the use of local bonding symmetry (irreducible representations) as a material design hypothesis enables the identification of anion antisite defects as promising spin qubits and quantum emitters in six monolayer transition metal dichalcogenides. The expansion of the high-throughput search in all known binary 2D materials led to the identification of more than 40 quantum defect candidates in a large set of host systems that can be utilized as qubits and/or quantum emitters. The work creates a technically accessible 2D platform for the fabrication of defect-based multi-qubit systems for quantum computing and quantum information technologies.

Biography:

Qimin Yan is an Associate Professor of Physics at Northeastern University. His research focuses on computational condensed matter physics and data-driven materials science. He received his Ph.D. in Materials from University of California, Santa Barbara in 2012. From 2013 to 2016, he was a postdoctoral researcher at Lawrence Berkeley Lab and University of California, Berkeley. He worked in the Department of Physics at Temple University as an Assistant Professor from 2016 to 2022 and joined the Department of Physics Northeastern in 2022 as an Associate Professor. He received the US DOE Early Career Award in 2019 and the US NSF CAREER Award in 2022.

Greenbuilding construction products –Sophisticated use of plant biodiversity

Simon Aicher

University of Stuttgart, Germany

Abstract:

Today in structural engineered applications timber products made from softwoods prevail by far. This fact is bound to several reasons being the timber availability, which is i.a. highly related to forestry policies. Further, easy sawing, machining and bonding properties of softwoods enable cost effective manufacture of today's most important engineered timber products, such as glued-laminated timber (GLT), cross-laminated timber (CLT) and I-beams. These building materials

form the basis for number- and height-wise increasing multi-storey timber buildings worldwide. However, the growing use of softwood timber, which is superimposed by the softwood-species detrimental global warming issue, is raising the options, demands and necessity of using the hardwood species resource to a much higher extent than previously. This is even more logical when bearing in mind that hardwoods very often incorporate superior physical and mechanical properties as compared to softwoods. Despite a highly resembling chemical and microstructural fiber wall build-up, softwoods and hardwoods differ significantly in many macrostructural properties. Hereby a higher density of many hardwoods as compared to softwoods is an important fact. Increased density is immediately related to a higher amount of crystalline cellulosic fibers of high tensile strength and an increased content of amorphous lignin enhancing the compressive strength. Beyond density the interface between successive annual rings or growth periods differs significantly between softwoods and diffuse porous hardwoods. In case of softwoods such as e.g. spruce and fir, the annual ring transition is sharply defined by an extreme step function-like density and cell wall thickness difference between so-called late and early wood. This material singularity represents a predestined onset for shear and tensile perpendicular to fiber failure. In contrast hereto, diffuse porous hardwood species are excelled by a rather smooth, steady wood matrix transition between growth periods related with highly increased shear and tensile properties of the annual ring interface. The higher density and the rather steady annual ring interface conditions make many hardwood species a superior building construction material as compared to softwoods. A composite-type combination of softwoods and hardwoods often presents superior solutions for structural timber building products. The build-up, the underlying composite idea and the resulting properties of three different hybrid softwood-hardwood composites are highlighted in the presentation. In detail the advanced green structural building products i) hybrid GLT designed for high bending capacity, ii) hybrid GLT designed for incorporation of very large openings and iii) hybrid CLT plates with superior rolling shear properties – are highlighted as examples of sophisticated use of plant biodiversity.

Biomimetic Composite Laminates Inspired by Odontodactylus Scyllarus' Appendages, FEM and Experimental Study

Karolina Gocyk*

AGH University of Science and Technology, Faculty of Materials Science and Ceramics

Abstract:

Nowadays materials face very high demands for quality and durability. In order to achieve that engineers often turn to biomimetics for inspiration. In this work Odontodactylus Scyllarus otherwise known as the Mantis Shrimp was the inspiration for a composite laminate with specific layer orientation that makes the composite extremely durable. Samples were prepared by hand lay-up lamination method and fabricated from carbon fiber and epoxy resin. In order to examine laminates properties Finite Element Method (FEM) simulations were conducted and real life tests performed. For FEM analysis ANSYS Workbench and ACP(Pre) were used. As a result it was observed that samples have a large tendency to asymmetrically deform and dissipate energy within their inner structure (known as the Bouligand structure) in a distinct way. Furthermore FEM simulations provided opportunity of analyzing singular layers instead of only getting results for the whole sample. Stress and strain in every segment of the laminate could be then observed. Results of simulations were compared to mechanical experiments on carbon fiber samples. The obtained results provided an understanding of the material behavior and shed light on the potential applications of this composite laminate.

Biography:

Karolina Gocyk is a Batchelor of Engineering and a student at AGH University of Science and Technology. She is a member of AGH Space Systems students' association. She is fascinated by materials science and works on new biomimetic solutions incorporated in AGH Space Systems newest rocket 3-TTK. She gave many scientific presentations on events such as 2019 MILSET Expo International Abu-Dhabi or Women in Tech Summit (2018). Her passion is science, especially materials engineering and mechanical engineering. She is fascinated with space related research and took part in LunAres Analog Astronaut mission and research in June 2022.

Poster Presentations

Structural Dependence of Electro-mechanical Properties of Knitted Strain Sensors and its Application for the Sign Language Glove

Jaegab Lee[1*]
Seung Hyeok Lee[2]
Juwon Jun[2]
Byoung-Joon Kim[2]
Youn-Hee Kim[3]
Ho-Seok Nam[1]

[1]School of Advanced Materials Engineering, Kookmin University, Korea
[2]Department of Advanced Materials Engineering, Tech University of Korea, Korea
[3]Dept. of Convergence Design and Technology, Kookmin University, Korea

Abstract

Conductive knitted fabrics have attracted huge attentions in wearable strain sensors due to their unique elastic properties, compared with those of other fabric structures such as woven and braid. What's more important, they can provide softness and comfortability for the wearers because of the loop structures. Recently, the sensing mechanism of the knitting devices, based on the change of the fabric electric resistance as a function of an applied force, has been explored, revealing the key factors affecting the performance. As for the electrical performance of the knitted devices, the contact resistances of the knitted loops such as interlocking loops and jamming ones are major contributors to the electrical change with an applied force. Few studies take into account the two types of contact resistance to develop theoretical model for the equivalent resistance of the knitted sensors under the state of strain.

In this study, we have developed the theoretical model by considering the two contact structures for various structures of knitted strain sensors, revealing the dependence of the electro-mechanical properties of kitted strain sensors on the structures. Finally, the structure was optimized and applied to the fabrication of the sign language glove.

Biography:

Jaegab Lee, a professor at Kookmin University in Seoul of Korea, is a director of CRC (Convergence of Research Center) funded by Korean NRF: CRC has focusing the developing of the smart fashion by implementing the wearable technology into whole garments.

Bi_2Se_3/CNT Binder-free Anodes for Sodium-ion Batteries.

Raimonds Meija*
Vitalijs Lazarenko
Yelyzaveta Rublova
Jana Andzane
Didzis Salnajs
Donats Erts

Institute of Chemical Physics, University of Latvia, Latvia

Abstract

One of the most important challenges in the world is effective storage of electrical energy for portable devices and electric vehicles as well as for energy storage and redistribution units for solar and wind power plants to manage short-run fluctuations in supply and demand. For these applications, Li-ion batteries (LIB) have been the dominant electrical power storage devices since 1990s.

Sodium-ion batteries (SIBs) have attracted significant attention as a possible replacement candidate for LIBs. It uses abundant sodium, which could lead to potentially low-cost large-scale storage systems. Although sodium and lithium have similar chemical and physical properties, the higher ionic radius, mass, and standard potential of Na+ in comparison to Li+ mostly lead to a worse reversible capacity, smaller energy density, and shorter lifespan. The efficiency of the SIBs can be improved by modification of electrodes, electrolytes, and separators between anode and cathode.

We report results on the development of Bi2Se3/CNT heterostructured anodes for SIBs. Bi2Se3 is a metal chalcogenide class material, that can provide high theoretical capacity and the CNT network backbone provides a conductive structural backbone. Also, the porous CNT network can accommodate the volume changes of the anode electrode during the sodiation/desodiation reactions.

Biography:

Raimonds Meija is a senior researcher at the Institute of Chemical Physics University of Latvia and is a member of its Scientific Council. He is a member of the expert committee of the Latvian Council of Science. His early work was dedicated to the application of nanowires, including metal chalcogenide nanowires in electronic devices: the main subfields were mechanical and electrical characterization of the nanowires. Recently the focus shifted to high-yield synthesis, and electrical and electrochemical characterization of metal chalcogenide heterostructures (coupled with carbon nanotube networks) to accelerate their use in thermoelectric devices and as battery anode materials.

First-principles Investigations of the Physical Properties of Experimentally Feasible Novel Aluminum Nitride Polytypes

Mowafaq Alsardia[1*]
I. B. Khadka[1]
Bakhtiar Ul Haq[1]
Se-Hun Kim[2*]

[1]Research Institute of Education Science, Jeju National University, Korea
[2]Faculty of Science Education, Jeju National University, Korea

Abstract

We present the results of a first-principles study on the structural stability and electronic and optical properties of new aluminum nitride (AlN) polytypes. The study includes the experimentally or theoretically known phases of AlN wurtzite (WZ), zincblende (ZB), and rock salt (RS) structures, which complement the pressure-dependent phase diagram of this industrially important compound. In addition to the structures of AlN considered in previous studies, we evaluated the dynamic stability of various novel phases: viz., SiC(4H), ZnS(15R), BeO, 5-5, TiAs, NiAs, MoC, Li2O2, and NiS. These were predicted recently in a high-pressure data-mining study of more than 140000 variations of the AlN structure, which claimed that they were either stable or nearly stable based on first-principles calculations. On the basis of the new AlN polytypes, the physical

properties of all considered phases were compared, and the common trends and differences were determined. According to the phonon band structure calculations, nine phases of these new polytypes are free from imaginary frequencies. This indicates adequate dynamic stability and the experimental accessibility of the polytypes. Additionally, the calculated cohesive energies of the dynamically stable phases are comparable to those of WZ-AlN and those specified in the available literature. Furthermore, the observed electronic structures and optical properties indicate that the polytypism of AlN can be a practical tool for refining its physical and chemical properties. The new phases show significant potential for use in future AlN electronic and optoelectronic applications.

Biography:

Mowafaq is a postdoc at the Research Institute of Education Science, Jeju National University. He received his M.S. degree from the University of Technology Malaysia and Ph.D. from Sungkyunkwan University, all in Condensed matter physics. His research expertise is first-principles density-functional theory calculations on materials to gain a fundamental understanding of the materials' properties at an atomic level. Now he is working on investigating structural response obtained by a first-Principles method when semiconductor materials are subjected to high pressures.

A Novel Technique to Repair the Scratches of Zirconia Surface after Occlusal Adjustment

Ting-Hsun Lan[1,2*]
Chih-Te Liu[1,2]
Chin-Yun Pan[1,2]
Yun-Chu Lai[2]

[1]School of Dentistry, College of Dental Medicine, Kaohsiung Medical University, Kaohsiung, Taiwan
[2]Division of Prosthodontics, Department of Dentistry, Kaohsiung Medical University Hospital, Kaohsiung, Taiwan

Abstract

After occlusal adjustment or function in the oral cavity, monolithic zirconia crowns often leave some scratches on the occlusal surface. A novel way to mend the scratches by brushing the solution of photopolymerization adhesive bonding agent and ZrO2 nanopowders to the zirconia was to find the proper proportion of the solution that can reduce the surface roughness of the specimen and sustain the durable test. 108 φ12.0 mm * 4.0 mm zirconia specimens with the same surface treatment smeared with mixing ZrO2 nanopowders (TZ-3Y-E, Tosoh Corp., Japan) and adhesive (3M ESPE Single Bond Universal Adhesive, 91125C) according to 2:8, 5:5 and 0:10 weight ratios, then light cure for 40 seconds. The solubility test was carried out by soaking the specimen in 100 ml of deionized water and recording the flake situation and mass loss of the coating layer (1 week, 2 week, 1 month, and 3 months). Another 27 zirconia specimens (2:8, 5:5, and 0:10 weight ratios) were implemented the abrasion test, which was soaking the specimens in the deionized water and conducted by an automatic abrasion tester (PAT-2012, PROES, Taiwan) under 200 gw and 60 times/mins till 48000 times. The morphology and thickness of specimens were observed by the optical microscope (OM, Olympus BX51, Japan), and the roughness was measured by the surface roughness tester (SJ-301, Mitutoyo, Japan). All data were statistically analyzed by SPSS software. For abrasion and solubility tests, sample 2Z8A has a statistically significant difference for anti-wear and less weight loss than 5Z5A and 0Z10A. From the abrasion test and solubility test, 2Z8A can get better adhesion, and the application in the oral cavity can be further explored in the future.

Biography:

Ting-Hsun Lan received his dental education and Dr. med. dent. Degree from the College of

Dental Medicine, Kaohsiung Medical University, Taiwan, in 2011/ 2017. In 2014 Dr. Lan received an Assistant Professorship at the College of Dental Medicine, Kaohsiung Medical University in Taiwan. From 2021 on, he was an Associate Professor at the same University. In 2018 Dr. Lan was a Visiting Scholar at the Minnesota Dental Research Center for Biomaterials and Biomechanics (MDRCBB), Minnesota University, USA. Additionally, since 2019 he has been the director of the Division of Prosthodontics, Department of Dentistry at the Kaohsiung Medical University Hospital, Taiwan.

Anchoring MoS_2 on Ethanol-etched Prussian Blue Analog for Enhanced Electrocatalytic Efficiency for Oxygen Evolution Reaction

Poulami Mukherjee*
Krishnamoorthy Sathiyan
Vishwanath R. S
Tomer Zidki

Ariel University, Israel

Abstract

The present work highlightsthe significance of combining the etching effect and decorative effect of molybdenum disulfide (MoS2) on the edges and surfaces of Co-Fe Prussian Blue Analog (PBA) for the electrochemical oxygen evolution reaction (OER). We introduce a mild etching agent, ethanol-water, to convert solid PBA nanocubes into hollow nanocages. It eliminates the need for a capping or stabilizing agent. The synthesis, structural modification, and electrochemical activity of the derived Etched-PBA-MoS2 catalyst towards O2 evolution are explicitly investigated. We also emphasize the usage of a 3D microporous carbon cloth (CC) substrate to boost the OER activity of the Etched-PBA-MoS2; the porous CC substrate influences the OER rate by promoting electrolyte diffusion and increasing active site accessibility. The potent catalyst exhibits excellent OER activity, requiring an overpotential of only 340 mV (on glassy carbon electrode) and 260 mV (on CC) to obtain a current density of 10 mA cm^{-2} . The catalyst benefits from two structural advantages: 1) hollowing PBA nanocubes by the etching process increases the density of active sites and promotes mass transport; 2) binding MoS2 on the surface of PBA nanocages induces a synergistic effect – the electronic interactions among the active components tune the electronic structures of Co, Fe, and Mo sites. This work can render a workable pathway to optimize the etching effect and fasten different metal sulfide heterostructures on PBAs to achieve an excellent OER performance.

Biography:

Poulami Mukherjee of Ariel University is pursuing her Ph.D. under the supervision of Dr. Tomer Zidki. She obtained her B.Sc. (2017) and M.Sc. (2019) in Inorganic Chemistry from Calcutta University (India) with high distinction. Her research focuses on hybrid metal-organic framework (MOF)-based nanostructures and its electrocatalytic applications, such as oxygen evolution reaction (OER), Na-ion, and Li-ion batteries. She specializes in hybridizing Prussian Blue Analog (PBA)-based materials and altering their structural properties for better catalytic performance.

Small-scale Mechanical Recycling of Solid Thermoplastic Wastes: A Review of PET, PEs, and PP

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Lachlan H. Yee[1,2]
Ricardo Vasquez Padilla[1]

[1]Faculty of Science and Engineering, Southern Cross University, Australia
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Mechanical recycling of thermoplastic products can be achieved with the right approaches. Thermoplastics such as high-density and low-density polyethylene are mostly considered for recycling because of their physical properties as well as ease of reprocessing. In this project, a review of the plastic recycling industry, mainly small-scale mechanical reprocessing, is carried out. Analysis of the selected thermoplastics' (polyolefins) key chemical and physical properties to determine possible changes before and after reprocessing is initiated. Furthermore, modelling of the reprocessing operation using the design of experiment method to explore the proper recycling process that allows the simultaneous optimisation of both energy and mechanical strength of the plastics is engaged. A clearer understanding and addressing of the process-related challenges will ultimately lead to successfully establishing and managing small-scale mechanical recycling facilities to produce plastic products and benefit communities. Efficient small-scale mechanical reprocessing establishments have become essential in reducing the environmental impacts of solid plastic wastes and for energy conservation.

Biography:

Canice Uzosike is a postgraduate research scholar at Southern Cross University, focusing on analysing the key chemical and physical properties of recycled plastics to ascertain the process limitations and modelling the small-scale extrusion process to determine the right parameters that allow the simultaneous optimisation of both energy and mechanical strength. Canice holds a bachelor's degree (B.Eng.) in mechanical engineering (industrial and production technology majors) and a Master of Management for engineers (M.Mgt.Eng.) degree. He is also a member of the Institution of Engineers Australia (MIEAust), having several years of industry experience spanning maintenance and field projects as a mechanical engineer.

Influence of Anodization Parameters on the Surface and Corrosion Resistant Characteristics of Titanium Nanotubes Formed on Ti Substrate in Simulated Body Fluids.

Faisal Abdelrahim*
Arumugam Madhan Kumar

King Fahd University of Petroleum and Minerals, Saudi Arabia

Abstract

Biomaterials are materials that can be repaired or replaced the broken or diseased parts to interact with the biological systems to serve the body for a more extended period with minimal failure. In this study, titanium (Ti) substrate was used as bio-implant material because it matches several mechanical properties in the human body, including the modulus of elasticity. Although using bare titanium as an implant treat, for example, bone fracture, its corrosion resistance is still weak. Therefore, an electrochemical anodization process will be conducted to form titanium dioxide nanotubes (TNTs), which will enhance the corrosion resistance. The electrolyte used for anodization was ethylene glycol containing H2O and ammonium fluoride NH4F. The anodization experiments were carried out under three different voltages (40V, 50V, 60V) corresponding to three different periods (30 min, 60 min, 90 min). Then, the annealing process was performed at 450 ^{0}C for 2 h. After that, electrochemical tests (potentiodynamic polarization measurements) were conducted in Simulated Body Fluid (SBF) to pick the best time that held higher corrosion resistance in different voltages, which was 30 min. Additionally, the optimum voltage value was selected according to the excellent distribution of the TNTs using field emission scanning electron microscope (FE-SEM) and X-ray diffraction (XRD). 50 V was the optimum voltage value because the TNTs were distributed perfectly, and the anatase phase existed. Forming TNTs will be a preparation for the next step, which is filling these tubes with an antibiotic (antibacterial) solution

and performing as drug delivery to the infection that might harm the implant.

Biography:

I'm senior undergraduate mechanical engineering student interested in material science field. This research project considers my first research experience which was conducted under interdisciplinary research center for advanced materials. My internship program was BAKER HUGHES – R&D center with two different departments: Additive Manufacturing Team & Non-Metallic Team. I published one conference paper during my internship about life cycle analysis of two different method of well construction: liner hanger vs long string.

Plenary

Design and Characterization of Functional Materials Based on Energy-resolved Distribution of Electron Traps

Bunsho Ohtani

Hokkaido University and Nonprofitable Organization touche NPO, Japan

Abstract

How can we design functional solid materials, such as catalysts and photocatalysts? What is the decisive structural parameters controlling their activities, performance or properties? What is obtained as structural properties by popular conventional analytical methods, such as X-ray diffraction (XRD) or nitrogen-adsorption measurement, is limited to bulk crystalline structure and specific surface area, i.e., no structural characterization on amorphous phases, if present, and surface structure has been made so far. This is because there have been no macroscopic analytical methods to give surface structural information including possibly present amorphous phases. Recently, we have developed reversed double-beam photoacoustic spectroscopy (RDB-PAS) which enables measure energy-resolved distribution of electron traps (ERDT) for semiconducting materials such as metal oxides [1,2]. Those detected electron traps (ETs) seem to be predominantly located on the surface for almost all the metal oxide particles, and therefore they reflect macroscopic surface structure, including amorphous phases, in ERDT patterns. Using an ERDT pattern with the data of CB bottom position (CBB), i.e., an ERDT/CBB pattern, it has been shown that metal oxide powders, and the other semiconducting materials such as carbon nitride, can be identified without using the other analytical data such as XRD patterns or specific surface area, and similarity/differentness of a pair of metal-oxide samples can be quantitatively evaluated as degree of coincidence of ERDT/CBB patterns. In this talk, an approach of material design based on the ERDT/CBB-pattern analyses is introduced [3]. [1] Chem. Commun., 2016, 52, 12096–12099. [2] Electrochim. Acta, 2018, 264, 83–90. [3] Catal. Today,

Biography

The research work on photocatalysis by Professor Bunsho Ohtani started in 1981 when he was a Ph. D. course student in Kyoto University. Since then, he has been studying photocatalysis and related topics for 40 years and published more than 300 original papers (h-index: 70) and two single-author books. After gaining his Ph. D. degree from Kyoto University in 1985, he became an assistant professor in the university. In 1996, he was promoted to an associate professor in Graduate School of Science, Hokkaido University and was then awarded a full professor position in the Catalysis Research Center (presently Institute for Catalysis), Hokkaido University in 1998 and retired at the end of March 2022. He was awarded several times form the societies related to chemistry, photochemistry, electrochemistry and catalysis chemistry.

Advanced Concepts for Ultra- High Conversion Efficiency of Solar Photons into Photovoltaics and Solar Fuels Based on Quantization Effects in Nanostructures and Molecular Singlet Fission

Arthur J. Nozik

Department of Chemistry and Renewable & Sustainable Energy Institute (RASEI)

University of Colorado, Boulder, CO
National Renewable Energy Laboratory (NREL), Golden, CO

Abstract

In order to utilize solar power for the production of solar electricity and solar fuels on a global scale, it will be necessary to develop solar photon conversion systems that have an appropriate combination of high efficiency (delivered watts/m2) and low capital cost ($/m2). One potential, long-term approach to attain high conversion efficiencies above the well-known Shockley-Queisser thermodynamic limit of 33% is to utilize the unique properties of quantum dot/rod (QD/QR) nanostructures and Singlet Fission (SF) in molecular chromophores, to control the relaxation dynamics of photogenerated hot carriers and excited states in photoexcited molecules to produce either enhanced photocurrent through efficient photogenerated electron-hole pair (ie, exciton) multiplication or enhanced photopotential through hot electron transport and transfer processes. To achieve these desirable effects, it is necessary to understand and control the dynamics of SF and hot electron and hole cooling, charge transport, and interfacial charge transfer of the photogenerated carriers. These fundamental dynamics in various bulk and quantied nanoscale semiconductors and SF molecules have been studied for many years using various spectroscopies with fs to ns time resolution. The prediction that the generation of more than one electron-hole pair (which exist as excitons in size-quantized nanostructures and photoexcited molecules) per absorbed photon would be an efficient process in QDs,QRs, and SF molecules has been confirmed over the past years in different classes of materials, molecules, and their architectures. Very efficient and ultrafast multiple exciton generation (MEG), also called Carrier Multiplication (CM), and SF from absorbed single higher energy photons has been reported in many quantized semiconductors and molecules and associated solar photon conversion devices for solar electricity and solar fuels (e.g. H2) production. Selected aspects of this work will be summarized, and recent advances will be discussed, including the very remarkable and extremely large beneficial theoretical effects of combining MEG with solar concentration. The analogous MEG effect in SF molecules and its use in molecular-based solar cells will also be discussed.

Keynote Presentations

Heterojunction Nanostructured Materials for Photothermal Catalysis

Ghim Wei Ho[*1,2]
Minmin. Gao[1]
Serene Wen Ling. Ng[1]
Tianxi Zhang[1]

[1]Department of Electrical and Computer Engineering, National University of Singapore, Singapore
[2]Department of Materials Science and Engineering, National University of Singapore, Singapore

Abstract

Interest in hydrogen as a zero-carbon energy carrier has increased significantly in recent years, given that hydrogen-based economy is the best energy alternative to the increasing concerns over carbon emissions, energy security, and climate change. Using readily available renewable resources i.e. solar energy and seawater to secure sustainable fuel and freshwater for humanity is an impactful quest. The utilization of photothermal materials with broad solar absorption, in parallel to engineered nanocatalyst, offers new approach to achieve efficient solar light conversion. Hoewever, the incorporation of multimaterials into a unitary photocatalyst configuration for efficient full solar spectrum catalysis with maximized photochemical and photothermal effects is particularly challenging. Here, we have designed solar thermal collector nanocomposites that possess efficient photothermal properties for highly targeted interfacial phase transition

reactions that are synergistically favorable for catalytic hydrogen production. The photothermal effect arises from plasmonic metal, semiconductor and carbon nanomaterials exhibit localized interfacial heating which directly triggers surface-dominated catalysis processes, with minimal heat losses, thermal masses and optics implementation. We propose a spectrum-designated solar harnessing photocatalyst that has uncompromised bilateral photothermal and photocatalytic functions. Tailored spectrum photocatalysts whereby high-frequency solar photon is exclusively captured for photochemical, while low-frequency photon is assigned to photothermal effect. The solar thermal collector nanocomposites are photo stable for practical solar conversion to simultaneously produce clean energy and water. Finally, proof-of-concept prototypes demonstrate the viability of sustainable photothermic driven catalysis and desalination under natural sunlight.

Biography:

Ghim Wei Ho is currently a professor of the Department of Electrical & Computer Engineering at the National University of Singapore (NUS). She has co-authored more than 200 papers in the international refereed journals. She was an elected Scholar at Selwyn College, University of Cambridge and is a Cambridge Commonwealth Society Fellow since 2006. She is also a Fellow of Royal Society of Chemistry (FRSC). In 2014, she was awarded the L'OREAL UNESCO for Women in Science Fellowship. In 2015, she was the honoree winner of the JCI's Ten Outstanding Young Persons (TOYP) Award in the Science and/or Technological Development category. In 2016, she was honoured as the Science & Technology winner for the Great Women of Our Time as well as the ASEAN-US Science Prize for women.

Do New-NonClassical Materials Need New-NonClassical Models?

Elias C. Aifantis

[1] Aristotle University of Thessaloniki, Greece

[2] Michigan Technological University, Houghton, MI, USA

[3] Mercator Fellow, Friedrich-Alexander University, Erlangen-Nuremberg, Germany

Abstract

The answer to the above question is YES! Several examples are presented in the lecture to confirm it. They range from Hooke's Law of Elasticity and Newton's Law of Gravitation to Fourier's Law of heat conduction and Fick's Law of diffusion. Additional examples include preciously advanced models of material behavior such as von-Mises criterion of plasticity and Coulonb's failure criterion. A suggestion of how to extend this approach to electrostatics and electrodynamics is also outlined.

Biography:

Elias C. Aifantis is currently an Emeritus Professor of Mechanics at Aristotle University of Thessaloniki/Greece and Michigan Technological University/USA, as well as Mercator fellow at Friedrich-Alexander University/Germany and a Distinguished Professor at Beijing University of Civil Engineering and Architecture/China. Formerly, he has also been a Distinguished Faculty Advisor at King Abdulaziz University/Saudi Arabia, Distinguished Visiting Expert at ITMO University/ Russia and Southwest Jiaotong University/China, as well as MegaGrant Director at Togliatti State University /Russia. He has promoted highly interdisciplinary work in mechanics of materials by bringing into the field of solid mechanics ideas from diffusion theory, chemical reactions, and nonlinear physics. He has coined the terms dislocation patterning, material instabilities, gradient plasticity/elasticity, chemo/nanomechanics, and pioneered internal length gradient (ILG) theories in these fields. Currently, he is extending the ILG framework to revisit electromagnetism and Maxwell's equations, as well as gravitation and Newton's Law. He has published over 350 articles and received about 13,402 citations with 59 h-index (Scopus); 12,450 citations with 55 h-index

(Web of Science); 20,580 citations with 70 h-index (Google Scholar). He is included in the ISI Web of knowledge list of the world's most highly cited authors in engineering.

A Superficial Tale: Semiconductor Nanowires as a Remarkable Platform for Nanoelectronics and Sensing

Harry E. Ruda*
David Lynall
David Gutstein
Selva Nair
Kris Burne
Alex Shik
Igor Savelyev
Marina Blumin
Jacky Lau
Carlos Fernandes
Christina de Souza

Centre for Advanced Nanotechnology, University of Toronto, Canada

Abstract

The first foray into semiconductor micron-scale 'whiskers' came from work by Wagner and Ellis in 1964, only to applied in the late 1990's to realise nanowires with diameters of tens of nanometers. With the possibility of strong confinement in two dimensions, these structures present ideal vehicles for 1d physics and devices. However, surface related phenomena can provide a curse or opportunity in this quest - the latter is the focus of this presentation. Here, I focus on the opportunities in a few areas including ballistic conductance, random telegraph noise, and scattering from individual surface charges. Harnessing these phenomena can enable a host of new opportunities including making inroads in the quest to tame the elusive Majorana Fermion, in ultra-sensitive elevated temperature single charge electrometry and in single molecule level sensing.

Biography:

Harry Ruda obtained his PhD from MIT in 1982 for work on optoelectronic properties of II-VI based infrared materials. After as IBM postdoctoral fellow, he developed one of the first theories for electron transport in 2DEGs. After he led the 3M Corporation II-VI blue laser program, joining University of Toronto in 1989 where he currently holds Stanley Meek Chair in Nanotechnology and is Director of Centre for Nanotechnology. He has about 300 journal publications (8,200 citations and h-index of 44). He is a Fellow of Royal Society of Canada, Institute of Physics, Institute of Nanotechnology, and Canadian Academy of Engineering.

Oral Presentation

Back Interface Engineering of $Cu_2(Cd,Zn)SnS_4$ Thin Film Solar Cells by Ultrathin CuO Interfacial Layer

Terence K.S. Wong

School of Electrical and Electronic Engineering, Nanyang Technological University, Singapore

Abstract

Cu2ZnSnS4 (CZTS) is a sustainable semiconductor absorber with a bandgap compatible with photovoltaics. Its kesterite structure is similar to the chalcopyrite semiconductors (e.g. CIGS).

Although it does not contain scare metals such as indium, it is prone to solid state reaction with molybdenum at the back contact during annealing. The resulting molybdenum disulfide layer can increase parasitic series resistance and reduce solar cell fill factor. In this talk, we present the use of amorphous cupric oxide (CuO) as an effective back interface layer and demonstrate kesterite thin film solar cells with above 10% power conversion efficiency (PCE). CuO is chosen for investigation because unlike previous back interfacial layers, it is a material with photovoltaic properties.

CuO (~10nm) was deposited by reactive magnetron sputtering onto molybdenum/soda lime glass substrates. The structure and composition of CuO were studied by XPS and XRD respectively. The effectiveness of CuO in blocking Mo diffusion was evaluated by secondary ion mass spectrometry. Cd substituted CZTS absorber (Cu2(Cd,Zn)SnS4) was deposited by a sol-gel method. The front CdS buffer layer was deposited by chemical bath deposition followed by sputter deposition of indium tin oxide. Under 1 Sun, AM1.5G illumination, a PCE of 10.8% maximum was measured for small area devices. After a period of storage in air in dark conditions, unencapsulated Cu2(Cd,Zn)SnS4 devices with optimized CuO thickness showed a slight gain in PCE relative to the control device.

Biography:

Terence Wong obtained the BA (first class) and PhD degrees in electrical engineering from the University of Cambridge. He is a tenured associate professor in electrical and electronic engineering at the Nanyang Technological University Singapore. His research expertise includes microfabrication for semiconductor manufacturing, semiconductor device physics, photovoltaics (organic/inorganic thin film) and OLEDs for information displays. Dr. Wong was principal investigator for several funded projects and supervisor of master's and PhD students. He is a senior member of the IEEE and SPIE.

The Electronic Structure of 2H-MoS2: Experiment & Theory

Manuel Ramos

Departamento de Física y Matemáticas, Instituto de Ingeniería y Tecnología, Universidad Autónoma de Cd. Juárez, Cd. Juárez, Chihuahua, México.

Abstract

The Molybdenum Disulfide (MoS2) have been studied with intensity in the past 20 years, its chemical structure was first reported by Linus Pauling, proposing a series of two-dimensional sheets stacked by weak van der Waals interaction. Later, the mineral was first used as lubricant to avoid the wear/tear of mechanical parts, and as "workhorse" in catalytic procedure known as hydrodesulphurization of crude oil and recently in the field of nanoelectronics. This talk will present a comprehensive panorama of the exceptional properties of this low dimension material, with special emphasis in the electronic structure when interacts with indium-tin-oxide (ITO) by theoretical and experimental data from RF-sputtering deposits of ITO-MoS2 thin films (~100nm-300nm), moreover, the talk presents data of I-V curves, atom probe tomography, scanning and transmission electron microscopy and density functional theory calculations. Results, indicate ⟨110⟩-orientation are aligned perpendicular to the ITO film with principal reflections at (002), (100), (101), (201), APT reveals MoS+2, MoS+3 as major evaporated molecular ions and indicates no significant diffusion/segregation of Mo or S species within ITO layer. Density functional theory calculations indicate ITO and MoS2 conform a Schottky barrier due to d-orbital interactions creating an ohmic contact with n-type Schottky barrier height (Φn) of − 1.6 eV for 2H and − 1.2 eV for 3R MoS2 and contact resistance of about 1 Ωcm2 when in contact with transparent ITO and semiconducting MoS2 can produce an efficiency of 2.48% as measured in proposed hybrid organic semiconductor solar cell prototype.

Biography

Manuel Ramos is a Mexican American native of Ciudad Juárez and a full-time professor in the Department of Physics and Mathematics at the Autonomous University of Ciudad Juárez. He has been a research assistant at the National High Magnetic Field Laboratory-Tallahassee, Fl. 2004-2006. Research Professor at Materials Institute of UTEP 2010-2015 and is currently visiting researcher at the Center for Integration of Nanotechnologies of Sandia National Labs at Albuquerque, NM and Karlsruhe Nano and Micro Facility in Germany. His area of study is a combination of theory and experiments to study the structure/functionality of energy and catalytic materials that includes the use of AFM, SEM, TEM and APT microscopy. He is the co-author about 35 peer-review manuscripts and conference proceedings. He is member of the National System of Researchers of CONACyTMexico since 2010. From 2013 to present has served as co-organizer and director of the Advanced Catalytic Materials Symposium held within framework of IMRC a joint scientific meeting between Mexican Society of Materials and Materials Research Society (USA). In addition, he has served as special editor for the Journal of Materials Research, Catalysis Today, MRS Advances, and Springer Book Series and is a peer reviewer for more than 20 JCR journals.

Wound Healing, Antioxidant and Antibacterial Potential of Sericin Mediated Silver Nanoparticles: Synthesis and Applications

Gitishree Das[1]
Han-Seung Shin[2]
Jayanta Kumar Patra[1*]

[1] Research Institute of Integrative Life Sciences, Dongguk University-Seoul, Goyang-si, Republic of Korea
[2] Department of Food Science and Biotechnology, Dongguk University-Seoul, Goyangsi, Republic of Korea.

Abstract

The silk protein (named sericin) possesses abundant amount of bioactive properties and has ample applications in the field of pharmaceutical, biomedical, cosmetic and food industries. Usually, sericin is a waste material that is removed from the silk cocoon in the process of manufacturing silk by the sericulture and textile industries. In view of the vast potential of the sericin protein, in the current investigation, an attempt has been made to use the waste sericin in the synthesis of silver nanoparticles by bio-reduction method, characterize them and study its biopotential in terms of wound healing, antioxidant and antimicrobial properties. Synthesis of silver nanoparticles are carried out by using the sericin extract as the reducing agent. Following synthesis, it was characterized by UV-Vis spectroscopy, FT-IR and TEM- EDS, Particle size and Zeta potential analysis. Further, the biopotential of the sericin-based silver nanoparticles are studied against a number of Gram-positive and Gram-negative foodborne pathogenic bacteria and its activity was recorded in terms of diameter of inhibition zones. The minimum inhibitory concentrations and the minimum bactericidal concentrations were also calculated. The antioxidant potential of the sericin-based silver nanoparticles was evaluated in terms of the DPPH assay, ABTS assay and the reducing power assay. The wound healing potential of the synthesized silver nanoparticles was evaluated by the starch wound assay and the results were promising. Taken together, the synthesized silver nanoparticles could be exploited for its potential applications as antibacterial agents and in wound dressing and other related biomedical applications.

Biography:

Jayanta Kumar Patra, Ph.D., is currently working as Associate Professor at Dongguk University, Republic of Korea. His current research is focused on nanoparticle biosynthesis and their application in bio-medical and agricultural fields. Dr. Patra has published more than 150 papers in various national and international peer-reviewed journals, 18 books, 38 book chapters. He is also editing two book series on Nanotechnology and Biotechnology for Elsevier and Springer Nature publications. Besides, he is editorial board member of several International Journals. Besides, Dr. Patra is listed under World's Top 2% Scientists based on citation impact during the single calendar year 2020-2021.

Sustainable Biosorbents and Nanomaterials Preparation from Agricultural Wastes for Water Decontamination

Roberta Del Sole*
Lucia Mergola

University of Salento, Italy

Abstract

In the last years, the serious environmental problems caused from pollution have addressed the efforts of scientific community to follow a green chemistry approach in its research. For instance, in nanotechnology field the implementation of the principles of green chemistry represents a fundamental issue in the latest nanoscience research such as using nontoxic chemicals, eco-friendly solvents and renewable or waste materials. In this context, our research group have been focusing on the development of innovative eco-sustainable technologies to produce new sorbents and nanomaterials in compliance with the principle of green chemistry, for water decontamination from organic and inorganic pollutants. Our recent research results on the use of product wastes of winery industry for water remediation will be discussed.

Grape marcs, which are a waste product of the wine industry, were used as starting materials for a green production of new biosorbents able to remove heavy metals from aqueous solutions. Grape marcs were pretreated to remove organic and inorganic components, using only green solvents, such as water and ethanol. The lignocellulosic components of the obtained biosorbents showed a high capacity to remove heavy metals from aqueous solutions.

Moreover, the reducing and stabilizing capacity of these compounds has been also exploited to synthesize green metal nanoparticles with interesting catalytic and antimicrobial properties that can be used for organic pollutants remediation. This strategy permits not only to reduce the environmental impact of grape marc wastes but also to reuse them for the decontamination and remediation of aquifers from organic and inorganic pollutants.

Biography:

She graduated in Chemistry at University of Bari (Italy) in 1999. Since 2000 she has been working in the chemistry lab of the department of Engineering for Innovation of University of Salento. She received her PhD degree in Material Engineering in 2003 and from January 2005 she is Assistant Professor in Chemical Foundation of Technologies at the Department of Engineering for Innovation of University of Salento where she carries out teaching activity in academic courses and research activities. Her main research interest is synthesis and characterization of molecularly imprinted polymers (MIPs) for biomolecules and metal ions recognition and their application in the environmental and biomedical field and development of innovative sorbents or nanomaterials from agricultural wastes.

Application of Polymeric Nanomaterials and their Nanocomposite in the Construction of Ion-selective Electrodes with Solid Contact

Cecylia Wardak[1*]
Karolina Pietrzak[1]
Szymon Malinowski[2]

[1]Maria Curie-Sklodowska University in Lublin, Poland

[2]Lublin University of Technology, Poland

Abstract

Among the various types of ISEs, electrodes without an internal electrolyte solution, the so-called solid contact ISEs (SCISEs), are becoming more and more popular. Unfortunately, in the simplest design version, SCISEs often exhibited large potential drift and poor potential reproducibility. These problems are caused by the blocked interface and the difficult charge transport between the ion-selective membrane and the electron conductor. Various electroactive conductive materials are used to overcome these drawbacks and obtain electrodes exhibiting a stable and reproducible potential.

In this study various types of nanomaterials including polyaniline nanofibers dopped with chloride or nitrate(V) ions, multiwalled carbon nanotubes and the nanocomposite of both materials were used for the electrode construction. Many types of electrodes were tested, differing in the composition of the solid contact material and the thickness of its layer placed between the electrode material and the ion-selective membrane. An extensive analysis of the electrical and analytical parameters of the sensors was carried out. It was found that in the case of electrodes containing polyaniline nanofibers as solid contact, a significant improvement in the analytical parameters of the electrodes was obtained compared to the unmodified electrodes without the solid contact layer. Comparing both types of nanofibers, it can be noticed that slightly better parameters were shown for electrodes based on nanofibers doped with chloride ions. Taking into account the sensors obtained with the use of nanocomposite, a further improvement in the stability of the electrodes was observed compared to the electrodes with permanent contact based on polyaniline nanofibers and on carbon nanotubes, respectively.

Biography:

Cecylia Wardak received her Ph.D. degree in analytical chemistry in 2004 and her DSc degree in analytical chemistry and electrochemistry in 2015 from Maria Curie Sklodowska University (MCSU), Lublin, Poland. Since then she has been working as associate professor in the Department of Analytical Chemistry of Maria Curie-Sklodowska University. She is an active COST member. Her main scientific interests are research, development, and analytical applications of electrochemical sensors and biosensors. Her latest research focused on the use of nanomaterials and composite materials in the construction of ion-selective electrodes with solid contact. She has published over 75 peer-reviewed papers.

Pulsed Laser Induced Membrane Disruptions of Gold Nanoparticle Loaded Micron and Nanoscale Polymersomes

Julianne C. Griepenburg[1,2*]
Ajay N. Shah[1]
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[2]Center for Computational and Integrative Biology, Rutgers University-Camden, USA.

Abstract

The ability to encapsulate and release molecules on-demand from smart carrier vesicles would be transformative for a wide range of applications. Polymersomes are a class of synthetic vesicles which self-assemble from diblock copolymer amphiphiles, resulting in an aqueous lumen and thick bilayer membrane; however, vesicles assembled from robust poly(butadiene)-b-poly(ethylene oxide) are not inherently stimuli responsive. Herein, we demonstrate that hydrophobic gold nanoparticles can be incorporated into the membrane to serve as photosensitizers, rendering

the vesicles responsive to pulsed laser irradiation congruent with their localized surface plasmon resonance. Studies on micron-scale polymersomes have demonstrated that membrane disruption resulting in cargo release can range from transient poration to complete rupture, depending on parameters such as laser pulse duration and energy. While direct investigation of membrane disruptions on the nano-scale proves challenging, this size regime is advantageous for many delivery applications in biological systems. Thus, this combined study on micron and nano-scale polymersomes seeks to leverage the mechanistic insight gained from the micron-scale towards development of a tunable system for future applications.

Biography:

Julianne Griepenburg received her PhD in Chemistry from the University of Pennsylvania in 2014 and is currently an Assistant Professor in the Department of Physics and Center for Computational and Integrative Biology at Rutgers University-Camden in the USA. Her research interests include light-material interactions, including harvesting plasmonic responses to induce structural changes in macromolecules.

Ultra-high Dielectric Strength and Capacitive Energy Density of Polymer Nanocapacitors

Alamgir Karim[1*]
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Jack Douglas[2]
Nihar R. Pradhan[3]

[1]Department of Chemical and Biomolecular Engineering, University of Houston, Houston, TX, USA
[2]Material Science and Engineering Division, National Institute of Standards and Technology, Gaithersburg, MD, USA
[3]Department of Chemistry, Physics & Atmospheric Sciences, Jackson State University, Jackson, MS, USA

Abstract

Understanding the influence of high-intensity electric fields on the stability of polymeric materials is a problem of interest for designing next-generation energy storage and electronic devices. Here, we show that the dielectric strength of entangled glassy polymer films increases sharply as the film thickness decreases in the sub-micron film thickness regime, reaching ≈ 2 GV/m for ≈ 100 nm films. We use these ultra-thin glassy polymer films to develop the first-ofits-kind polymeric nanocapacitors, which demonstrate an ultra-high discharge energy density (Udmax) of 27.5 J/cm3 with an efficiency (η) higher than 80%. The efficiency of the linear glassy polymeric nanocapacitors stays higher than 90% till Ud ≈ 40% of Udmax, which is significantly higher than those of competing ferroelectric polymers and their composites (η < 80% for 0.2 Udmax < U < 0.7 Udmax). We also we report a thin film heterostructure capacitor based on poly(vinylidene fluoride)/poly(methyl methacrylate)/poly(vinylidene fluoride) with stratified 2D nanofillers (Mica or h-BN nanosheets) (PVDF/PMMA-2D fillers/PVDF), that shows enhanced permittivity, high dielectric strength and an ultra-high energy density of ≈ 75 J/cm3 with efficiency over 79%. We envision that these results will inspire a new era of high-energy density nanocapacitors for advanced energy storage applications.

Biography:

Alamgir Karim is Dow Chair Professor in William A. Brookshire Department of Chemical and Biomolecular Engineering at University of Houston (UH), where he is Director of the Materials Engineering Program. He is Fellows of American Physical Society, American Association for the Advancement of Science, and the Neutron Scattering Society of America. His areas of interest and research include polymer thin films, surfaces and interfaces for energy and sustainability.

Feasible Technology of Rotataed Graphene Drastically Improves the Capacity of Li-ion Batteries

Tereza M. Paronyan

HeXalayer, LLC, Louisville, KY,

Abstract

Lithium-ion batteries (LIBs) remain the most reliable energy storage for many portable electronics, Unmanned Aerial Systems (UAS), electric vehicles (EV), electric grid storage, and the Internet of Things (IoT). Exponentially increasing demand for those batteries would face a big challenge in providing Lithium due to the limited amount of Lithium on our planet. The inefficient use of cathode material as a Lithium source with a low-capacity anode (currently, graphite) increases the demand of Lithium for the higher energy demand. Besides their high voltage and safety, graphite-based anodes provide a very limited capacity (372 mAh/g) that keeps the energy density of these batteries relatively lower. The strength of repulsive forces within interlayer spaces of graphite limits the lithium diffusion into the anode structure during the battery charge.

HeXalayer develops and scales up the new class of high-capacity graphene as an anode for LiBs. This anode is a newly discovered layered graphene consisting of rotated graphene layers (referred also as incommensurate). The reversible capacity of this layered graphene anode has demonstrated up to 1,800 mAh/g throughout hundreds of charge-discharge cycles with over 97% Coulombic efficiency. The feasibility of this graphene technology promises a significant improvement of the energy density of Li-ion batteries and therefore efficient use of battery components.

Biography:

Tereza M. Paronyan is a Founder and a Chief Scientist of HeXalayer, LLC. Dr. Paronyan earned her Doctorate degree in Physics at the National Science Academy of Armenia in 2003. She has many years of postdoctoral experience working in Renewable Energy and Energy storage fields. Her current research focus is developing a novel graphene structure as an advanced material for secondary batteries. She is currently leading HeXalayer's projects toward commercializing graphene innovative technology for next-generation high-energy batteries and other applications. Her innovations and monographs have been published in high-impact journals, Encyclopedias, and handbooks as well.

A Spectral Selective Solar Harvesting Module for Synergistic Photothermal, Thermoelectric, and Photovoltaic Energy Generation

Donglu Shi[1*]
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Abstract

The efficiencies of photovoltaic (PV) and thermoelectric (TE) have been limited by the intrinsic properties to ~ 25 % and ~ 10 %, respectively. In current applications, photovoltaics utilizes the shorter wavelength end of the solar spectrum but suffer decreases in efficiency from heating caused by IR absorption. The novel tunable nanostructures of new hybrids eliminate this problem by directing thermal energy from longer wavelengths to the thermoelectric device. Solar light is harvested through transparent hybrid and segregated into different wavelengths:

the IR is absorbed by the hybrid which is photothermally heated up to 66.4 °C for the required thermoelectric temperature span; the UV/visible is directed to PV with reduced IR components, therefore significantly reducing heating. In this way, both PV and TE operate jointly by separately utilizing the full spectrum of solar light. The novel hybrid functions not only as a photothermal heater for TE but also a wavelength segregator enabling the PV and TE devices to synergistically produce electrical energy with much greater system efficiency. Also identified is the operating structural mechanism on spectral tunability and photothermal effect of the photonic hybrids.

Biography:

Donglu Shi is currently the Chair and Graduate Director of the Materials Science and Engineering Program at the University of Cincinnati. Donglu Shi's main interests include fundamental studies in nanoscience and novel applications in energy and biomedicine. Donglu Shi has so far published 300 refereed SCI journal publications including ones in Physical Review Letters, Nature, and Advanced Materials. He is currently the Editor-in-Chief of Nano LIFE, Editorial Board of Biomaterials Advances, and Associate Editor of J. of Nanomaterials. Donglu Shi has been elected as a Fellow of ASM International and a Graduate College Fellow at the University of Cincinnati. He has received Rieveschl Award for Distinguished Scientific Research, SIGMA XI Research Recognition Award, and Neil Wandmecher Teaching Award.

Evolution of Electrochemically Active Materials – Meeting the High-energy Density Challenge

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Abstract:

Energy storage is currently the primary engine critical for an energy independent global economy currently still very much dependent on tapping into the earth's natural reserves aided by natural oil and gas exports. The Li-ion battery chemistry has emerged at the forefront of secondary rechargeable battery systems and has witnessed burgeoning and ever-increasing research activity ever since the commercialization of the first Li-ion battery in 1990. There has been alarming advances in all areas of cathodes, anodes, and electrolytes. Despite much progress, lithiated transition metal oxides and carbon remain the preferred mainstream systems that have made it into the commercial systems deployed in electric vehicles (EVs) at present. The search for higher energy density systems has drawn the attention of Li-air and Li-S systems, of late. The Li-S systems are of particular interest due to the promise of achieving 500 Wh kg-1 , a "holy-grail" in energy density for next generation EVs matching and exceeding the performance metrics of the internal combustion engine (ICE). This presentation will discuss the materials challenges in generating high-energy density cathodes and anodes as well as electrolyte additives to meet the grand challenge of 500 Whkg-1. Efforts made in the areas of new sulfur confinement systems with ability to confine high sulfur loadings combined with unique electrocatalysts exhibiting the propensity to trap polysulfides while also catalyzing the formation of Li2S will be discussed. Concurrently, research directions in generating new dendrite-free anodes and current collectors as well as electrolyte additives matching the cathode performance will be outlined.

Biography:

Prashant N. Kumta is the Edward R. Weidlein Endowed Chair Professor in the Swanson School of Engineering at the University of Pittsburgh, Pittsburgh, PA. Dr. Kumta holds appointments in the Department of Bioengineering, Department of Chemical and Petroleum Engineering, Department of Mechanical Engineering and Materials Science in the Swanson School of Engineering as well as the Department of Oral and Craniofacial Sciences in the School of Dental Medicine. Dr. Kumta 's research interests span energy storage, energy conversion, and biomaterials for hard and soft tissue engineering, non-viral gene, and drug delivery including developing impedimetric biosensors for various disease detection.

Protecting users Against Covid-19 via Essential Oil-loaded Electrospun Mats

Helena P. Felgueiras

Centre for Textile Science and Technology, University of Minho, Portugal

Abstract

Face mask usage is one of the most important measures to reduce SARS-CoV-2 transmission. Yet, most masks display a passive-like action. Here, we propose to overcome this limitation by incorporating antiviral essential oils (EOs) within polycaprolactone (PCL) electrospun fibrous mats.

Twenty EOs were examined for the first time against the Escherichia coli MS2 virus (potential surrogate of SARS-CoV-2). The most effective were the lemongrass (LGO), Niaouli (NO) and eucalyptus (ELO) with a virucidal concentration (VC) of 356.0, 365.2 and 586.0 mg/mL, respectively. PCL was processed via electrospinning and EOs were loaded via: (1) physisorption on pre-existing mats (PCLaEOs), and (2) EOs blending with the polymer prior to fiber extrusion (PCLbEOs). In both cases, 10% VC was used as loading concentration. EOs presence and release from mats was confirmed by UV-visible spectroscopy (≈5257-631 μg) and gas chromatography-mass spectrometry (≈14.3% EOs release over 4 h), respectively. PCLbEOs mats were considered the more mechanically and thermal resilient, with LGO promoting the strongest bonds with PCL. Mats modified with the EOs were all identified as superhydrophobic. Air and water-vapor permeabilities were affected by the mats' porosity (PCL<PCLaEOs<PCLbEOs). Antimicrobial testing revealed the mats' ability to retain the virus (preventing infiltration) and to inhibit its action (log reduction >1). The most effective combination against the MS2 viral particles was the PCLbLGO. These mats were also deemed the most pleasant during sensory evaluation. Overall, data demonstrated the potential of these EOs-loaded PCL fibrous mats to work as COVID-19 active barriers for individual protection masks.

Biography:

Helena Felgueiras is a Biomedical Engineering from University of Minho (Portugal) with a PhD in the same field (specialization in biomaterials) from Université Paris 13 (France). Presently, she works has an Auxiliary Researcher at the Centre for Textile Science and Technology (2C2T, Portugal), developing antimicrobial surfaces resorting to biological cues, and heading the line of research in medical textiles. She is the author of 63 publications, with a h-factor of 17 (Scopus). HF has international collaborations with >10 countries, reflected in published work (110 co-authors). She has given 128 national/international communications and has received 12 awards and 12 distinctions.

Assessing the Light-induced Electron Transfer for Developing Photoelectrodes

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Abstract

Lithium-ion batteries are widely used to power a range of portable devices. While the use of such electronics and their portability has improved the overall quality of life, it comes with a drawback. The batteries need to be recharged. Although the electricity consumed for recharging a single device has little effect on a power grid, the sheer number of electronics worldwide collectively contribute to global electricity demands. Battery charging with fossil fuel producing electricity also contributes to greenhouse gas emissions. Alternative means for battery charging that are reliant on clean and renewable energy would mitigate greenhouse gas emissions. Solar energy is an ideal source of clean and sustainable energy that can be exploited to charge batteries. Indeed, batteries can be successfully charged by coupling to solar cells panels. This requires two unique components: the battery and a solar cell. Scaling the sun charging process to occur on a molecular level in the battery would have the benefit of consolidated the two otherwise separate devices into one. Towards such an all-in-one battery that can be charged with light, we will present the fundamental light triggered electron transfer process between a photoactive dye and the active components of a lithium-ion battery. Different solid-state electrode architectures will be presented along with systematic studies that confirm the light triggered process indeed results in electronic transfer at the molecular level.

Biography:

The Skene group research focuses on the design and preparation of functional materials for a broad range of tangible applications. The research team establishes structure-property relationships to guide in their rational design of functional materials having targeted properties for improving the performance of plastic electronics. Testing platforms to validate the opto-electronic properties of materials prepared include electrochromic devices, OLEDs, light emitting electrochemical cells, electrofluorochromic devices, and batteries. Recent efforts have focused on integrating green practices into device assembly by developing in situ polymerization method as well as using renewable feedstocks and environmentally benign solvents for materials preparation and processing.

Ligand Targeted Therapy: Role of the Surface Density of Anti- Avβ3 Peptides on Peg-B-PPS Micelles for Anti-angiogenic Activity

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Evan A Scott[2]

[1]Nanomedicine Lab, Department of Biomedical Sciences, University of Illinois College of Medicine at Rockford, IL, USA
[2]Department of Biomedical Sciences, Northwestern University, Evanston, IL, USA

Abstract

Diabetic retinopathy is one of the most prominent disabilities that cause vision impairment/irreversible blindness through retinal neovascularization. The current treatment options involve the administration of anti-VEGF agents through frequent intravitreal injections which may cause severe adverse effects. The anti-VEGFs currently used can interfere with the normal physiological process involving VEGF and may cause hypertension, myocardial infarction, and stroke. Ligand-targeted therapy was recently established as a promising strategy for the angiogenesis-related

disease. In this study, we developed an αvβ3 integrin-targeted PEG-b-PPS micelles (PEG-b-PPS-aANG MC) and reduce the side effects associated with non-specific binding. We evaluated the optimum density of anti-integrin peptides on MC to induce anti-angiogenesis using primary human umbilical vein endothelial cells. PEG-b-PPS-MCs were synthesized using the co-solvent evaporation method. Characterization of the micelles was carried out by dynamic light scattering (DLS) and Cryo-TEM. The integrin blocking after short-term exposure with peptide-bound micelles was evaluated by immunocytochemistry using Anti-human CD51/CD61. The average particle size of the blank micelles and SDV peptides was between ~60-80 nm. Detailed investigation on the anti-angiogenic effect in vitro demonstrated a surface peptide density-dependent effect by the MCs compared to random-peptide and cRGD-MCs, primarily through the AKT signaling pathway. Moreover, the developed nanomedicine showed a potential anti-inflammatory response in activated macrophages as well as endothelial cells. The study demonstrated that peptide density on the micellar surface is crucial in enhancing integrin clustering for anti-angiogenesis. Continued research is underway for the development of a sustained-release PEG-b-PPS-aANGP depot to reduce intravitreal injection frequency.

Biography:

Divya Bijukumar received her MS in biotechnology from Mahatma Gandhi University, India in 2005. In 2012 she received her Ph.D. degree in Nanobiotechnology from Amrita University, India. After graduation, she worked as a Postdoctoral research fellow at Amrita University (India), University of Witwatersrand (South Africa), and the University of Illinois College of Medicine (USA). Currently, she is an Assistant professor at Nanomedicine Lab under Biomedical Sciences at UIC College of Medicine Rockford, USA. She has more than 60 peered reviewed research publications, 4 book chapters, and several conference presentations. Bijukumar is part of three NIH grants (Two R03- PI and one R01-co-I). She won the prestigious William. H. Harris Award from the Orthopedic Research Society in 2020.

The Influence of Alkanethiols on the Production of Hydrophobic Gold Nanoparticles via Pulsed Laser Ablation in Liquids

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Abstract

The ability to suspend plasmonic metal nanoparticles in apolar environments is an important feat towards harnessing their optical properties for use in amphiphilic biological environments. Pulsed Laser Ablation in Liquids (PLAL) is a well-established method for the production of gold nanoparticles (AuNPs) in aqueous environments; however, ablation in organic liquids for the synthesis of hydrophobic AuNPs still has many unknowns, such as the relationship between colloidal stability and the ligand shell. In this study, hydrophobic AuNPs were produced by PLAL of gold in a 1-alkanethiol/n-decane solution and treated with laser fragmentation. Results demonstrate that longer chain length ATs produced particles with a smaller average size; however, there was no strong correlation between alkanethiol (AT) concentration and particle size. Stability was investigated by monitoring the temporal evolution of the extinction spectra which revealed that lower concentrations of AT stabilize the colloids while higher concentrations tend to result

in quicker particle aggregation. Furthermore, longer chain length ATs demonstrated improved stability. Additionally, vibrational spectroscopy was employed to examine the AuNP surface chemistry, which pointed to the presence of oxidized carbon species and graphitic carbon.

Biography:

Cory Trout is an Assistant Teaching Professor at Rutgers-Camden University where he also received his bachelor's degrees in both physics and mathematics. He has received his master's and is currently pursuing his PhD in applied physics from the collaborative NJIT-Rutgers Newark Applied Physics Program. Mr. Trout is currently working under Dr. Sean O'Malley studying light-material interactions for the purpose of nanomaterial production and light-activatable nanoscale technologies.

Green Synthesis of De Novo Bioinspired Porous Iron-Tannate Microstructures with Amphoteric Surface Properties

Sheeba Dawood*
Hemali Rathnayake
Gayani Pathiraja
Kelvin Adrah
Olubunmi Ayodele

Abstract

Bioinspired porous microstructures of iron-tannate (Fe (III)-TA) coordination polymer framework were synthesized by catenating natural tannic acid with iron (II), using a scalable aqueous synthesis method in ambient conditions. The chemical composition, morphology, physiochemical properties, and colloidal stability of microstructures were elucidated. The surface area (SBET) and the desorption pore volume were measured to be 70.47 m2/g and 0. 44 cm3/g, respectively, and the porous structure was confirmed with an average pore dimension of ~27 nm. Microstructures were thermally stable up to 180 ◦C, with an initial weight loss of 13.7% at 180 ◦C. They exhibited high chemical stability with pH-responsive amphoteric properties in aqueous media at pH levels ranging from 2 to 12. Supporting their amphoteric sorption, microstructures exhibited rapid removal of Pb+2 from water, with 99% removal efficiency, yielding a maximum sorption capacity of 166.66 mg/g. Amphoteric microstructures of bioinspired metal–phenolate coordination polymers remain largely unexplored. Additionally, natural polyphenols have seldomly been used as polytopic linkers to construct both porous and pH-responsive amphoteric coordination polymer frameworks with a robust structure in both acidic and basic media. Thus, this de novo porous microstructure of Fe (III)-TA and its physiochemical surface properties have opened new avenues to design thermally and chemically stable, eco-friendly, low-cost amphoteric sorbents with multifunctionality for adsorption, ion exchange, separation, storage, and sensing of both anions and cations present in heterogeneous media.

Influence of Thermoplastic Polyurethanes in Polymer Blends for Additive Manufacturing

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Abstract

Acrylonitrile-butadiene-styrene (ABS) and acrylonitrile-styrene-butylacrylate (ASA) are currently two of the most used polymeric materials in additive manufacturing technologies such as fused filament fabrication (FFF) and fused granular fabrication (FGF) due to their good mechanical

properties, good range of operating temperatures and weatherability. However, materials printed via FFF or FGF present high anisotropy in the mechanical properties due to poor adhesion between the printed layers. This may lead to a decrease below 1/3 in tensile strength. Moreover, adequate 3D printing of ABS and ASA requires the previous heating of a printing platform or chamber above 90 ºC to ensure good adhesion of the first deposited layer and minimize undesired effects as warping. To overcome these issues, in this work we present a set of materials suitable for FFF and FGF prepared from blends containing either ABS or ASA and thermoplastic polyurethanes (TPUs). TPU is expected to enhance the adhesion between layers, thus reducing the anisotropy in the mechanical properties. The printing conditions were optimized for different blends with contents up to 50 wt% TPU and the mechanical properties of standard specimens printed in different directions were tested. ABS: TPU blends containing less than 30 wt% TPU exhibited enhanced tensile strength when compared to pure ABS, suggesting an enhancement of the adhesion between the layers caused by TPU. Moreover, blends containing 30 wt% TPU allowed successful fabrication of objects without heating the printing platform. The mechanical properties of this material did not vary when the printing platform was increased up to 90 ºC.

Biography

Alberto Sanz de León started his scientific career in the Institute of Polymer Science and Technology (ICTP-CSIC), where he received his PhD in Polymer Chemistry in 2015. Then, he became a postdoctoral researcher at the Max Plank Institute of Colloids and Interfaces (MPIKG), where he worked for 2 years in the development of polymers for mechanical sensing. Since 2018, he works at the University of Cadiz in the development of new polymers and polymer-based nanocomposite materials for additive manufacturing.

Polymer-based Membranes for NGL Recovery from Natural Gas

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Abstract:

Raw natural gas consists primarily of CH4 as the prevailing element, but also contains significant amounts of impurities (e.g., CO2, H2S, N2, He, and hydrocarbons). The separation & removal of C3+ hydrocarbons (i.e., natural gas liquid, NGL) from natural gas is necessary to prevent condensation during transportation by reducing the dew point and heating value to pipeline specification. In addition, these C3+ hydrocarbons are valuable chemical feedstocks, and can be used as a liquid fuel for power generation. Polymer membrane-based separation technology offers a low-cost alternative to traditionally energy intensive adsorption processes. Conventional rubbery polymers, such as PDMS, are utilized industrially for the rejection of N2 and for the concentration of C2+ hydrocarbons in the membrane permeate streams, but these membranes exhibit low C3+/CH4 selectivities due to high degree swelling under C3+ rich hydrocarbon feed streams. In this talk, the application of synthetic polymeric membranes for NGL separation and recovery is reviewed. We demonstrate strategies to overcome this limitation by developing novel siloxane rubbery and reverse-selective glassy polymers for NGL recovery from natural gas. These novel polymer membranes showed enhanced separation performance under industrially relevant feed streams and testing conditions. Results emphasize the observations that membrane separation performance is strongly related to the testing conditions and feed compositions, highlighting the importance of exploring and designing better polymer-based membranes for the actual industrial process.

Biography:

John Yang received his Ph.D. in Polymer Science from Chinese Academy of Sciences and completed his postdoctoral training in the Department of Materials Science & Engineering at University of Michigan, Ann Arbor. Dr. Yang joined Aramco Boston Research Center in 2013, and is now leading Material Technology Group to develop advanced materials for gas separation and carbon capture, utilization and storage. Before joined Aramco, he worked with Dow Chemical Company in the fields of polyolefin and thermoplastic product development, membrane for water purification & wastewater treatment. Dr. Yang is coauthor on 36 peer-reviewed articles and 16 patents.

Thermogravimetric Analysis of Polymers and Polymer-based Nanocomposites

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Karen Lozano
Dorina M. Chipara
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Abstract

Thermogravimetric analysis TGA) is a well-established method in the study of the thermal features of polymers and polymer-based nanocomposites (obtained by dispersing nanoparticles within polymeric matrices). The lecture provides a critical review of the method, focusing on the thermograms obtain in different environments (air and inert atmosphere). The analysis will include a detail discussion of our recently approach to the modeling of the experimental thermograms (for the case of a single isolated sigmoid). The proposed model will be checked for thermal degradation processes characterized by an overlap of two sigmoid (as in the degradation of polyvinylidene chloride). Recent spectrometers have the capability to record also the derivative of the thermograms with respect to the temperature. This allows the transition from some empirical definitions (such as temperature at which the residual mass is dropped to 50 %) by some parameters with scientific significance such as the inflection temperature (or the temperature at which the mass loss rate is highest) as well as the residual mass at the inflection temperature. The approach allows for the introduction of a new parameter which is the width of the dependence of the thermogram derivative on temperature. This parameter Is typically not used in the analysis of TGA data. TGA capability to reveal the presence of an interphase is also investigated. While in most cases, TGA is not yet capable to quantify the amount of interphase, it is still capable to sense and to warn the user about the potential formation of an interphase.

Lead-Iron Perovskites - Room Temperature Nanoscale Multiferroic Thin Films with Strong Magnetoelectric Coupling

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Dilsom Sanchez
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Department of Physics, University of Puerto Rico, San Juan
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Abstract:

The coexistence of magnetization and electric polarization in a multiferroic material gives rise to extra atypical properties that can be utilized in designing several novel multifunctional devices including next generation logic and non-volatile memories devices. In this talk, we will be reporting fabrication, dielectric, ferroelectric, piezo-response force microscopy, magnetic force microscopy, magnetization and magnetoelectric coupling measurements of some interesting lead-iron perovskites, such as (1-x)Pb(Zr0.52Ti0.48)O3-xPb(Fe0.5Nb0.5)O3 (PZTFNx), and (1-x) Pb(Zr0.52Ti0.48)O3-xPb(Fe0.5Ta0.5)O3 (PZTFTx) for x = 0.2-0.3 single phase room-temperature magnetoelectric multiferroic thin films that were deposited on suitable substrates by laser ablation processes in oxygen atmosphere. A saturated magnetization (M-H curve) loop with a strong remanent magnetization was observed at room temperature and the films retain the ferromagnetic ordering from 5- 400 K. The magnetization orderings are argued based on Fe3+-O-Fe3+ exchange interaction. Ferroelectric piezoelectric nature of strong domain switching in the films is confirmed from phase and amplitude image contrasts using piezo-response force microscopy (PFM). The magnetic domains profiles were studied using magnetic force microscopy (MFM). We carried out temperature dependent dielectric measurement on these metal-insulator-metal (M-I-M) heterostructure capacitors to understand the ferroelectric ordering in these materials. P-E loops measured from the M-I-M reveal their ferroelectric ordering at room temperature. These thin films exhibited very large magnetoelectric couplings at room temperature for an in-plane bias field of around 350 Oe. These studies demonstrate that PZTFNx and PZTFTx thin films are room temperature multiferroic with reasonably large magnetoelectric couplings and are suitable materials for magnetic sensors and spintronic device applications.

Biography:

Ram Katiyar is a Professor of Physics at the University of Puerto Rico, San Juan (USA) where he has been leading Advanced Materials Research Laboratory for investigations in the area of nano-structured materials and thin films for energy, memory, and sensor applications. His expertise include ceramic processing and growth of oxide films by PVD techniques and their characterization to understand size:structure:property relationships in various ferroelectric, multiferroic, semiconductor, and energy storage materials. His immense contributions in these fields are represented by his excellent publication record (>1200) in the reviewed scientific journals. He is a fellow of American Physical Society, Materials Research Society, Electrochemical Society, and also a fellow of American Ceramic Society for his contributions in the area of growth and characterization of nanostructured ferroelectric materials.

GaAsSb Nanowires-based Short Wave Infrared Photodetectors

Shanthi Iyer

Nanoengineering, North Carolina A&T State University, USA

Abstract

Nanowire-based structures offer opportunities to create the next generation of advanced devices by exploiting scale-dependent unique material properties that arise due to its anisotropic geometry in the nanoscale regime. In addition, the large surface-to-volume of the NW configuration relaxes lattice mismatch constraints, expanding the material combinations that can be used and enabling the implementation of a variety of architectures, which are not conceivable in thin films. These, combined with their remarkable quantum, surface, and outstanding optical absorption properties, permit innovative bandgap engineering of the NWbased heterostructures to achieve high-performance III-V-based optoelectronic devices integrated onto Si and other 2D substrates. This talk will be focused on ongoing research findings at North Carolina A&T State University on the Ga-assisted molecular beam epitaxial growth of GaAsSb nanowires on Si and graphene in

axial and core-shell architectures. The performance of various NW-based photodetector devices, p-i-n junction, and avalanche photodetectors will be presented.

Biography

Shanthi Iyer, Professor in the Nanoengineering Department at the Joint School of Nanoscience and Nanoengineering has been responsible for initiating and developing NCA&TSU's state-of-theart Molecular Beam Epitaxy (MBE) Laboratory and associated academic and research programs. Her current research is MBE growth, characterization, and fabrication of next-generation compound semiconductor nanowire-based photodetectors for various applications. She has published over 65 journal papers and proceedings and has been granted a patent.

Percutaneous Stent Graft Deployment to Treat Arterial Aneurysms: is the Lack of Smart Materials Responsible for the Plateau to be Reached Prematurely?

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Jing Lin
Yvan Douville
Eric Philippe
François Côté
Lu Wang
Ze Zhang

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College of Textiles, Donghua University, Songjiang District, Shanghai, China.

Abstract

Since the early percutaneous deployments of endografts to treat arterial aneurysms in the early 1990s by Volodos in Ukraine and Parodi in Argentina, stent grafts have been acknowledged as the most elegant technique preferably performed compared to open surgery. The frail older patients were first to benefit from this milestone technique. Progressively the indications were extended for the treatment of younger people. Dake deployed stent grafts in the thoracic aorta. The basic design of all endografts is somewhat similar: tubular grafts supported by self-deployable or balloon-deployable stents. The first generation was in manufacturing startups with less than optimal materials. Fabrics were fragile and nitinol wires corroded rapidly. The evolution to get devices with satisfying biofunctionality and biodurability was achieved at the turn of the previous century. Research-oriented companies as Cook & Gore proved to be successful. In the meantime, multiple startups were agglomerated in major manufacturing key players such as Medtronic, Torumo, MicroPort. Biofunctionality and biostability of stents were quickly reached, whereas only polyester and ePTFE survived as tubular grafts. Polyurethane tubes ended up as medical disasters being underreported. The indications were expanded with branched endografts to treat suprarenal and aortic arch aneurysms. New generation of medical imaging devices and developing ancillary equipment were key determinants in order get more patients treated, whatever their age. The infections were on the decline after the setup of hybrid operating rooms. Currently, deployment of chimney grafts and fenestrations (customized, on-site or in situ) made more people amenable to standard recanalization of blood flow through aneurysms. Regretfully the biocompatibility issue is still to be addressed. The search for devices made with polyester fabrics that are resistant to abrasion and pitting, and capable of biointegration still represents a considerable challenge. Development of mass spider silk through targeted gene replacement has gone nowhere, and is probably reaching a dead end. The ongoing efforts to develop smart materials look hopeless, as there is no flag in the field. Bioinspiration presents theoretically a great potential in the long term. However, crowds of patients demand immediate treatments. Yes, a plateau has been rapidly reached for the care of patients benefiting from an efficient

treatment. New generations of devices will tackle some specific niches but marginal progress can only be anticipated in the forthcoming decades: they come from improved medical practice, better ancillary equipment and more sophisticated imaging techniques. As we enter the Fourth Industrial Revolution, the relationship with biomaterial science is lagging behind.

Current and Future of Red and Black Phosphorus Nanomaterials

Hai-Feng Ji

Department of Chemistry, Drexel University, Philadelphia PA, USA

Abstract:

I will present a summary of some optoelectronic applications of red and black phosphorus nanomaterials. The synthesis, characterization, stability improvement of the materials will also be discussed.

Biography

Hai-Feng (Frank) Ji is current a professor of Department of Chemistry, Drexel university. His research interests focus on MEMS devices, nanomaterials for energy and environmental applications, drug discovery, nanopillars and phosphene for energy applications, and surface chemistry. He is currently a co-author of 210 peer-viewed journal articles and book chapters. He has an H-index of 42. He is an editorial board member of several chemistry journals.

Geopolymer Concrete Railroad Crossties Prestressed with Basalt FRP Bars

Mohsen Issa*
Mounir Kassem
Alain Saroufim

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Abstract:

Railways constitute the primary transportation systems in the US. Their integrity and durability are a main concern for economy and safety. The condition of the railway system depends mainly on the interaction between the fastening components including the rails, plates, and railroad ties, in addition to their interaction with the crossties. The railway crossties play a key role in distributing loads from the wheel rail interface into the subgrade and hold tracks gauge. Given these performance requirements, their integrity is of great importance. This newly materials-related crosstie may provide an opportunity to increase the service life of these components while also mitigating the environmental impact of any treatment methods that were used on the original product. The objective of this research project is to demonstrate and validate the use of an innovative prestressed BFRP polymer concrete crosstie that have very good mechanical and durability characteristics. The crossties were tested for center negative moment region and rail seat positive moment region in accordance with the AREMA Manual for Railway Engineering testing standards. Very good performance test results were observed for the center negative moment and rail seat positive moments for both crossties. The BFRP material proved to be a suitable alternative to steel tendons where corrosion problems are more evident. In addition, the inclusion of synthetic fiber reinforcement in the concrete matrix has significantly improved the rail tie performance in the considered tests.

Biography:

Mohsen A Issa, PhD, PE, SE, F.ACI, F.ASCE, and F.SEI is a professor of structural and materials engineering at the University of Illinois at Chicago. His research interests include structural buildings and bridges, advanced composites, concrete durability, recycled plastic materials, and sustainability. He is a Fellow of the American Concrete Institute (ACI), Fellow of American Society of Civil Engineers (ASCE), and fellow of the Structural Engineering Institute (SEI) as well as a member of several professional organizations and societies including ACI, ASCE, PCI, and TRB. Dr. Issa is a registered Structural Engineer in the State of Illinois as well as Professional Engineer in the State of Florida.

Microstructural Modification and Mechanical Properties Improvement of Titanium and Titanium Alloys through High-Density Pulsed Electric Current

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Yang Ju*

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Abstract

Titanium and its alloys are versatile materials that find widespread use in various applications, including aircraft parts, steam turbines, medical devices, etc. Thermomechanical processing is typically necessary during the manufacturing of titanium and its alloys to improve their microstructure and performance. However, the conventional thermal process often involves high temperatures and long processing times, which can increase costs and pose environmental challenges. Recently, we developed a novel method based on high-density pulsed electric current (HDPEC) treatment to enhance the microstructure and mechanical properties of metallic materials. Our study demonstrates that low current input HDPEC treatment can increase the strength and ductility of pure titanium. Microstructural characterization reveals that the treatment enhances the twin boundary and dislocation density, which contributes to improving mechanical properties. In the case of the dual-phase α/β titanium alloy Ti-6Al-4V, the situation is more complex but interesting. The HDPEC treatment results in grain refinement and increased dislocation density, leading to enhanced strength. Additionally, the improved β-Ti and α/β coherent grain boundaries contribute to increased ductility. Overall, this novel method shows promise for achieving low-cost and high-efficiency manufacturing of titanium and its alloys.

Biography

Yang Ju received a B. Eng. in 1985 and a Ms. Eng. in 1991 in Electrical Engineering from Shandong University of Technology and Tsinghua University, China, respectively. He received a Dr. Eng. in 1999 in Mechanical Engineering from Tohoku University, Japan. He became an associate professor in 2003 at Tohoku University, and a professor in 2007 at Nagoya University, Japan. Professor Ju's research interests include damage recovery, crack healing and property enhancement of metallic materials, creation and development of functional nano and biomaterials. He has published more than 200 manuscripts in Archival Journals and has 16 patents in Japan and United States. Prof. Ju received The Japan Society of Mechanical Engineers Medal in 2006. He became a Fellow of The Japan Society of Mechanical Engineers in 2018, and a member of The Engineering Academy of Japan in 2021.

The Microstructures and Creep Deformation Mechanisms of a Superalloy Fabricated by Electron Beam Layer Solidification

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Masao Takeyama[3]
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[4] Institute of Metal Research, Chinese Academy of Sciences, China.

Abstract

A new additive manufacturing method, namely electron beam layer solidification (EBLS) technology is put forward to prepare the Inconel 718 alloy with refined microstructures and high purity, which shows an extended creep life of 1266.3 h at 953 K/500 MPa. Detailed microstructure-property relationship of the EBLS alloy has been obtained for the first time and compared with a traditional alloy. The alloy prepared by EBLS shows refined microstructures with dendrite spacing of less than 23 μm, in which the microsegregation coefficient of Nb remains 1.97, and thus formation of large carbides in the inter-dendrite areas can be restrained. The EBLS alloy exhibits a typical intergranular failure mode, while the transgranular fracture is observed for the conventional alloy. The inter-dendritic MC carbides formed by the abnormal reverse diffusion of Nb could impede grain boundary sliding or initiate cracks, depending on their size and morphology. The tiny grain boundary δ precipitates in the EBLS alloy could reduce the critical stress for microvoids nucleation to 161.07 MPa by decohering the particle/matrix interface or vacancy condensation near the δ interface, and thus contribute greatly to grain boundary microcracks formation. For the conventional alloy, the large size MC carbides inherited from the solidification process, although accounting for merely 0.36 vol.%, could nucleate microcracks by particle fracturing.

Biography:

Xiaogang You is a research fellow at Zhengzhou University. His research interests include the preparation of metals and alloys with high purity and homogeneity by electron beam metallurgy, and the controlling of the microstructures and properties of the alloys. He has published over 50 papers on Journals such as Journal of Materials Science & Technology, Journal of Cleaner Production, Separation and Purification Technology, Scripta Materialia, and so on, and has been authorized more than 20 national or international patents. He is also the guest editor and reviewer of many SCI journals, and the member of several international and national academic organizations.

Tungsten Trioxide Films Produced by Ultrasonic Spray Deposition for Electrochromic Devices

Chi-Ping Li*
Bing Ze Li

Department of Chemical Engineering, National United University, Maioli, Taiwan

Abstract

Template-assisted sol gel chemistry provides a versatile approach to introduce order and porosity into nanostructured materials. However conventional evaporation induced self-assembly techniques are not easily scaled to produce films with sufficient thickness over large areas at the throughput required by electrochromic windows. The principles of sol gel chemistry may be deployed using ultrasonic spray deposition (USD) for scalable synthesis of nanocrystalline WO3 films with unrivalled electrochromic performance are demonstrated [1-4]. Systematic manipulation of sol chemistry enabled the production of mesoporous films with high specific surface area (>100 m2/g), mean pore sizes of ~5 nm, and narrow pore size distributions. Film thickness is found to be proportional to the sol concentration and number of spray passes, and various combinations are shown to produce films capable of modulating >98% of incident solar radiation in the visible spectrum (450–900 nm). Elimination of haze enables full transmission in the bleached state, while the broadband coloration is attributed to the exceptionally high charge density (>120 mC/cm2). The materials have good switching speeds which improve with specific surface area, and the long term durability is promising.

Biography:

Chi-Ping Li received his PhD of Materials Science from Colorado School of Mines (USA) in 2014 and followed by postdoctoral research in National Renewable Energy Laboratory (NREL, USA) in 2015. He joined Department of Chemical Engineering in National United University in Taiwan as an assistant professor in 2018. His research interests are mainly focused on synthesis of nanostructured films, nanocomposite films and nanoparticles. Those materials are used in electrochromic windows, lithium batteries, organic photovoltaics and LED encapsulants. His goal is to overcome the challenges and produce great but low cost materials in the fields of green and renewable energy.

Functionalized Bioelectronic Materials for Multiplexed Leukocytes Enumeration

Umer Hassan*

Rutgers The State University of New Jersey, USA

Abstract

Functionalized bioelectronic materials finds many biomedical applications. Here, we present out work in developing biomedical platforms where multiplex biomarker detection is enabled by functionalized bioelectronic materials. Bioelectronic materials in particular hydrogel microparticles with different electrical properties were utilized for targeting different biomarkers in complex sample matrices. Recently, we have shown the target application for leukocyte multiplex detection. Hydrogel microparticles were probed at different frequencies to generate unique electrical signatures. Once these particles are functionalized with specific antibodies, they can target different corresponding leukocyte antigens. Such conjugated were detected in a microfluidic impedance cytometer. We tested the multiplexing system with human blood samples collected from the patients.

Biography:

Umer Hassan is an Assistant Professor at the Department of Electrical and Computer Engineering (ECE) and Global Health Institute at Rutgers University. He is the director of the Laboratory of Immunoengineering and Micro-nano technologies for Personalized Healthcare (LIMPH). Dr. Hassan completed his Ph.D. studies in ECE from UIUC in 2015. His research has been focused on developing point-of-care (PoC) translational biosensors for infectious disease diagnostic applications for global health settings. Dr. Hassan has received many awards including Brandt Early Career Investigator Award in Precision Medicine (2017), BMES Career Development Award (2017), Baxter Young Investigator Award (2016, 17) among others.

Computational Insight into the Electrochemical Stability of Hexamethylphosphoramide as Electrolyte Additive for Graphite Dual-ion Battery

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Zie Zin Khoo[2]
Kai Yi Chow[2]
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[2]Xiamen University Malaysia Campus, School of Energy and Chemical Engineering, Jalan Sunsuria, Bandar Sunsuria, Selangor

Abstract

In this study, molecular dynamics (MD) simulations and density functional theory was used to investigate the behavior of a ternary electrolyte solution consisting of ethyl methyl carbonate (EMC) with hexamethylphosphoramide (HMPA) as an additive and lithium hexafluorophosphate (LiPF6) as a salt for a lithium-ion battery. The MD trajectories of the electrolyte solution and the radial distribution function (RDF) of the solvent molecules around the lithium and PF6 ions were generated. Additionally, we perform density functional theory (DFT) calculations to determine the HOMO-LUMO energy levels of EMC and their impact on its stability in the presence of HMPA. Small amounts of HMPA to the electrolyte solution alter the solvation structure of the solvent molecules around the lithium and PF6 ions, leading to an increase in the strength of the solvation shell. The polar and acidic nature of HMPA can enhance the solvation of PF6 ions and improve its mobility by forming stable solvated complexes with the anion. We also find that EMC with higher HOMO-LUMO energy levels is less stable in the electrolyte solution, with a greater tendency towards degradation and formation of unwanted side products. However, the presence of HMPA can mitigate the degradation of EMC by stabilizing its HOMO-LUMO energy levels and improving its solvation properties. Our RDF analysis and DFT calculations provide insights into the solvation structure of the ternary electrolyte solution and the impact of the HOMO-LUMO energy levels of EMC on its stability, as well as the effect of adding HMPA as an additive. These findings are crucial for designing more efficient and stable lithium-ion batteries.

Biography:

Zhafran is from Universiti Malaya, Malaysia; currently he is pursuing MSc. (research) in Computational Chemistry, under the supervisions of Assoc. Prof. Dr. Vannajan Sanghiran Lee, Prof. Dr. Sharifuddin Md. Zain, and Dr. Chong Woon Gie from Xiamen University Malaysia Campus. His present research interest includes material design, where he grows interest in energy storage design: 2D Materials; supercapacitor and other electronic devices, rechargeable dual-graphite battery, hydrogen storage, polymer, LED, ionic liquids, and protein-ligand interactions by using molecular dynamics simulations, density functional theory (DFT) and Ab Initio simulation.

Nanocrystallization of Fe-based Rapid Quenched Alloys

Motoki Ohta

[1] PROTERIAL. Ltd. (previously Hitachi Metals), Japan
[2] Shimane University, Japan (Concurrent post)

Abstract

Fe-based nanocrystalline alloy ribbons are beginning to attract attention as a candidate for new iron core materials to replace electrical steel sheets and amorphous alloy ribbons. By using this nanocrystalline structure powder in resin-molded cores, it is expected to achieve both high

superposition characteristics and low core loss when applied to high-frequency inductors. In order to obtain this structure with powder, it is necessary to solve problems specific to powder. First, let us briefly touch on the mechanism of nanocrystal appearance in ribbon materials. The nanocrystalline phase of this material is obtained by heat treatment after obtaining the Fe phase amorphous phase by liquid quenching. In this case, Cu is used as the nucleus of the nanocrystals, and the number density of the nuclei depends on the Cu concentration and the cooling rate. It has been confirmed that when the number density of nuclei is low in the As-Q state, a nanocrystalline phase can be obtained by performing a rapid heating heat treatment. It is not realistic to subject the powder to rapid heating heat treatment. In addition, since the cooling rate of the powder is highly dependent on the powder size, the number density of nuclei also varies from particle to particle. Tuning by composition is difficult. Therefore, we tried to solve it by adding a certain element so as to the nuclei can be stably supplied in any state.

Biography:

2002 Received Ph.D. from Tohoku University. 2003~2005 Assistant Professor at Tohoku University. Joined Hitachi Metals (HML) in 2005 as a researcher. In 2013, seconded to Metglas, a subsidiary of HML, as a senior researcher. 2015 Returned to HML. In 2019, concurrently served as a professor at Shimane University. At Tohoku University, he studied magnetic properties, and after joining HML, he was engaged in the development of soft magnetic materials. Currently, the project leader of a Next Generation Co-creation project in which HML and Shimane University participate.

Surface Engineering of Electrospun Fibrous Scaffolds for Enhancing Cell Attachment, Infiltration and Proliferation

Kyriakos Komvopoulos*

Department of Mechanical Engineering, University of California, Berkeley, CA, USA

Abstract

The morphology and chemistry of bio-surfaces play influential roles in cell behavior. Specifically, surface texture impacts cytoskeletal components affecting cell shape, growth, and motility, whereas surface chemical functionalities control cell surface affinity. Surface micro-patterning by lithographic techniques and surface texture and chemistry modification by plasma treatment are effective methods for creating morphological and chemical surface cues, respectively, which can elicit cell attachment and enhance cell infiltration and proliferation. For instance, scaffolds with aligned fibers can affect cell migration, organization, and differentiation. However, cell attachment and growth on polymeric surfaces is fairly limited due to the lack of suitable biochemistry. Plasma surface treatment is a versatile method for tuning surface chemical and mechanical properties to specific application needs. This method yields a wide range of surface functionalities, which can greatly improve biocompatibility either directly or indirectly through biomolecule surface immobilization. This presentation will highlight advances in plasma surface chemical modification and micro-patterning of polymeric fibrous scaffolds, using select results to illustrate the efficacy of the former methods to produce scaffolds with different structural and biochemical characteristics, including fiber alignment, locally relatively high or low porosity, micro-wells of different dimensions, and different biochemical surface characteristics. The substantial improvement in cell attachment, infiltration, and proliferation produced by the foregoing surface engineering techniques reveals the high potential of these methods for various tissue engineering applications.

Biography

Kyriakos Komvopoulos holds the position of Distinguished Professor in the Department of Mechanical Engineering, University of California, Berkeley. He is also the founder and director of the Surface Sciences and Engineering Laboratory and the Computational Surface Mechanics Laboratory, and Faculty Scientist, Materials Sciences Division, Lawrence Berkeley National Laboratory; Principal Investigator, Center for Information Technology in the Interest of Society; and Principal Investigator, The Berkeley Stem Cell Center. He is internationally known for pioneering research in surface nanosciences and nanoengineering, with important implications in several emerging technologies including ultrathin films, microelectronics, information storage, and biotechnology.

Surface Functionalization for Improved Osseointegration on Additively Manufactured Materials

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Maria Rosaria Saffioti[2]
Domenico Umbrello[2]

[1]Department of Management, Finance and Technology, University LUM Giuseppe Degennaro, Italy
[2]Department of Mechanical, Energy and Management Engineering, University of Calabria, Rende, Italy

Abstract

Additively manufactured parts are increasingly gaining interest for biomedical applications. In fact, the possibility to customize a medical device reducing the risk of infection and post operation complications is becoming a fact. Thus, it is necessary to understand how the additively manufactured part can influence the human response to implantation and how their surface characteristics can be modulated in order to optimize their performance. In this work an experimental campaign in order to modify the additively manufactured Ti6Al4V surfaces for bone implants fabrication has been performed. In particular, cell culture has been carried out over the samples and compared with the wrought one in order to understand how the surface state and the fabrication methodology influences the cell response over the samples. Results demonstrate that both fabrication and post processing influence the surface state which, in turn, dictates the cell behavior on the implant.

Biography:

Giovanna Rotella is currently an associate professor at LUM University, Bari, Italy. She holds a PhD in Production Systems at Politecnico di Torino (Italy) where she graduated in February 2013. She holds a master's degree in mechanical engineering from University of Calabria. Her research activities have been focused on surface modifications for biomedical applications, surface integrity by Severe Plastic Deformation processes, wear and corrosion, surface modification of engineering materials for improved wettability and adhesive bonding, but also on the interrelation between machining processes, surface integrity and sustainability which was the subject of her PhD dissertation.

Dual-functional Fibrous Filter Incorporating Conductive Nanowire and Photocatalytic Nanoparticle for Indoor Air Quality Control

Gen-Wen Hsieh*
Ren-Yao Zheng

Laboratory for Organic and Nano Electron Devices & Materials, Institute of Lighting and Energy Photonics, College of Photonics, National Yang Ming Chiao Tung University, Tainan, Taiwan

Abstract

In light of the substantial threat to public health and life quality brought on by air pollution, it is high time to think of how we can protect human health, and deal with particulate matters (PMs) and volatile organic compounds in efficient and economical manners. Although a variety of porous and fibrous filters based on mechanical filtration mechanism have been reported with high PM removal efficiency. More PMs captured deeply by these filters can cause excessive pressure drop and unfavourable clogging effect, leading to small dust holding capacity and short service life as well as high energy consumption. Therefore, deep insight into the augmentative materials and feasible fabrication systems would be very helpful in the quest for high efficient, sustainable, and affordable air pollution control.

Herein, we demonstrate a dual-functional polyester fibrous air filter consisting of self-assembled titanium dioxide nanoparticles and percolated silver nanowires for high air permeability, electrostatic PM removal, and photocatalytic formaldehyde decomposition. The surface-functionalized polyester air filter reveals a remarkable PM removal efficiency of up to 99.5% and a quality factor of 0.42 Pa^{-1} during heavy hazardous smoke. The re-useable filter is also able to maintain high removal efficiency after five cleaning cycles. Further, with the aid of the decorated photocatalytic titanium dioxide nanoparticles the same network can effectively degrade gaseous formaldehyde under UV irradiation. This strategy of surface-functionalizing nonwoven fabrics, which is reliable, easy-to-handle and low-cost, may open up a promising alternative route in tackling global air pollution-related crises.

Biography:

GEN-WEN HSIEH has been an Associate Professor of Institute of Lighting and Energy Photonics, National Yang Ming Chiao Tung University, Taiwan, since 2018. He holds a BSc in Chemistry and a MSc in Chemical Engineering from National Tsing Hua University, Taiwan. From 2002-2006, he was an R&D engineer in the Industrial Technology and Research Institute, Taiwan. Then he went on to read for a PhD in the Electronic Devices and Materials Group at Engineering Department, University of Cambridge, UK, under the supervision of Prof. Bill Milne. Gen-Wen's research interests include wearable tactile sensors, organic electronics, and air purification.

Structural Investigation of Ca2(Mn,Ti)O4 Black Pigments by using Synchrotron Xrd, Xafs and Dft Calculation

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Tomokatsu Hayakawa

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Abstract

In recent years, functional inorganic pigments, which exhibit color properties as well as near-infrared (NIR) reflective ability, have attracted attention as materials used to prevent heat storage due to NIR light absorption. In a previous study, Ca2MnO4 was found to be an ideal NIR-reflective black pigment among several calcium manganese oxide pigments. Recently, we analyzed crystal structures and electronic states for Ca2(Mn,Ti)O4 ceramics and reported that there was the presence of the Ti–Ti correlation with a certain distance in the lattice.

In this study, valence states, local structure, and electronic states of constituent elements of Ca2(Mn,Ti)O4 ceramics were analyzed by using X-ray synchrotron radiation. White line peak positions of Mn and Ti K-edges did not shift with increasing Ti4+ contents, and the valence states of Mn and Ti were dominantly 4+. From the results of pre-edge peak analysis, the local symmetry of MnO6 octahedra was found to be changed by introducing Ti4+ into Mn4+ site. Based on the results of Rietveld analysis, XANES, EXAFS, and first principle calculations, it is considered that the Mn/Ti atoms were located at positions that deviated from the ideal position defined by the space group in the c-axis direction. In addition, the displacement of them would become large as the content of Ti4+ increases.

Biography:

Ryohei Oka graduated doctoral degree at Tottori University in March 2021. He is Assistant Professor at Nagoya Institute of Technology from April 2021. He specializes in synthesis and characterization of inorganic pigments and optical materials containing transition metal ions.

Method for Viscosity Measurement of Silicate Melts by Hot Stage Microscopy

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Chiara Zanelli
Daniele Giordano
Michele Dondi

CNR-ISTEC, Istituto di Scienza e Tecnologia dei Materiali Ceramici

Abstract

The viscosity of silicate melts represents a key parameter to control the manufacturing processes in the ceramic and glass industries and to understand nature phenomena (e.g., volcanic eruptions). The techniques generally used are time wasting, requiring equilibrium conditions, and limited to small viscosity ranges. The reduction of testing time represents a challenge for both academic and industrial aims. For this purpose, hot stage microscope (HSM) technique was selected as alternative for a rapid viscosity determination and an experimental methodology was set up. Specimens (pressed powders) were heated at 10°C/min till melting. Characteristic shapes (Start sintering, End sintering, Softening, Sphere, Hemisphere and Melting) were found at characteristic temperatures (CT). Seven natural glasses, with a measured viscosity-temperature dependence (Vogel-Fulcher-Tammann, VFT) were selected. Each CT viscosity was calculated based on the experimental VFT parameters. The observed shape is given by a cumulative viscosity-surface tension effect. This circumstance let the viscosity values at each CT linearly scale with the surface tension. The viscosity was calibrated introducing correction factors based on glass chemistry. By this way, two independent data sets can be obtained – CT (by HSM) and the corresponding characteristic viscosity (from the glass composition) – to be used to calculate the VFT parameters. The comparison between the calculated and the experimental viscosity shows a good correspondence, significantly improved with respect to previous attempts in the literature using HSM data only. These results also disclose a promising prospect of this noncontact technique in evaluating the effects of crystalline particles and porosity on silicate rheological properties.

3D Printing of Artistic and Technical Ceramics: from Pottery to Industrial Objects

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Abstract

As an emerging technology, 3D printing offers increased complexity and greater freedom in the design of functional ceramic objects. The definition of a ‘model’ ceramic with its “drying sequences” and “high temperature of firing and sintering” are key sequences in 3D shaping. The sequences must be well controlled due to, among other things, shrinkage and compression. The choice of the corresponding temperatures is driven by fine inspections of thermal analyses (weight loss and dilatometry).

Two ways to process 3D ceramics are presented. i. Based on a Pressure-Assisted Deposition Modelling (PADM), that needs to prior control the formulation of kaolin doughs. ii. Based on a Fused Deposition Modeling (FDM), that uses hybrids filaments (polylactid acid (PLA) + ceramic powder). Both the ways are with a subsequent drying/debonding and sintering stages.

The ability to generate fine controlled structures with freedom in 3D-design is discussed together with the needed functionality, for example (but not reductively) artistic design and heat exchanger.

Biography

Functional Microstructures activities (MINES Paris PSL - CNRS) aim to conduct combinations of physics / morphologies / structures / interfaces and surfaces in hybrids materials (ceramics and polymers composites) to meet the challenges of tomorrow, i.e. to develop new materials, news model-experiments and new numerical models based on physical phenomena.

Origin of Piezoelectric Response by Nano-domain Dynamics in Lead-free Bibased Piezoelectrics

Sangwook Kim*

Hiroshima University

Abstract

It is generally accepted that physical origin of piezoelectricity can be coupled intrinsic by lattice

dynamics and extrinsic by domain dynamics. However, piezoelectricity often occurs without extrinsic effect. BiFeO3-based lead-free system is one of replacement for lead-based piezoelectric materials, because their high Curie temperature. An interesting property of the Bi-based lead-free ceramics is that piezoelectric response is exhibited without extrinsic effect in the pseudo-cubic structure. In this study, we revealed an extrinsic effect by nano-domain rearrangement, which is distinctly different extrinsic by domain dynamics. The nano-domain formed by Bi ion anisotropy, and it is aligned in a certain direction by external electrical stimulation, which play a similar role of ferroelectric domain switching. The nano-domain by Bi ion disordering is contributed direct origin of piezoelectricity in pseudo-cubic structure.

Biography:

Sangwook Kim is an assistant professor in Physics program on Graduate School of Advanced Science and Engineering at Hiroshima University, Japan. He received his PhD degree from the University of Yamanashi, Japan. His research interests include piezoelectric and ferroelectric materials with material structural physics.

Effect of the Oxygen Content in Cathodic Copper on the Ductility of Copper Wires

Carlos Camurri*
Yasmin Maril

University of Concepcion, Chile

Abstract

The oxygen content on cathodic copper, among other impurities, determines the mechanical properties of the derived copper wires. From traction tests on copper wires and observation of their fracture surfaces it has been concluded that the principal impurity affecting the ductility of the copper wires is oxygen over 600 ppm, mainly incorporated during the melting of the cathodes and casting the rods for the further drawing of the copper wires. In addition, the probes been mechanically tested must not have been annealed, since in this case cuprous oxide particles are more dispersed in the matrix, and not only segregated at grains limits in the non annealed condition, and so the deleterious effect of the oxide on the ductility does not manifest.

Biography:

Carlos Camurri is a Metallurgical Engineer and DSc in Metallurgy , Full Professor and Director (up to March 2022) of the Materials Department at the University of Concepcion, Chile. His working areas are mechanical characterization of materials, metal forming and simulation. He has more than 60 SCI publications, H index of 15 and over 1 million USD grants for research and development from Chilean government and industries

Nanostructured Carbon for Electrochemical Energy Applications

Ram Gupta

National Institute for Materials Advancement, Department of Chemistry, Pittsburg State University, USA

Abstract:

Carbon-based materials such as carbon nanotubes, graphene, mesoporous carbons, etc. possess some unique characteristics which make them very suitable for energy applications. Their electrochemical properties can be tuned by doping and synthesizing them in a highly porous structure. We will provide an update on the recent development in our lab regarding applications of nanostructured carbons for electrochemical energy production and storage. Carbons derived from bioresources, used fabrics, and polymers will be covered. Various approaches to tuning their properties and the effect of such modifications on structural and electrochemical behavior

will be discussed. The performance of coin-cell-type supercapacitors using these materials will be explored. The effect of temperature and electrolytes on the energy storage capacity will be discussed. Finally, their applications as electrocatalysts for water splitting will be provided. The effect of doping on the electrochemical behavior of the electrocatalysts and their long-term performance will be explored.

Biography:

Ram Gupta is an Associate Professor at Pittsburg State University. Dr. Gupta's research focuses on green energy production and storage, electrocatalysts, supercapacitors, batteries, optoelectronics and photovoltaics devices, sensors, nanomagnetism, bio-based polymers, bio-compatible nanofibers for tissue regeneration, scaffold and antibacterial applications, bio-degradable metallic implants. Dr. Gupta published over 250 peer-reviewed articles, made over 320 national/ international/ regional presentations, chaired many sessions at national/ international meetings, wrote several book chapters (55+), working as an Editor for many books (20+), and received several million dollars for research and educational activities. He is serving as Associate Editor, Guest editor, and editorial board member for various journals.

Flexible, lightweight, and Low-Voltage Carbon Nanotube Heaters

Kavitha Joseph

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Abstract

Flexible and low-voltage heaters that can be easily integrated into devices are attracting increasing attention in aerospace, medical, textile, and other industries. The goal of the research is to design and fabricate flexible, efficient, and lightweight Carbon Nanotube (CNT) heaters that can be integrated into various electronic devices and wearables like garments (to combat cold weather). This work takes advantage of the efficiency and relative ease of fabrication of carbon nanotube sheets. The CNT sheet was obtained from a vertical array of spinnable carbon nanotubes synthesized by chemical vapor deposition. The copper electrode contacts of the CNT heater were made by copper electrodeposition. The fabricated heater was characterized for morphology (SEM), defects (Raman Spectroscopy), resistivity (non-contact sheet resistance test), and heating efficiency by thermal imaging technique (IR camera). The number of CNT layers forming the heater determines the efficiency of the heater. 40 and 80 layers of CNT heater were fabricated and tested. The 80-layer heater proved to be highly efficient with low voltage and low power conditions with faster heating and cooling responses (It took only a few seconds to reach 40oC at 1.1V and 0.5 W). The CNT heater meets the requirements of a potential heating material to be used in future wearable electronic devices in various application sectors.

Photoactive Carbon Dots-Antimicrobial Functions and Mechanistic Implications

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[1]Department of Pharmaceutical Sciences, North Carolina Central University, Durham, North Carolina, USA
[2]Department of Chemistry and Laboratory for Emerging Materials and Technology, Clemson University, Clemson, South Carolina, USA.

Abstract

We have recently developed carbon dots (CDots) as a new class of highly effective visible/natural light-activated antimicrobial agents. CDots, generally defined as small carbon nanoparticles with various surface passivation schemes. Attributed to the π-plasmon-associated electronic

transitions, CDots have remarkable broad optical absorptions in the entire visible spectrum, extending into both near-UV and near-IR, making them excellent visible light-excitable agents. Our teams have demonstrated the highly effective photoactive antimicrobial activities of CDots against various bacteria and viruses, ranging from laboratory model bacteria (E. coli, Bacillus Subtilis), pathogenic foodborne bacteria (Listeria, Salmonella), to multi-drug resistant nosocomial pathogens (Enterococcus), and biofilms, as well as various viruses (model MS2 virus, vesicular stomatitis virus, and marine norovirus). Mechanistically, upon photoexcitation on CDots, there are rapid charge transfers and separation to form electron/hole redox pairs, followed up by the radiative recombinations of the separated redox pairs resulting in emissive excited states, which are responsible for photodynamic production of classical reactive oxygen species (ROS). It is the combined action of the initially formed redox pairs and the generated classical ROS that are responsible for the effective photoinduced antimicrobial function of CDots. Associated oxidative damages in CDots-treated bacterial cells and viruses, are evident. Our studies on property-function correlations have revealed that the optical properties, the surface functional groups/charges, and the synthesis processes, are highly correlated with their antimicrobial functions, which make CDots tunable and expandable material platforms for further improvement. Together with their non-toxic nature, CDots present new opportunities for non-traditional photodynamic antimicrobial agents.

Biography:

Liju Yang is a Professor in the Department of Pharmaceutical Sciences at North Carolina Central University. Dr. Yang received her B.S. (1991) from Hangzhou Normal University, and M.S. (1996) from Hangzhou University in China, both in Chemistry. She received her Ph.D. (2003) in Biological Engineering from University of Arkansas. Dr. Ya-Ping Sun is the Frank Henry Leslie Professor of Materials/Organic Chemistry in the Department of Chemistry, Clemson University. Dr. Sun received his B.Eng. (1982) from the Zhejiang Institute of Technology and his M.S. (1985) from the Zhejiang University, both in Hangzhou, China. He earned his Ph.D. (1989) at the Florida State University.

Additive/Subtractive Hybrid Manufacturing of Steels

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Josh Soostr

National Research Council Canada, Aerospace Research Center, Montreal, H3T 1J4, Canada. r Matsuura Machinery USA Inc., USA.

Abstract

Additive/subtractive hybrid manufacturing (ASHM) leverages the benefits of laser powder bed fusion (LPBF) with high speed milling to create parts that have complex geometries, high quality surface finishes and tight dimensional tolerances in an in-envelope process. Development of this hybrid process, however, entails detailed grasping of the interactions and synergies of the additive and subtractive sequences that affect the heating/cooling cycles and, in turn, impact the resulting microstructure, defects, and dimensional integrity of the final part. An overview of the ASHM research on two heat resisting materials – 316L stainless steel & 18Ni-300 maraging steel– is provided to bridge key knowledge gaps and establish the process-microstructure-property relationships. Based on the findings, the presentation will discuss future areas for research and technology advancement and the application of ASHM in the relevant industrial sectors.

Optimizing Process and Geometry Parameters in Bulging of Pipelines

Shabbir Memon*

L&T Technology Services, 2035 Lincoln Highway, Edison, NJ, USA

Abstract

The objective of this work is to determine the optimum process and geometry parameters to attain maximum bulge height without necking / splitting failure. The effect of process parameters on strain path and its correlation with bulge height is also carried out., ANOVA is used to study the relative contribution of geometry properties, process parameters and tube thickness. It is found that the strain hardening exponent has the highest impact on bulging followed by plastic anisotropy and thickness of tube has a relatively lesser contribution to limit strains of tube bulging. The effects of process parameters, at a specific bulge height, are studied on effective strain distribution and thinning distribution, the homogeneity of which is expressed in the terms of real Kurtosis value. It is concluded that optimum process parameters not only give less thinning and greater bulge height, it also gives more uniform deformation pattern (thinning and effective strain). The validation of optimum process parameters obtained through Taguchi is carried out using additive model and it is found that the observed value is well in agreement with the predicted value. It is also found that friction has a negative impact on bulge height as well as thinning. This is because higher friction resists the flow of material and causes the material to thin more rapidly at the critical area where necking is taking place. It is also found that bulge height is maximum at higher pressure and higher bulge length and thinning is minimum at lower pressure and higher bulge length.

Biography:

Currently Dr.Memon is Senior research engineer at L&T Technology Services. Dr.Memon received his PhD from Wichita state University in Mechanical Engineering in May 2018. Dr.Memon pursued his masters in Manufacturing engineering from Indian Institute of Technology Bombay in June 2013. Dr.Memon pursued his Bachelors in Mechanical engineering from Sardar Patel University in June 2009. Dr.Memon works in the field of Metal forming, Metal joining and Advance Manufacturing engineering.

General Generalized Thermoelasticity Theory (GGTT)

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[2]Department of Mathematics, Faculty of Education, Alexandria University, Alexandria, EGYPT

Abstract

The major goal of this research is to establish a new theory of generalized thermoelasticity for thermomass gas flow with low velocity and linear resistance based on the general non-Fourier law of heat conduction. The resistance effect has been included in the general heat conduction equation, which is based on the total derivative of the thermomass gas velocity. Using the governing equations of that unique model, two numerical applications of homogeneous, isotropic, and thermoelastic one-dimensional rods have been constructed. The two applications were solved using the Laplace transform and numerical inversion methods. In terms of thermal and mechanical wave distributions, the latest findings illustrate the contrasts between the Lord-Shulman model and the present revolutionary thermoelasticity model. The parameters of the current general nonFourier equation of heat conduction have a major impact on thermomechanical waves.

Design of Sugar-based Surfactants: Challenges and Opportunities

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Abstract

Non-ionic surfactants are indispensable industrial products with wide application potential. Growing concerns of biocompatibility and focus on renewable resources have created high interest in carbohydrate-derived products. The variety differs significantly in chemical stability. While sugar esters exhibit high sensitivity towards hydrolysis, amides and particularly glycosides enable applications relying on chemical stability, without affecting biodegradability requirements. The chemical synthesis of glycoside-based surfactants, however, poses challenges in terms of solubility. This reflects poor miscibility of the surfactant antipodes and competing chemical reactions in solvents enabling the formation of a solution for both precursors. Amides, on the other hand, easily suffer from strong intermolecular interactions, resulting in unfavorable temperature constraints for applications. Both, synthetic obstacles and thermo-constraints, limit the optimization of a surfactant for a target application.

The packing theory enables a simple optimization of the surfactant design for a target application, by identifying a suitable aggregate to facilitate the required interphase. The geometric pattern can be translated into a molecular shape, based on the ratio of surface areas for the surfactant antipodes. However, the experimental realization of such optimized surfactant design is affected by the synthetic constraints indicated above. In order to overcome the issue, we have separated the functionalization of the carbohydrate surfactant precursor, including the biodegradable glycosidic linkage between the final surfactant antipodes, from the chemical coupling of the domain precursors. Triazole-linked glycosides, varying in the overall surfactant design to cater different applications, have been prepared and their surface properties were studied. The analysis indicates potential and limitations.

Biography:

Thorsten Heidelberg studied chemistry at the University of Hamburg, Germany. After his Ph.D. in synthetic carbohydrate chemistry, he spent time as a postdoctoral researcher in New York and in France, before joining a startup company on hard-particle based nanotechnology. He joined the University of Malaya as lecturer in 2006. His current research is focusing on the synthesis of carbohydrate-based surfactants and their application for the creation of nanosized drug carriers.

The Use of Steel Making Wastes as Raw Materials for Soil-cement Bricks

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Georgia Serafim Araújo
Viviana Possamai Della Sagrillo
Alexandre Ferreira Mohaupt
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Abstract

World Steel Association reported that steel crude production was 1,911.9 Mt in 2021. For each tone, approximately 600 kg of wastes are generated and steel industry is searching for new destination for these wastes, that may be called by-products after a correct destination is achieved. Aiming to contribute to new destination for steel making wastes, this work reports the use of flue gas dessulfuration waste (FGDW), off-gas Blast Furnace dust (OGBFD), and Kambara reactor slag (KRS) as soil and/or cement partially replacement for manufacturing soil-cement bricks. The raw materials were 50 wt% clay – 50 wt% sand from the north of Espírito Santo, Brazil, CP V ARI Portland cement, and FGDW, OGBFD, and KRS, all donated from a steel company in Brazil. All raw materials were characterized by SEM, XRF, XRD, particle size distribution. A reference sample was made constituted of 90 wt% soil – 10 wt% cement. FGDW partially replaced soil (5 wt%, 10 wt%); OGBFD partially replaced soil (4 wt%, 8 wt%, 12 wt%); KRS partially replaced soil (15 wt%, 25 wt%, 35 wt%) and cement (2.5 wt%, 5 wt%). KRS was also partially replaced cement (0.5 wt%, 1.0 wt%) with ornamental rock waste (ORW) partially replacing soil (18 wt%, 36 wt%). Water absorption and compressive strength were evaluated according to Brazilian standards. Results showed that FGDW cannot partially replace soil (compressive strength decreased compared to reference sample), but OGBFD and KRS can partially substitute soil and/or cement as raw materials for soil-cement bricks manufacturing.

Biography:

André Gustavo de Sousa Galdino is a Materials Engineer from Federal University of Paraíba (1997), Material Engineering and Science master from Federal University of Ceará (2003) and Mechanical Engineering doctorate from State University of Campinas (2011), Brazil. Since 2012 is professor at Federal Institute of Espirito Santo, Vitoria Campus, Mechanical Coordination. Has experience in Material and Metallurgical Engineering, focusing on metallic and ceramic materials, acting on the following subjects: porous ceramics, physic-mechanical properties, red clay, powder metallurgy, composites, biomaterials, refractories and materials teaching. Besides is leader of research groups “Materials and fabrication processes” and “Civil construction materials” at campus Vitoria.

Charge Transport Ability Evaluation with Dynamic Surface Potentional Mapping

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Abstract

The pivotal property of organic semiconductors (OSCs) to achieve high performance devices is a high charge carrier mobility. However, the mobility is commonly measured from a model device, most often a field-effect transistor, making the mobility value material- and device-dependent. Both, the intrinsic factors - such as energy levels of all materials involved, molecular packing of the OSC, its crystalline domain size and orientation - and the extrinsic factors - likewise device structure, morphological defect, contact defect - will influence the final result. On the other hand, computational methods can provide intrinsic mobilities, which deviate frequently over several orders of magnitudes from the experimental data. Thus, material scientists need a reliable method to (re-)evaluate the existing and newly developed materials in order to gain a rational structure-function-relationship.

Herein, we present an electron-spectroscopic method to evaluate the charge carrier mobility directly from thin-films or microcrystals. Such samples can easily be obtained for most materials. With the proposed method the effects of the extrinsic impact factors are reduced to only one - the contact resistance. Depending on n-type or p-type OSCs, suitable charging conditions that results in negative or positive charging can be deliberately selected. By comparing the electron fluence flowing through different OSC thin films, one can evaluate OSCs in terms of lateral charge

carrier mobility. In addition, space charge, impacts from crystal orientation and molecular packing on mobility can be observed. The relative lateral mobilities between different OCSs can thus be directly determined.

Biography:

Wen-Shan Zhang receiced her Ph.D degree at Ulm University, Germany un der the supervision of Prof. Peter Bäuerle. After 2 years postdoctoral research in the group of Prof. Rene Janssen at Technical University Eindhoven, the Netherlands, she joined Bioquant of University Heidelberg. Her research focuses on investigating charge transport of organic semiconductors using ultra-low voltage spectral scanning electron microscopy.

A Journey to High-efficiency, Low-cost Perovskite Solar Cells/Module

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Abstract:

The understanding of ultrafast carrier dynamics is the foundation of quantum materials applications in renewable energy, nanotechnology, and quantum information and technology. To reveal the ultrafast dynamics, the majority research groups rely on classic ultrafast optical spectroscopies such as pump-probe transient absorption spectroscopy and time-resolved photoluminescence. Although these non-contact photon-in and photon-out approaches have made revolutionary discoveries, which have been demonstrated by our pioneers' work in Femtochemistry (Zewail, 1999), super resolution microscopy (Hell, 2014), and chirped pulsed amplification (Strickland, 2018), they lack an in-situ feature for characterizing building block devices such as solar cells, LEDs, photoconductors, transistors, etc.. In this talk, I will highlight the ultrafast photocurrent spectroscopy that we have developed to bridge the gap between classic optical spectroscopies and carrier dynamics in-situ devices. In particular, I will focus on quantum materials including perovskite nanocrystals and 2D layer transition metal dichalcogenide (TMDC). Because of their unique quantum confinement effect, leading to the novel phenomena such as hot carrier and exciton condensation, the understanding of ultrafast dynamics may lead to next generation hot carrier solar cells and room temperature superconductors.

Biography:

Currently, Dr. Jianbo Gao is an assistant professor in the Department of Chemistry at Brock University, Ontario, Canada. Upon he received a Ph.D. degree from the University of Alberta (2009), Dr. Gao had postdoc trainings at the National Renewable Energy Laboratory (2009-2013), the Los Alamos National Laboratory (2013-2014), and the Department of Materials Science and Engineering, and Chemistry at University of California, Berkeley (2014-2017). Dr. Gao's research interests include A) novel ultrafast carrier dynamics of quantum materials; B) next generation quantum devices application in renewable energy and optical quantum communication; and C) nanomaterials synthesis. His research is highly interdisciplinary and is at the interface of Materials Physics, Materials Sciences and Engineering, Electrical Engineering, and Chemistry.

The Impact of Drying Rate and Specimen Size on the Shrinkage and Creep Behavior of Cementitious Materials

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Abstract Not Available!!!

Posters

Phase Transitions in Polymer – based Nanocomposites.

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Alexandro Trevino
Karen Martirosyan
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Dorina M. Chipara
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Abstract

Most polymers do show several phase transitions such as crystallization and melting within the ordered domains of the polymer and melting within the amorphous polymeric domains. With few exceptions, polymers exhibit a certain degree of crystallinity (they are neither fully amorphous nor completely crystalline. For decades, the differential Scanning Calorimetry (DSC) data were analyzed by assuming that the standard amorphous-crystalline polymer is a two component system. This may have resulted in an overestimation of the degree of crystallinity. Recent data point towards a non-negligible contribution of the interphase that mediates between the crystalline and amorphous blocks. The role of this interphase becomes more complex in the case of polymer based nanocomposites where the huge surface area of the nanoparticles coupled with the wetting of the nanofiller by the macromolecular chains further enhance the thickness of the interface, magnifying its role. It is speculated that under certain circumstances a transition from a volume dominated nanocomposite to a surface dominated nanocomposite may be possible. DSC investigations of fluorinated polymers as well as on the blends of fluorinated polymers with polyethylene oxide are reported and analyzed in detail. The glass transition temperature is obtained from the derivative of the DSC signal versus temperature and the crystallization and melting peaks are simulated by a superposition of a sigmoidal and a Lorentzian component.

Biography:

1. Victor Kuncser, Dorina Chipara, Karen S. Martirosyan, Gabriel Alexandru Schinteie, Elamin Ibrahim, Mircea Chipara, Magnetic properties and thermal stability of polyvinylidene fluoride—Fe2O3 nanocomposites, JOURNAL OF MATERIALS RESEARCH, 35, 2, 132-140 (2020).

Smart Materials for Fabrication Atmospheric Water Generators

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Abstract:

The smart polymeric and network of gel materials have open a way to reduce the worldwide food and water stress, the most common natural resources that are depleting. Atmospheric water generators (AWGs) were presented as an innovative and complemental resource to reduce freshwater stresses since vapor is the third most abundant air ingredient. The passive AWGs use natural forces to collect water from fog and dew. Fog collectors operate in the specific locations where fogs are common; the ones made with newly developed materials have five times higher yields than the traditional ones. Fog collectors' AWG output depends on their structure and materials; the most efficient ones are inspired by nature. Passive dew collectors AWGs are simple tilde surfaces such as a roof of a building in rural areas, operating based on the variation of the humidity and temperatures during the day and night. Though they have one low-yield cycle, the amount of water they collect is enough to satisfy the essential needs of a small community. The advanced ones combine desiccants and hygroscopic materials within porous gels, photoabsrobamt material, and thermal-sensitive polymers resulting in multi-cycle absorption-desorption devices to harvest environmental water. Active AWGs have complex structures and require mechanical and electrical force to operate, such as the ones available in the market. Their efficiency depends on the environmental humidity, temperature, and condenser operating temperature.

Comparative Study of the Fundamental Properties of Ga2O3 Polymorph

Fatima Safieddine

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Abstract:

Full potential linearized augmented plane wave method plus local orbitals (FP-LAPW þ lo) on the basis of Density Functional Theory (DFT) is called to study the structural, electronic, elastic, optical, thermodynamic and transport properties of four different phases of Ga_2O_3 denoted by α, β, δ, and ε. The calculated gap energy Eg for the stable polymorph β-Ga_2O_3 using the modified Becke-Johnson (mBJ) exchange potential is 4.6 eV which lies in the deep ultraviolet range making Ga_2O_3 promising for optoelectronics. Thermal effects on some macroscopic properties such as heat capacity, thermal expansion coefficient, Grüneisen parameter and Debye temperature are predicted using the quasi-harmonic Debye model. The analysis of transport properties for β-Ga_2O_3 using semi-classical Boltzmann transport theory in temperature range between 300 and 1000 K showed high Seebeck coefficient S = -348.4 μVK-1 at room temperature with huge power factor PF = 39.5*10^10 WK-2 m-1 at T = 1000 K. This suggests that Ga_2O_3 is a potential thermoelectric material.

Computational Prior Guided Searching of Electrocatalysts for CO2 Reduction

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Huihui Yang
Ligang Lu

Shell, USA

Abstract

Electrochemical CO2 reduction can be used to store renewable energy produced intermittently and has been recognized as a promising solution in tackling human society's energy and environmental challenges. Scale-up of this reaction requires the discovery of effective electrocatalysts. However, the electrocatalyst search space is too large to explore exhaustively. The expense of quantum chemistry calculations and experimental catalyst validation significantly hinders the search for novel catalysts. Here, we provide a greedy search method for using an explainable and reliable numeric measure of chemical similarity called the Element Mover's Distance (EMD) [1] for the rapid discovery of catalysts based on the reference catalyst seed. In this work, we explore the feasibility and potential of using computational similarity measures to guide the nearest CO2 reduction catalyst neighbour search in chemical database retrieval systems. Our results show a considerable reduction of searching trails compared to the no-prior random searching when re-identifying 31 alloys from a Density functional theory (DFT) database retrieval.

Biography:

Yuan Zi received a B.S. degree in exploration technology and engineering (geophysical exploration) from the China University of Petroleum (East China), Qingdao, China, in 2019. He is currently pursuing a Ph.D. degree with the Department of Electrical and Computer Engineering, University of Houston, Houston, TX, USA, co-advised by Dr. Jiefu Chen and Dr. Zhu Han. He was a Summer Intern in machine learning with Siemens Sustainable Automation Solution (SAS) and Shell AI, Princeton, NJ, USA, in 2020, and Houston TX, USA, in 2021 respectively. His research interests include machine learning, anomaly detection, sustainability, optimization, and signal processing.

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