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ABSTRACT BOOK

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Milestones and Recent Advances in the Science and Technology of Corroles

Zeev Gross

Technion - Israel Institute of Technology, Israel

Abstract Not Available!!!

Fullertubes: Long Predicted, Missing Families of New Molecules are Finally Experimentally Verified and Isolated

Steven Stevenson

Purdue University (Fort Wayne), United States

Abstract:

In a recent series of JACS papers1-3 from 2020-2022, we showed the first experimental evidence that “fullertubes” really do indeed exist in nature. Our experimental findings reveal that fullertubes are present in soot as families of molecules, whose length is segmentally increased by adding belts of carbon atoms. [Note: “Fullertubes” have been mathematically and theoretically predicted since the 1990s, but nobody could experimentally verify their existence in the lab setting]. The irony is, for decades, fullertubes were globally present in everybody’s arc-generated soot, but nobody knew it.

In this talk, I discuss how these new families of fullertube molecules remained hidden for over 30 years in arc-generated soot, i.e., co-produced with empty-cage fullerenes (e.g., C60, C70, C76-C200) and also co-produced in metallofullerene generated carbon soot (e.g., Gd@C82, Sc3N@C80). As of this writing, the published family of [5,5] fullertubes has been increased from [5,5] C100 – D5d(1) in 20203 to now include [5,5] C120 – D5d(1) in 2022.1 I will also discuss our current efforts to isolate even longer fullertubes, e.g., [5,5] C130 – D5h(1) and [5,5] C150 – D5h(1). Seminal efforts with collaborators include the use of fullertubes as catalysts4 and photophysical agents.5 In this talk, I will also discuss openings for new collaborators and opportunities for new experiments (either fundamental science or applications). 1. JACS, 144, 16287–16291 (2022). https://doi.org/10.1021/jacs.2c06951 2. JACS, 143, 4593–4599 (2021). https://doi.org/10.1021/jacs.0c11357 3. JACS, 142, 15614–15623 (2020). https://doi.org/10.1021/jacs.0c08529 4. Angew. Chem., 61, e202116727 (2022). https://doi.org/10.1002/anie.202116727 5. JACS, 144, 10825–10829 (2022). https://doi.org/10.1021/jacs.2c02442

Biography:

Currently a Professor of Chemistry at Purdue University (Fort Wayne), Stevenson is a career “new molecule chaser.” For three decades, Stevenson has published newly discovered carbon-based molecules multiple times in Nature, JACS, and Angewandte Chemie. Stevenson’s career is multi-faceted, as he has worked at all three major types of employment sectors: academic, government, and industry. Having lived in France, Guatemala, and the US, Stevenson has a love of international languages and appreciates multicultural diversity. At Purdue University (Fort Wayne), Stevenson teaches both French and Chemistry courses. Stevenson is equally happy to speak Spanish with others.

2D Materials for Application in High Performance Devices

Martin Kalbac

UFCH JH, Czech Republic

Abstract Not Available!!!

Nanocarbons as the basis for hybrid energy-storage electrodes.

Pedro Gomez-Romero*

Catalan Institute of Nanoscience and Nanotechnology, ICN2 (CSIC, BIST), Spain

Abstract:

Nanocarbons with high active surface area are the materials of choice for the fabrication of supercapacitor electrodes. Yet, their electrophysical storage mechanism limits their capacity and energy density. The design of proper hybrid materials integrating redox-active clusters into these nanocarbon substrates leads to hybrid energy storage devices with improved energy densities that keep the advantages of supercaps, most notably, high power density, long cyclability and extended lifetimes. This conference will present some representative case studies of this type of hybrid materials developed in our lab based on 1D, 2D and 3D nanocarbons, and will discuss the many requirements needed for a successful hybrid design, including the building of synergies and the kinetic matching of the components.

Biography:

Pedro GOMEZ-ROMERO (FRSC) is Full professor of the National Research Council (CSIC, Spain) and Group Leader of the NEO-Energy Lab at ICN2, Barcelona, Spain. Leading projects on materials and devices for energy storage and conversion, with emphasis on batteries, supercapacitors and hybrid devices, pioneering the use of polyoxometalates as energy storing materials. Fellow of the Royal Society of Chemistry since 2014, CIDETEC Award to research on electrochemistry in 2017. Cofounder of the spin-off Napptilus Battery Labs. Author of four award-wining popular science books, as well as two technical books (Functional Hybrid Materials, Wiley-VCH, 2004) (Metal Oxides in Supercapacitors, Elsevier, 2017).

ORAL PRESENTATIONS

Plasma synthesis of 3D-graphene network

Mineo Hiramatsu*, Keigo Takeda, Hiroki Kondo, Masaru Hori

[1]*Meijo University, Japan,*

[2]*Nagoya University, Japan*

Abstract:

3-dimensional (3D) graphene network represents an aggregate of standing few-layer graphenes. This kind of carbon nanostructure is called as carbon nanowalls (CNWs), carbon nanoflakes, graphene nanowalls, and vertical graphenes. CNWs and similar carbon nanostructure are self-supported few-layer graphene sheets, standing almost vertically on the substrate to form 3D structure. They possess large specific surface area and space surrounded by graphene sheets. The maze-like architecture of CNWs with large-surface-area graphene planes would be useful as electrodes for energy storage devices and scaffold for cell culturing. CNWs can be synthesized by several plasma-enhanced chemical vapor deposition (PECVD) techniques on heated substrates (600-800 ˚C) employing methane and hydrogen mixtures. After the nucleation, the height of CNWs increases almost linearly with the growth period, while the thickness of each sheet and interspaces between adjacent sheets are almost constant. From TEM observation, each sheet is not a single crystal, but is composed of nanographene domains. These domain boundaries are chemically reactive, and metal nanoparticles such as Pt nanoparticles stick selectively at the grain boundaries. Therefore, combined with surface functionalization including surface termination and decoration with nanoparticles and biomolecules, CNWs can be suitable as platform in electrochemical and biosensing applications. We have carried out CNW growth using several PECVD techniques. Moreover, we report the performances of hydrogen peroxide sensor and fuel cell, where CNW electrode was used. Electrochemical experiments demonstrate that CNWs offer great promise for providing a new class of nanostructured electrodes for electrochemical sensing, biosensing and energy conversion applications.

Biography:

Prof. Mineo Hiramatsu received Ph.D. from Nagoya University and is a Full Professor of

Department of Electrical and Electronic Engineering, Meijo University, Japan. He serves as the Director of The Japan Society of Applied Physics. His main fields of research are plasma diagnostics and plasma processing for the synthesis of thin films and nanostructured materials. He is an author of more than 150 scientific papers and patents on plasma processes for materials science. He was awarded the Japan Society of Applied Physics Fellow in 2017.

Chiral Helicenes and Nanographenes as Important Carbon Materials

Marc Gingras*

Aix-Marseille Université, CNRS, CINAM, Marseille, France

Abstract:

Helicenes are part of helicoidal molecules known for over 120 years. 1 They were considered as an intellectual curiosity for several decades because of their chiral distorted p-system. Their attractiveness is not only due to their syntheses2 and helicity, but mostly to their exalted chiroptical, electronic and supramolecular properties.1 They recently became the center of expanding subfields in asymmetric catalysis, advanced materials, molecular electronics, optics, spintronics and supramolecular assemblies.1b Some assemblies of helicenes on metal surfaces2b,3 and on insulators led chiral supramolecular carbon surfaces. Thus, helicenes have become crucial carbon building blocks. Triple-fused helicenes embedding six helicene motifs are reported as stable chiral nanographenes with a record distortion of a benzene ring, bond length alternation, local aromaticity and metal ions complexation.5,6 It contributes to the expanding field of stable chiral nanographenes.

Biography:

M.G. obtained his PhD degree at McGill Univ. in 1989. He joined Univ. of Wisc.-Madison (USA) as postdoct. with Pr. E. Vedejs and Pr. L. L. Kiessling (now at MIT). He worked with Pr. J.-M. Lehn at Strasbourg (1993-95). A faculty position was held at ULB (1995-99) and at Univ. of Nice (1999- 2007). He moved to CNRS CINAM at Aix-Marseille Univ.. He supervised >85 research trainees, >74 publications (> 4200 cit.), 125 conferences, 38 oral comm. He is an editorial member of Austin J. of Biosensors and Bioelectronics, General Chemistry (2018-), J. Funct. BioMater. (2021-), and a former member of J. Sulfur Chem. (2010-14).

A Calcium-deficient Hydroxyapatite Coated Carbon Fiber Cloth as a Promising Patch for Bone Reconstruction

Florian Olivier[2], Nathalie Rochet[2], Sylvie Bonnamy*[1]

[1]CNRS, Univ. Orléans, ICMN, F-45071 Orléans, France;

[2]Univ. Côte d'Azur, CNRS, Inserm, Institut de Biologie Valrose, F-06107 Nice, France

Abstract:

Reconstruction of large bone defects after trauma or pathological fractures is still a challenge in tissue engineering. Our work is focused on the demonstration that an activated carbon fiber cloth (ACC) coated with hydroxyapatite could be used as an efficient tissue patch in vivo to accelerate wounded bone healing and reconstruction. We already shown that the sono-electrodeposition process allows to perform a highly biomimetic calcium-deficient hydroxyapatite (CDA) coating on carbon fiber cloth. Moreover, we demonstrated that this CDA could be doped in particular with strontium leading to a Sr-substituted CDA coating quantitatively controlled up to 10 at.%. Strontium is chosen for its pre-osteoblast activity and differentiation and its use in osteoporosis treatment. We also took benefit of the activated carbon fiber cloth microporosity to study the adsorption/desorption of bioactive molecules (aspirin and tetracycline) into the CDA/ACC composite, showing the possibility to obtain dual drug delivery systems and thereby bone patches with controlled (multi) drug release. Results of in vitro and in vivo biological assays are discussed. For in vitro tests, human primary osteoblast cells are cultured on ACC/CDA materials. The positive effect of strontium and aspirin on the viability and proliferation of cells is evidenced. For in vivo assays, performed in using a rat bone defect model, it is shown that (Sr)-CDA/ACC patches are efficient for cortical bone healing in having a double effect: as a guide effect of ACC on bone formation and as an acceleration effect of (Sr)-CDA/ACC on bone reconstruction.

Biography:

Dr. Sylvie Bonnamy is Director of Research at CNRS, ICMN-Orleans-France. She is renowned for her expertises in the multiscale characterization (HRTEM) and the physicochemical studies of carbon materials (carbon-based biomaterials, nanotubes, porous carbons, carbon fibers, C/C composites). She was recipient of Carbon Schunck award in Berlin in 2000. She directed 18 PhD. A track-record of 85 publications in peer-reviewed journals, 5 patents, 9 book chapters, 28 invited lectures/keynotes and about 230 presentations in conferences. She participated as coordinator of partner to 60 international and national research programs. She is member of the director board of the French Carbon Group.

Adsorption Behavior of Polar and Non-polar Organic Solvent on Carbon Nanotube Films

Shuhei Inoue[1], *, Mengli Zhang[2], Yukihiko Matsumura[2]

[1]*Kindai University, Japan*

[2]*Hiroshima University, Japan*

Abstract:

Here we would like to report a progress in our research, which is an effect of molecular adsorption on carbon nanotube (CNT) film. Previously, we found the mechanism of electrical resistance changes of CNT film, which is induced by molecular adsorption. Even a small piece of CNT film can detect gas molecules, so that we can apply it as a cheap and disposable sensing materials. So far, we have clarified that a gas molecule adsorbed at the CNT-CNT junction modified permittivity that resulted in increase of electric resistance. Therefore, even less reactive molecules such as methane and ethanol appear as changes in electric resistance; even though, they do not chemisorb with CNT. Hence, a CNT-CNT junction behaves as a specific adsorption site and the phenomenon follows Langmuir adsorption isotherm. Based on Langmuir model, a number of adsorbed molecule must be one; however, we recently we found like two layer adsorption for non-polar organic solvent. As for polar organic solvent, the behavior showed Langmuir model. We used DFT calculations to clarify the adsorption mechanism for this seemingly contradictory phenomenon.

Biography:

Dr. Shuhei INOUE earned Ph. D (mechanical engineering) at the University of Tokyo in 2003. He became an assistant professor in the School of Engineering, Hiroshima University, Japan; and currently he is a professor in the Faculty of Engineering, Kindai University. During his early career, he visited Prof. Kappes group in Karlsruhe Institute of Technology, Germany from 2005-2006. Now he focuses on photochromic material, wavelength conversion material, and gas sensor using carbon nanotube.

Application of Diamond-like Carbon Thin films to Control of Cell Behavior

Masahito Ban*

Nippon Institute of Technology, Japan

Abstract:

Diamond-like carbon (DLC) thin films, which consist of mainly carbon and hydrogen, present the biocompatible, excellent tribological and chemically inert properties, and have been widely applied to medical uses as biomedical components. Our group has

created wrinkle microstructures and their patterns by means of depositions of the DLC thin films on polydimethylsiloxane (PDMS) substrates by a plasma chemical vapor deposition (CVD) method, and applied the technology to control of cell behavior. Cross-sectionally a wave-like concavo-convex shape can be created at the size of about 3 to 12 μm in width and about 1 to 3 μm in height, which are controllable by the deposition conditions. Our research indicated that the DLC deposited PDMS substrates have the ability to be adhered various kinds of cells more tightly and changed the cell shapes by designing the adequate patterns composed of the deposited areas. Moreover, we applied these functions to effective control of neuronal cells, positioning cell bodies and guiding axons, and fabricated distinguishing plane-type substrates, on which the distinctive interconnection structures of axons were created. In addition, from the recent research we report a rope-like structure composed of axon bundle, which is individually taut in a straight line apart from a base substrate, expected of uses for evaluating the axon behaviors of neuronal cells in brain-on-chip models.

Biography:

Masahito Ban is Professor in Department of Applied Chemistry at Nippon Institute of Technology. He received a Master's Degree in material processing from Nagoya University in 1991 and a Doctor of Engineering Degree in functional thin films by plasma processing from Nagoya University in 2002. From 1991 to 2005, he worked in Technical Institute of Kawasaki Heavy Industries Ltd., and during that time his research was based on plasma and thin film technologies. His current research is focused on applications of carbon-based nanomaterials such as diamond-like carbon (DLC) thin films, graphenes and fullerenes to biomaterials, cell scaffolds and organ-on-chips.

Overcoming the Physical and Chemical Limitations of Lipid Nanoparticles for the Stabilisation and Delivery of RNA

Suzanne Saffie-Siebert, Flavia Sutera, Ashkan Dehsorki, Negeen Kargar, Uttom Nandi, Mukhtar Ahmed, Michael Welsh & Nissim Torabi-pour

SiSaf Ltd, 3 Huxley Road, Surrey Research Park, Guildford, GU2

Abstract:

Lipid Nanoparticles (LNP) are efficient RNA delivery vehicles, and LNP-RNA formulations have successfully entered the clinic with the widespread use of COVID-19 LNP-RNA vaccines representing a milestone for RNA therapeutics. However, challenges associated with targeting and transfection, cytotoxicity, and immunogenicity remain important considerations when it comes to effective and safe RNA delivery. These challenges are primarily due to the physical and chemical instability of LNPs which can lead to premature dissociation and 'leakage' of the encapsulated RNA. Physical instability results in the collapse of the LNP under physical/mechanical stress. Chemical instability occurs because of lipid susceptibility to hydrolysis and oxidation, leading to LNP degradation. Common strategies to address physical and chemical instability, such as PEGylation, typically cause new issues, such as potential immunogenicity in the case of PEGylated lipids.

We have developed a unique silicon-stabilized LNP platform as a promising solution for the targeted delivery of RNA. Our innovative Bio-Courier technology is a biocompatible hybrid of porous silicon nanoparticles and lipids with a demonstrated ability to increase stability of lipid micellar vesicles that offer controlled release and delivery of functional RNA to targeted tissues. The high structural integrity of Bio-Courier provides thermostability and prevents the physical collapse of the LNP on lyophilisation, thereby avoiding ultra-cold supply chain storage. BioCourier, as a biodegradable RNA delivery vehicle, has also demonstrated efficacy for in vivo and in vitro delivery of RNA to corneal cells and to the bone. This makes Bio-Courier technology a promising alternative to conventional LNPs.

Biography:

Dr Saffie-Siebert has over 20 years' experience in the fields of pharmaceuticals and drug delivery. Her previous positions include Director of Research at pSiMedica Ltd (spin out from QinetiQ) and Head of the Drug Delivery Centre at Dompe SpA (Italy). She obtained her PhD in Pharmaceutical Science from the School of Pharmacy at the University of London. She is named as the inventor or co-inventor on more than twenty worldwide drug delivery patents and is Visiting Professor at Ulster University.

Formation of Defect-free Monolayer Graphene on Si Interfacial Film *via* SiSn Cointercalation and Sn Deintercalation

Hidong Kim[1]*, Nyamaa Tsogtbaatar[2],[3], Bolortsetseg Tuvdendorj[2],[3], Jae M. Seo[2]

[1]*Nuclear Research Institute, Pusan National University, Korea;*

[2]*Department of Nanoscience and Technology and Institute of Photonics, Electronics and Information Technology, Jeonbuk National University, Korea;*

[3]*Quantum Spin Team, Korea Research Institute of Standards and Science, Korea*

Abstract:

Normally, when silicon atoms are intercalated beneath the graphene-like zero layer (ZL) formed on a silicon carbide (SiC) substrate, the resulting QFMLG contains numerous crater-like defects due to a strong reaction between silicon and carbon. We explored a technique to create a defect-free quasi-free-standing monolayer graphene (QFMLG) above a silicon (Si) interfacial film. The technique involves the formation of a precursor interfacial film composed of silicon and tin (SiSn) by sequentially depositing tin and silicon on the ZL at room temperature, followed by post-annealing at 650-700 °C. By doing so, the tin atoms act as a barrier, preventing the reactive silicon atoms from directly interacting with

the ZL and causing defects. Subsequently, the sample undergoes annealing at 750 °C to selectively eliminate the tin atoms from the SiSn interfacial film, resulting in a well-ordered silicon film. The SiSn interfacial film consists of a silicon layer at the bottom and tin atoms on top, and its structure exhibits a short-range-ordered “2×2” or a long-range-ordered 2×√7 superstructure, depending on the annealing temperature and the coverage of tin. Both of these superstructures are semiconducting and induce fewer n-doped QFMLG regions compared to a pure silicon film.

Biography:

Hidong Kim received his PhD degree in physics from Korea Advance Institute of Science and Technology in 2001. Then he started his study on the high-index Si surfaces with Prof. Jae M. Seo in Jeonbuk National University in Korea. He is currently studying graphene on silicon carbide substrates and magnetic two-diemsional materials using scanning tunneling microscopy, photoemission spectroscopy, etc. in Nuclear Research Institute, Pusan National University, Korea.

Carbon Nanozyme with Elevated Phosphatase Activity Induces Cell Cytoskeleton Collapse and Membrane Bursting

Timur Elebessov[1], Lazzat Nurtay[2], Ayazhan Dauletova[1], Haiyan Fan[2], Tri Thanh Pham[1]*

[1]*Department of Biology, Nazarbayev University, Kazakhstan;*

[2]*Department of Chemistry, Nazarbayev University, Kazakhstan*

Abstract:

Nanozymes have sparked substantial attention in recent years due to their ease of production, low cost, low toxicity, greater flexibility, high stability, and excellent electronic/optical properties. However, the impacts of nanozymes with substantial catalytic activity on cells have not been thoroughly investigated. Here, we investigated the effects of sulfur and nitrogen co-doped carbon nanoparticles (SN-CNPs) with strong phosphatase activity on Drosophila neural stem cells. Live cell imaging and atomic force microscopy were employed to evaluate the influence of SN-CNPs on the physical and mechanical properties of neural stem cells in both intact brain and in primary culture. Our live cell imaging data revealed that SN-CNPs induced hyperactive actomyosin contraction, resulting in actin cytoskeleton separation from the cell membrane and subsequent collapse. Additionally, it caused the depolymerization of microtubules, an increase in cell size, and ultimately the bursting of the membrane. The outcomes of the biochemical experiments revealed that SN-CNPs exhibit strong ATPase and GTPase activity. Thus, our SN-CNPs possessed two crucial biological enzymatic activities commonly observed in cells: ATPase and GTPase activities. Due to elevated level of ATPase and GTPase activites, the cell’s internal osmotic

pressure increases, resulting in uncontrolled expansion and ultimately cell explosion. This study is the first to report the existence of carbon-based nanoparticles with high ATPase and GTPase activities as well as a dual cell-destructive mechanism based on phosphatase activity. This novel class of carbon nanozymes has the potential to be used in cancer therapy.

Biography:

Tri T. Pham is an Assistant Professor in Biology Department at Nazarbayev University. He received a Double Degree in Advanced Science and Aerospace Engineering from the University of Sydney in 2005, as well as a Ph.D. in Computational Biophysics from Monash University in Australia in 2009. He recently established the Mechanobiology Laboratory to study how therapeutic drugs, antibiotics, nanoparticles, nanomaterials, and material surfaces such as metal implants or polymer scaffolds affect cellular viability, biomechanical properties, and biofilm formation. Light microscopy, atomic force microscopy, live cell imaging, mechanobiology, biosensors, and biomaterials are some of his areas of interest in research.

Biodegradable Amphiphilic Copolymers with Enhanced Drug Loading Capacity and Their Toxicity Evaluation Through Microfluidics

Mihaela C. Stefan*, Michael C. Biewer, Abhi Bhadran, Himanshu Polara, Tejas Shah, Godwin Babanyinah

Department of Chemistry and Biochemistry, University of Texas at Dallas, Richardson, TX, USA

Abstract:

Amphiphilic diblock copolymers were synthesized by the ring-opening polymerization of various g-substituted e-caprolactone monomers and self-assembled into the water to form micelles, which can improve the loading of anticancer drugs. The drug-loaded micelles can passively target tumors through enhanced permeability and retention (EPR) effect. Our research has been focused on two strategies to increase the drug loading capacity of the amphiphilic diblock copolymer micelles; a) tuning substituents at the hydrophobic polycaprolactone block, and b) co-loading with polyphenols, such as resveratrol and quercetin, when benzyloxy substituents were employed at the hydrophobic polycaprolactone block. The non-covalent interaction, such as p-stacking and hydrogen bonding interaction between the anticancer drug, doxorubicin, and polyphenol, can increase the drug loading capacity. The co-loading approach can significantly reduce the cardiotoxicity caused by the anticancer drug. Moreover, we reported a microfluidic device to cultivate stem cell-derived organoids to simulate the dynamic microenvironment of the organ and test the toxicity of drug-loaded micelles. The cell-cell and cell-matrix interactions found in living organs can improve the evaluation of ex vivo toxicity of drug-loaded micelles.

Biography:

Mihaela C. Stefan received her Ph.D. in Chemistry from Politehnica University Bucharest, Romania. She joined the Department of Chemistry and Biochemistry at the University of Texas at Dallas in 2007, and she is currently a Eugene McDermott Professor and Department Head. Her research group is developing novel organic semiconductors for organic electronics, biodegradable and biocompatible polymers for drug delivery applications, and rare novel catalysts for polymerization of dienes and cyclic esters. At the University of Texas at Dallas, she supervised 36 graduate students and 24 Ph.D. students graduated with a Ph.D. in Chemistry under her supervision.

Nano-structured Diamond Sensors for Extreme Environments: Taking SERS from the laboratory to the Ocean

Richard B. Jackman

London Centre for Nanotechnology and Department of Electronic Engineering, UCL (University College London), 17-19 Gordon Street, London, WC1H 0AH, UK.

Abstract:

The treasures within the pyramids of ancient Egypt contained much that was gold. In this work, diamond nanopyramids with a base dimension of ~60nm have been fabricated which encase gold nanoparticles (NPs) with a diameter of ~20nm. The plasmonic nature of the gold NPs, along with the optical properties of the diamond host matrix make these nanostructures of great interest in numerous applications; here we will discuss the realisation of robust sensors for marine applications. Diamond is chemically resilient, and is transparent at optical wavelengths. Diamond has also been shown to resist biofouling in marine environments. This leads to the idea that diamond may be an ideal platform for sensors destined for use in extreme environments, including ocean deployment. Surface plasmon excitations in NPs lead to electromagnetic field enhancement near the metal surface. The NPs effectively act like small antennae, capturing and amplifying the incident light. Their plasmonic natures offers opportunities for Surface Enhanced Raman spectroscopy (SERS) enabling trace levels of chemical detection, being significantly more sensitive than conventional Raman. This is of great interest for use within the marine environment where trace chemical sensing is important for pollution control and for climate change studies. However, SERS substrates tend to degrade over time and are not suitable for re-use. Moreover, they are simply too fragile for use in environmentally challenging situations such as ocean analysis. As a robust substrate for SERS, diamond has near-to ideal optical properties; however, the typical reliance of van-der-Waals forces for NP adhesion to the diamond offers little improvement over other substrates in terms of marine applications. A solution is the inclusion of the NPs in diamond, sufficiently near the surface of the diamond to retain their plasmonic enhancement of the SERS signal.

Biography:

Richard holds UCLs Chair in Electronic Devices and heads UCLs Diamond Electronics Group (DEG) whose laboratories are within the London Centre for Nanotechnology. Richard moved to UCL in 1988, having previously held the Royal Society Eliz. Challenor Research Fellowship at the University of Oxford, to establish one of the first teams dedicated to the then newly emerging material, diamond, grown by chemical vapour deposition (CVD) methods. Since then UCLs DEG has been responsible for licensing some of the first diamond device technology to reach commercial development by industry and has published patents relating to such. Professor Jackman has published more than 250 journal articles and is a Fellow of both the IET and IoP.

Flash Chemistry Makes Impossible Organolithium Chemistry Possible

Aiichiro Nagaki

Department of Chemistry, Faculty of Science, Hokkaido University, Sapporo, Japan

Abstract:

Many successful applications reported in the literature speak well for the power of the flowmicroreactor method in chemical synthesis. The reaction time in a flow microreactor is defined as the residence time between a reagent inlet and the quencher inlet, which can be controlled precisely and reduced to millisecond order by adjusting the length between these positions and the flow speed. Such a feature of flow microreactors enables the use of short-lived highly reactive intermediates for synthesis. Various chemical reactions using highly reactive short-lived organolithium species that are difficult or even impossible to perform in batch processes can be accomplished in flow microreactors using space integration of reactions. In this presentation, we slow our recent results to various synthetic reactions mediated by organolithium reagents based on flash chemistry conducted in flow reactors, especially utilizing space-integration of the flow reactions.

Biography:

Dr. Aiichiro Nagaki, now is a professor of department of chemistry, faculty of science, hokkaido university. Aiichiro Nagaki graduated from Doshisha University in 2000. He received his PhD in 2005 from Kyoto University under the supervision of Professor Junichi Yoshida. He worked with Professor Hiroaki Suga, Tokyo University, from 2005 as a postdoctoral fellow. In 2006, he became an assistant professor of Kyoto University. He was promoted to a junior associate professor in 2013, an associate professor in 2018 and became a full professor of Hokkaido University in 2022. He His current research interests are organic synthesis and microreactor synthesis. Awards: Takeda Pharmaceutical Co., Ltd. Award in Synthetic Organic Chemistry, Japan (2012), Incentive Award in Synthetic Organic Chemistry, Japan (2012), and Young Innovator Award on Chemistry, MicroNano

Systems (2013), ESPEC Prize for the Encouragement of Environmental Studies (2013), Flow Chemistry India 2014 Distinguished Presentation Award (2014), and SSOCJ Tosoh Award for Environment and Energy (2022).

Carbon-based Nanomaterials in Photothermal and Photocatalytic Applications

Dongling Ma*

Center of Energy, Materials and Telecommunications, Institut national de la recherche scientifique (INRS), Canada

Abstract:

Carbon-based nanomaterials, such as graphene, have played an important role in the clean energy environment sectors. In this presentation, I will present some of our recent works on this aspect [1-3]. One example is about using graphene materials for water purification and desalination. We have prepared a high-efficiency solar energy conversion material consisting of low-cost nonmetal, extremely thermally-stable plasmonic TiN nanoparticles (NPs) and hydrophilic semireduced graphene oxide (semirGO), with broadband solar absorption capability, by a fast in situ microwave reduction method. The two-dimensional semi-rGO serves as a support for the loading of plasmonic NPs, and meanwhile accelerates the transport and evaporation of water due to its hydrophilicity. Then, decoration of plasmonic TiN NPs further enhances the solar photon absorption and hydrophilicity while suppressing the heat loss, thanks to the layered structure of TiN/semi-rGO, improving overall solar energy utilization. Owing to the enhanced absorption and unique layered nanostructure with strong interfacial interaction, the optimal sample of TiN/semi-rGO-25% absorber achieves a high and stable water evaporation rate of ≈1.76 kg m−2 h−1 with an energy efficiency as high as 99.1% under 1 sun illumination. Furthermore, this plasmonic TiN/ semi-rGO absorber is capable of producing high-quality freshwater from sustainable seawater desalination and wastewater purification processes.

Biography:

Prof. Dongling Ma (FRSC, FIAAM, Canada Research Chair (Tier 1)) has been a professor at INRS since 2006. Her research interest consists in the development of nanomaterials for energy, environment, photocatalysis and biomedical applications. She has co-authored >170 articles (J. Am. Chem. Soc, Nat. Commun., Adv. Energy Mater., Adv. Funct. Mater., etc.), 5 patents and 4 book chapters. She is an associate editor of ACS Applied Nano Materials and also serves/served on multiple journal editorial advisory boards, including ACS Energy Lett. Her most recent award is the 2022 Clara Benson Award from the Chemical Institute of Canada.

Synthesis of Vertically Aligned Carbon Nanotubes on Conductive Substrates with Catalytic Chemical Vapor Deposition Technique

Lilla Nánai[1]*, Anna Szabó[2], George Kaptay[1,3], Klara Hernadi[1]

[1]*Institute of Physical Metallurgy, Metal Forming and Nanotechnology, University of Miskolc, Hungary*

[2]*Department of Applied and Environmental Chemistry, University of Szeged, Hungary*

[3]*ELKH-ME Materials Science Research Group, University of Miskolc, Hungary*

Abstract:

Potential application of vertically aligned carbon nanotubes (VACNT) structures can be significant due to their surface and electrical properties. The efficient fabrication of VACNTs by catalytic chemical vapor deposition (CCVD) is crucially dependent on both the formation of the catalyst thin film and the precise adjustment of the CCVD synthesis conditions. Current work presents the growth of VACNTs on support layer (Al2O3, TiO2) supported Fe – Co catalyst layers, which were grown by simple cost-effective techniques (spray coating and dip coating) onto titanium and aluminum doped zinc oxide (AZO) glass substrates. The effect of various parameters during catalyst layer deposition (substrate, heat treatment, composition, thickness, etc.) and during CCVD (reaction temperature, reaction time, gas feed, water vapor etc.) on VACNT properties was investigated in detail. The obtained VACNTs were characterized by scanning electron microscopy (SEM), transmission electron microscopy and Raman spectroscopy. As a result, multi-walled VACNTs with 5-9 µm height could be grown onto AZO and with 15-25 µm height could be grown onto titanium substrate. In the case of AZO substrate, it was observed that the CNTs synthesized at the more moderate synthesis temperature of 650 °C have better density, orientation and structure, besides the Al2O3 support layer is essential for the uniform adherence of catalyst particles on the AZO surface and indirectly for the growth of VACNTs.

Biography:

Lilla Nánai is currently a research fellow at the University of Miskolc. She received her BSc degree in chemistry from the University of Szeged in 2017, MSc degree in chemistry from the University of Szeged in 2020. She is currently employed at the Institute of Physical Metallurgy, Metal Forming and Nanotechnology, University of Miskolc as an assistant researcher with experience in scanning and transmission electron microscopy measurements. Her current research interest focuses on the key pathways involved in the synthesis of carbon nanotubes and nanocomposites.

Twistronics, Quasicrystals, and Exotic Composite Materials

Ken Golden*

University of Utah, Department of Mathematics, USA

Abstract:

From twisted bilayer graphene to quasicrystalline alloys, the study of material properties arising from quasiperiodic structure – ordered yet aperiodic – has driven advances in theory and applied science. Here we introduce a class of tunable composites, with the mixture geometry of two constituent materials determined by Moiré patterns from rotating one lattice relative to another. We find that these twisted bilayer composites, whose microstructure can be designed on almost any scale ranging from nanometers to meters depending on the application, display exotic behavior in their effective electrical, magnetic, diffusive, thermal, and optical properties. With a slight change in the twist angle, the microstructure can transition from periodic to quasiperiodic, and the transport properties switch from those of ordered to randomly disordered materials. We observe Anderson localization transitions, the appearance of mobility edges, and other phenomena normally connected to wave equations and quantum transport in solid state physics, even though there are no wave scattering or interference effects at play here. The results emerge by distilling the relationship between classical transport and microgeometry into the spectral properties of an operator analogous to the Hamiltonian in quantum mechanics. Surprisingly, our findings were motivated by studying the role of sea ice in the climate system, and the analysis of sea ice microstructures, such as the millimeter-scale brine inclusions whose geometry and connectivity govern fluid flow in sea ice, remote sensing signatures, and their suitability as habitats for microbial communities like algae that support the polar marine ecosystem.

Biography:

Kenneth M. Golden is a Distinguished Professor of Mathematics and Adjunct Professor of Biomedical Engineering at the University of Utah, with interests in sea ice, climate, polar ecology, and composite materials. He has been on 18 polar expeditions and given over 500 invited lectures, including three presentations to the U.S. Congress. His work has been covered by media around the world, including profiles in Science, Scientific American, Physics Today, and the BBC. Golden is a Fellow of the Society for Industrial and Applied Mathematics, the American Mathematical Society, the Electromagnetics Academy, and the Explorers Club.

Path Integral Molecular Dynamics Simulation for H/D Isotope Effect in Protonated/Deuterated Aqueous solution

Masanori Tachikawa

Graduate School of NanoBioScience, Yokohama City University, Yokohama, Japan

Abstract:

Water dissolves various substances, and many essential chemical reactions occur in aqueous solution. The proton (H+) behavior in an aqueous solution is also crucial in biochemical reactions and proton transfer in living organisms. On the other hand, the behavior of deuteron (D+) in heavy water (D2O), an isotope of water, is still unclear. In this study, thus, we have applied the on-the-fly path integral molecular dynamics simulation, which can include both the nuclear quantum effect and thermal effect. To elucidate the isotope effects of H+/D+ behavior in an aqueous solution, we calculated the systems of H+ in light water solvent and D+ in heavy water. We found a significant isotope effect around the Eigen H3O+/D3O+ region. First, the structures with Zundel H5O2+, H7O3+, and H9O4+ were confirmed at the system of H+ in a light water solvent, while such structures are less at that of D+ in heavy water. We also found the H/D isotope effect at the radial distribution function of O-O distances.

Biography:

Dr. Masanori Tachikawa obtained his Ph.D. in Chemistry from Waseda University in 1995, undertook “Research Fellowship for Young Scientists (PD)” from JSPS and “Special Postdoctoral Researcher (SPDR)” in RIKEN in 2000. In 2003, he moved to Yokohama City University as an Associate Professor, promoted to Professor in 2006. His research area is “Computational Chemistry” and “Quantum Chemistry”. He is developing new quantum simulation methods, in which both electrons and hydrogen nuclei are treated quantum mechanically. He has applied these methods to various systems from material science to biochemistry. He has earned awards for “Young Scholar Lectures of the Chemical Society of Japan, 2006”, “The Young Scientists’ Prize, The Commendation for Science and Technology by the Minister of Education, Culture, Sports, Science and Technology 2007”, “Award of Society of Computational Chemistry, Japan, 2017”, and “International Award of Japan Society of Molecular Science, 2019”.

A Thermodynamic Study on Swelling Stress of Bentonite as a Buffer Material Composing Engineered Barrier in Radioactive Waste Disposal

Haruo Sato

Okayama University, Japan

Abstract:

In many countries, bentonite is used as a buffer material composing engineered barrier (EB) in the geological disposal of a high-level radioactive waste (HLW). The EB system consists of vitrified waste, overpack (carbon steel container) and buffer material from inside, and the outside of the buffer material is rock mass. HLW is disposed of excavated tunnels in geological formation deeper than 300m (geological disposal). After being disposed, bentonite develops swelling stress by penetration of groundwater from the surrounding rock mass, and this parameter is important in designing buffer material and analyzing long-term behaviour of buffer material. We developed a thermodynamic model which can calculate the swelling stress of bentonite under standard condition (298.15K) based on the thermodynamic data (the activity of water and the relative partial molar Gibbs free energy) of interlayer water in montmorillonite which is the main component of bentonite and montmorillonite content in the bentonite in previous studies, and furthermore we also developed a thermodynamic model which can calculate the effect of temperature on the swelling stress of bentonite based on the relative partial molar enthalpy in recent studies. This talk introduces outline of the thermodynamic model and thermodynamic data of interlayer water in montmorillonite obtained so far. Furthermore, we also introduce practicality of the model by comparison with measured data of swelling stress.

Biography:

Haruo Sato graduated from Department of Geotechnology, Doctor's Program of Graduate School of Mining and Engineering, Akita University in 1997 (DE, 1997). He studied on geological disposal for HLW in Power Reactor and Nuclear Fuel Development Cooperation (PNC, presently Japan Atomic Energy Agency (JAEA)), 1989-2014. He joined in the Horonobe Underground Research Laboratory project in Hokkaido, 2006-2012. Furthermore, he also joined in the research of environmental dynamics in Fukushima, 2012- 2014. Since 2014 he has been employed as an Associate Professor at Okayama University. He is mainly specialized in backend engineering, environmental dynamics and radiation safety in the university.

Development of Organic Materials towards Sustainable Energy Applications

Kouki Oka

Osaka University, Japan

Abstract:

Toward the realization of a sustainable society, the development of innovative organic energy materials, which are composed of earth-abundant elements, and which play a role in energy conversion and storage, is highly required. In this lecture, I will describe several

examples of organic energy materials (organic polymeric materials) with the following energy-related functions (1)-(5). (1) Charge storage and transport. (2) Proton storage and transport. (3) Hydrogen gas production and storage. (4) CO2 selective adsorption and storage. (5) Photocatalysis and clean energy production. The latest efforts towards designing materials with both robust functionality and material decomposition will be also introduced.

In addition, this presentation will also cover the prototyping of applications or devices using these organic energy materials. For example, ① Organic secondary batteries which are composed of organic electrode-active materials. ② Compact fuel cells which use organic electrode-active materials as an anode. ③ Hydrogen carrier materials (Polymeric hydrogen storage materials) which chemically fix and release hydrogen gas (H2) even under mild conditions. ④ CO2 storage material. ⑤ On-site clean energy (e.g., H2 and H2O2) production which uses organic energy materials as a photo(electro)catalyst or electrocatalyst.

Biography:

Kouki Oka received his Ph.D. from Waseda University (Supervisor: Prof. Hiroyuki Nishide and Prof. Kenichi Oyaizu) in 2021, supported by the research fellowship for Young Scientists from the Japan Society for the Promotion of Science (JSPS). He also received joint supervision as a visiting student and researcher at Uppsala University during his doctoral course. After postdoctoral work at the University of Tokyo and Uppsala University, supported by the research fellowship for Young Scientists from JSPS, he is currently a tenure-track assistant professor at Osaka University. His research focuses on advanced polymers and functional materials for batteries, hydrogen storage, and catalysis.

Synthesis of Thermal Heat Storage Material Using Various Phosphate Composites Like Polythene Waste, Wall care putty, etc.

Trilochan Swain

Associate Professor, P.G. Department of Chemistry, Fakir Mohan University, Balasore, Odisha, India

Abstract:

The polythene was invented 75 years ago and this invention at that time was called the gift of God to human civilization. Now, it is called as hell to human civilization. The widely use of polythene in different purposes make this environment highly polluted. The level of pollution is so high that it also affects the aquatic life. To reduce the above problem at some extent, I used polythene bags to convert into carbon particles with some phosphate compounds. The alternate layers of polythene bags and phosphate compounds one after another were heated at 333 K in atmospheric pressure. All the heating products are crushed to powdered form using motor and pestle. The crushed products were

thermally analyzed using DSC and TG-DTA in N2 atmosphere. The FT-IR spectrum of crushed products indicate that vibration spectrum of polythene is completely absent. The elemental analysis like C, H, N, S and DRS were also carried out. The specific heat capacity (CP) shows endothermic behavior in temperature range 271 K to 343 K at heating rate 2K/min. The minimum CP is ~ 0.83 J/g/K at ~ 272 K and maximum CP is ~ 4.13 J/g/K observed at 329 K. These crushed products are mixed with black paint to evaluate the heating capacity of composite black paint. This composite black paint can be used in solar heater or solar cooker to enhance its heating efficiency.

Biography:

The author has more than 20 years of teaching experience in postgraduate and undergraduate course. The author published more than 40 research papers in reputed National and International Journals like Solar Energy, Journal of Energy Storage, Journal of Thermal Analysis and Calorimetry, etc. Out of which more than 25 publications related to composite building envelope materials. Taking to action of local problem, the author recently works on fluoride chemistry. The local soil, ground water and plant leafs are contaminated with high fluoride concentration. The author committed to provide WHO recommended fluoride concentrated drinking water towards the end of this year.

POSTER PRESENTATIONS

Sorbents Prepared by Microwave Pyrolysis of Waste

Zuzana Jankovská*[1], Lenka Matějová[1], Pavlína Peikertová[2] and Jonáš Tokarský[2]

[1]Institute of Environmental Technology, CEET, VSB-TUO, Czech Republic;

[2]Nanotechnology Centre, CEET, VBS-TUO, Czech Republic Presenter

Abstract:

Disposal of huge amounts of diverse wastes (polymers, biomass) for reduced costs accompanied with gaining of energy and valuable chemicals is an eager topic in waste-to-energy and fuel business. Microwave pyrolysis is a thermochemical route providing such benefits. Waste scrap tyres, biomass and/or their blends were pyrolyzed in microwave reactor at different conditions (power, time) without/with different type of activator. Quantity and quality of pyrolysis products, especially carbon blacks were investigated. Sorption capacity of xylene was also evaluated on prepared carbon black. It was found that determining physicochemical properties of carbon black in its sorption performance for xylene is microporosity and large volume of micropores.

Biography:

Ing. Zuzana Jankovská, Ph.D. (1980) – senior researcher, Ing. (2004, Chemical Engineering, VSB-TUO), Ph.D. (2009, Institute of Chemical Technology Prague, Ph.D. thesis "Total oxidation of volatile organic compounds over heterogeneous catalysts"), postdoctoral research fellow (2012-2013, VSB-TUO, Energy Research Centre). Publications totally: 10 (WoS), since 2018 (WoS): 3, total citations in ISI Web of Knowledge: 157 (154 without auto-citations), H-index 6. **Research areas**: heterogeneous catalyst preparation, VOCs catalytic oxidation and adsorption, characterization of solids using thermogravimetry, conventional and microwave pyrolysis of wastes.

Engineering Carbons Produced by Microwave Pyrolysis of Agricultural Biomass for Xylene Adsorption

Lenka Matějová[1*,] Michal Vaštyl[1], Zuzana Jankovská[1], Jonáš Tokarský[2], Milan Dopita[3], Ivana Šeděnková[4], Gerardo Juan Francisco Cruz[5]

[1]*Institute of Environmental Technology, CEET, VŠB– Technical University of Ostrava, Ostrava, Czech Republic*

[2]*Nanotechnology Centre, VŠB– Technical University of Ostrava, Ostrava, Czech Republic*

[3]*Department of Condensed Matter Physics, Faculty of Mathematics and Physics, Charles University Ke Karlovu, Prague, Czech Republic*

[4]*Department of Structure and Dynamics of Macromolecules, Institute of Macromolecular Chemistry CAS, v.v.i., Heyrovského náměstí, Prague 6, Czech Republic*

[5]*Departamento de Ingeniería Forestal y Gestión Ambiental, Universidad Nacional de Tumbes, Av. Universitaria s/n, Campus Universitario – Pampa Grande, Tumbes, Peru*

Abstract:

With respect to development of energy-save and sustainable technologies in the area of solid wastes valorization to energy, fuels and other technological solid products the microwave pyrolysis is currently very challenging. It represents a good alternative to conventional slow high-temperature pyrolysis. Moreover, microwave pyrolysis of polymer wastes (e.g. tires) is already industrialized, yielding hydrogen. However, some knowledge and obstacles still needs to be revealed and overcame for inhomogeneous agricultural biomass valorization by microwave pyrolysis before its industrialization.

This contribution deals with the optimization of micro/structural and surface properties of the solid carbon products (biochars and activated carbons) from microwave pyrolysis of agricultural biomass wastes (namely corn cob, coffee husk, cocoa pod husk, banana waste and red mombin seeds) to yield an efficient gaseous xylene adsorbent. The effect of chemical activator is studied. The xylene adsorption experiments are supported by the

results from molecular modelling of xylene adsorption in built-up carbon structure.

Acknowledgement: Experimental results were accomplished using Large Research Infrastructure ENREGAT supported by the Ministry of Education, Youth and Sports of the Czech Republic (projects No. LM2018098 and LM2023056).

Biography:

Dr. Lenka Matějová (1981) – Head of Laboratory of Materials and Waste Valorisation at Institute of Environmental Technology, CEET, VSB-Technical University of Ostrava, Czech Republic. Studies: Engineer (2004, Organic Technology, Institute of Chemical Technology, Prague), Doctor (2008, Organic Technology, Institute of Chemical Technology, Prague and Institute of Chemical Process Fundamentals ASCR, v.v.i.). Research stays/cooperation: University of Oulu (Finland), Engineering University in Lima (Peru), National University of Tumbes (Peru). Publications: 85, total citations: 1936, H-index: 22 (WoS). ORCID: 0000-0002-8816-0070. **Research areas:** environmental photo/catalysis, VOCs catalytic oxidation and adsorption, supercritical/subcritical fluids application in nanostructured material design and waste valorisation, microwave pyrolysis, carbon.

Conversion of RDF- fuel to Solid Carbon, Liquid and Gaseous Combustible Products with various Potential Applications

Ivanka Stoycheva*, Boyko Tsyntsarski, Bilyana Petrova, Angelina Kosateva, Nartzislav Petrov

Institute of Organic Chemistry with Centre of Phytochemistry, Bulgarian Academy of Sciences, Bulgaria

Abstract:

Composition RDF is a mixture of waste materials, characterized by a higher combustibility (e.g. organic compounds) as compared with the components in the total waste stream. RDF is successfully used as a fuel additive in coal-fired boilers in thermal power plants. A big problem with thermal power plants is the high content of hazardous organic substances in pyrolysis gases. This requires their purification as filters containing a carbon adsorbent are commonly used. The aim of the research is to develop a method for processing RDF fuel, which leads to production of liquid and gaseous combustible products and solid product with carbon adsorbent properties are obtained. RDF fuel from waste materials was tested. As a result of the treatment, a nanoporous materials with a high surface area of 600-700 m2 was obtained. The initial material was examined by TG and DSC analysis. The resulting carbon materials were characterized by Elemental Analysis, Nitrogen Porosimetry. The obtained results show that the material has a potential application for adsorption of contaminants and catalysts support.

ACKNOWLEDGEMENTS

The authors acknowledge support for this work from the EU Project BG05M2OP001-1.002-0019: (Clean & Circle) and Project KP-06-N59-12/22.11.2021

Biography:

Associated Professor (2022) in Institute of Organic Chemistry with Centre of Phytochemistry, Bulgarian Academy of Sciences. Born in 1989 in Sofia, Bulgaria. Publications- 30. **Main research area and subareas:**Technology and chemistry of natural and synthetic fuels, Carbon materials, Adsorption, Catalysis, Ecology. **Career and Education:** Institute of Organic Chemistry with Centre of Phytochemistry, Bulgarian Academy of Sciences, Associated Professor, 2022. Institute of Organic Chemistry with Centre of Phytochemistry, Bulgarian Academy of Sciences, PhD, 2016 Chemical Technology and Metallurgy, Sofia, Natural and Synthetic Fuels –M.Sc. (Engineer), 2013 Chemical Technology and Metallurgy, Sofia, Engineering Ecology and Environmental Protection – B.Sc., 2012.

Low Temperature Adsorption of N2 of Carbon Materials

Bilyana Petrova*, Ivanka Stoycheva, Angelina Kosateva, Boyko Tsyntzarski, Nartzislav Petrov

Institute of Organic Chemistry with Centre of Phytochemistry, Bulgarian Academy of Sciences, 1113 Sofia, Bulgaria

Abstract:

In order to evaluate the porous texture of porous carbon materials obtained in the laboratory, it was investigated by the amount of adsorbed nitrogen at 77 K. The investigation is performed on Autosorb iQ-MP, Quantachrome instrument. The results obtained for pore volume, pore size distribution and specific surface area of nanoporous carbons and carbon foam samples obtained from different raw materials and treatment conditions are presented. Preliminary assessment of the possibilities for carbon materials application was made. Nanoporous carbon has many advantages, such as high surface area, tunable pore structure and surface chemistry, resistance to acidic or basic media, stability at high temperatures in inert or reduction atmosphere, as well as ability for regeneration.

ACKNOWLEDGEMENTS

The authors acknowledge support for this work from the EU Project BG05M2OP001-1.002-0019: (Clean & Circle) and Project KP-06-27/9 from 08.12.2018

Biography:

Main research area and subareas

New nano-structured materials, Technology and chemistry of natural and synthetic fuels, Carbon materials, Adsorption, Catalysis, Ecology.

Additional research areas and subareas

Thermo-oxidative treatment of different organic materials(coal, polymer materials, lignin-cellulose materials, etc.), porous carbon, carbon-carbon composites, activated carbons, chemical-physical investigations of different carbon materials, characterization of carbon adsorbents, purification of drinking and potable water from organic and inorganic pollutants; purification of water and air from organic and inorganic pollutants.
Institute of Organic Chemistry, Bulgarian Academy of Sciences, PhD, 2007
Sofia University "St. Kliment Okhridski", Faculty of Chemistry, M.Sc., 2000

Thermal Properties of Polybenzoxazine Modified by Acetylene Functionalization

Kwang Soo Cho* and Hodong Kim

Dankook University, Korea(South)

Abstract:

Phenol resins have been used for years as advantages of low flammability and relatively high char yield, despite problems of brittleness, catalyst demand during polymerization, and water and formaldehyde release during manufacturing. As the need for resins to be applied to highperformance fields increases, there is a constant need for new resins that improve the shortcomings of phenol resins. Benzoxazine resin is attracting material as a type of highperformance thermosetting resin due to its excellent processability, high thermal stability, excellent mechanical properties and molecular design flexibility, low dielectric constant and low moisture absorption. Benzoxazine monomers can be easily synthesized from various phenols, formaldehyde, and primary amines through the Mannich reaction. In addition, catalysts and curing agents are not needed, and by-products are not released during curing. Based on these outstanding characteristics, they are now suitable for applications in high-performance fields such as electronic technology and aerospace. In order to further improve the thermal stability of benzoxazine resins, many researches have been actively carried out by the functionalization of monomer structure. In particular, it is confirmed that thermal stability can be greatly improved through thermal decomposition research on acetylene-functionalized polybenzoxazines. To study the improvement of thermal properties of benzoxazine monomers with acetylene functional groups, the isomeric effect of acetylene functional groups in benzoxazine monomers will be further discussed in details.

Biography:

2022.09 ~ Present : M.S. in Fiber system engineering, Dankook University, Korea(South)
2016.03~2022.09 : B.S. in Fiber system engineering, Dankook University, Korea(South)

Surface Reactions on 3D Printed MnOx-based Monoliths During the Oxidation of Volatile Compounds Through Heterogeneous Catalysis.

Santiago Suárez-Vázquez[1]*, Sonia Gil[2], Arquímedes Cruz López[1], Javier Ramírez-Lomán[1]

[1]Universidad Autónoma de Nuevo León, Environmental Engineering, Mexico.

[2]Université Claude Bernard Lyon I, CARE, France

Abstract:

The emission of volatile organic compounds (VOCs) is considered a major problem since they contribute to the formation of fine particulate matter with negative effects in human health and implications for global warming. Therefore, the interest in developing new technologies for the mitigation of VOCs has been increased. One of the most popular alternatives is heterogeneous catalysis, due to its high efficiency and selectivity to H2O and CO2. With the purpose of cost reductions, metal oxides such as FeOx, MnOx, CeOx or NiOx have been studied as alternatives to noble metals. In this sense, mixed oxides of Mn-Ce-Ox have been proposed with promising results. In addition, the use of 3D printing of catalysts has attracted great attention recently due to low costs and optimization of raw materials. This work shows the fabrication of catalytic monoliths based in Mn-Ce oxides supported on commercial resins printed in 3D and evaluated for the toluene oxidation reaction. We obtained several monoliths with different surface compositions with a new transitional design. Characterization results showed the formation of the Mn3O4 along the surface composition of the monolith. Surface analysis revealed the existence of Mn3O4 with Mn concentration between 5-25 Wt%. Promising results were obtained with the surface composition of Mn-Ce-OX achieving the total conversion of toluene to CO2. Since there are no studies on the reaction mechanism in monoliths with these characteristics, we set out to study it through an In-situ DRIFTS.

Biography:

Dr. Suárez-Vázquez obtained a Doctoral degree in Materials Science and Engineering from the Nagaoka University of Technology in Japan. He was a visiting professor at the Université Claude Bernard in Lyon, France, and at the University of Antioquia in Colombia. Currently, he is a Professor in the Civil Engineering Faculty of the Autonomous University of Nuevo Leon. Dr. Suárez-Vázquez has been working on the development of new catalytic materials based on 3D printing technologies. Dr. Suárez-Vázquez has published more than 25 scientific papers applied in the oxidation reaction of volatile organic compounds and several atmospheric pollutants.

Electrochemical Performance of Lithium-ion Battery Based on Petroleum Pitch/ Polymer Composite Binder

Hyeon Taek Jeong *

Division of Energy Engineering, Daejin University, 1007 Hoguk Road, Pocheon-si, Gyeonggi-do, 487-711, Korea

Abstract:

Conventional polymer-based binder including CMCSBR, PVdF and PU have been widely used in lithium ion battery with high cost that associated with the production and disposal of these binders have raised concerns in recent years. As a result, there has been a growing interest in finding alternative materials that can replace polymer binders while maintaining the desired performance. Petroleum pitch based composite binder is one of the promising candidates to use in lithium-ion batteries due to its low price and high carbonization yield with abundant aromatic hydrocarbon. In this work, the petroleum pitch/polymer composite have fabricated to various ratios between petroleum pitch and polymer in order to optimize physical and electrochemical performance of the lithium-ion battery. Physical and electrochemical performances of the prepared lithium ion battery have evaluated by using charge/discharge test, cyclic voltammetry (CV), electrochemical impedance spectroscopy (EIS) and universal testing machine (UTM). The petroleum pitch/ polymer composite binderbased lithiumion battery demonstrated higher electrochemical performances than PVdF binder based lithium ion battery. The petroleum pitch/polymer composite binder (with a 5:5 wt% ratio) based lithium ion battery gave a 35.4 gf mm-1 of adhesion strength with 371 mAh g-1 of specific discharge capacity and 91 % of ICE value. These results suggest that the petroleum pitch/polymer composite based binder has the potential to replace conventional polymer based binder in lithium-ion battery.

Biography:

Current Affiliation: Associate Professor, Division of Energy Engineering, Daejin University, 1007 Hoguk Road, Pocheon-si, Gyeonggi-do, 487-711, South Korea

Education: MS Korea University (in Materials Science and Engineering), 2009. Ph.D. University of Wollongong, Australia (in Chemistry), 2015.

Supervisor: Professor Gordon G. Wallace

Research Experience: Research Scientist at Korea Korea Institute of Science and Technology (KIST), 2007- 2010.

Research Interests: 1. Design and Fabrication of Energy Storage Devices Including Supercapacitor and Lithium Ion Battery by Using Nanocarbon Materials.

2. Synthesis of Intelligent and Multi-Functional Polymers Composite using Controlled Polymerizations with Nanocarbon Materials.

Lignin-protein Interaction and Adhesion Performance of Lignin-protein Adhesives

Donghai Wang[1] and Xiuzhi S. Sun[2]

[1]*Department of Biological and Agricultural Engineering, Kansas State University, Manhattan, KS*

[2]*Department of Grain Science and Industry, Kansas State University, Manhattan, KS 66506*

Abstract:

Soy protein adhesives (SPA) have a high potential to replace petroleum-based adhesives. However, the wet strength of SPA is related low compared with petroleum-based adhesives. Lignin has shown a potential to enhance the water resistance property of SPA. The objective of this research was to study the lignin-protein interaction and adhesion performance of lignin-protein adhesives. In this study, the behaviors of lignin, soy protein (SP) and lignin-soy protein complexes were formulated at varied pH and pH-shifting treatments. The lignin morphologies and protein folding degrees were observed. Lignin, SP and LSP were more soluble at higher pH. Comparing to SP films, LSP films had higher water resistance, especially at high pH. Lignin enhanced thermal resistance and induced alternative folding structures of SPA. The pH-shifting process promoted larger clump of protein particle observed under transmission electron microscope. Significant improvement in tensile strength in both wet and dry adhesion tests was observed over the 8.5-4.5 pH-shifting process. Lignin-blended adhesive showed significant improvement on wet adhesion strength. Results also showed that lignin-SP interaction, solubility, degree of penetration and the balance of those factors contributed significantly to adhesion strength.

An Efficient Electrocatalyst for Hydrogen Evolution Reaction Using Ru Nanoparticles Load on TiC-Support

Chanyong Yu[1*], Yebeen Kim[1], Sungkyun Park[2], Kang Hyun Park[1]

[1]*Department of Chemistry, Pusan National University, Busan 46241, Republic of Korea*

[2]*Department of Physics, Pusan National University, Busan 46241, Republic of Korea*

Abstract:

The uncontrolled use of fossil fuels has caused significant environmental pollution. To address this issue, researchers are exploring the hydrogen evolution reaction (HER) as a means to generate hydrogen in energy conversion devices and eco-friendly renewable energy sources. However, the HER suffers from slow reaction kinetics, necessitating the development of cost-effective, long-lasting, highly stable, and efficient electrocatalysts for practical applications. In this study, we successfully prepared ruthenium (Ru) particles supported on titanium carbide (Ru/TiC) using a reduction method. we employed

experimental techniques to examine the stability and electrocatalytic activity of Ru as a transition metal on a TiC support. The synthesized catalyst was characterized using X-ray powder diffraction, scanning electron microscopy, transmission electron microscopy, and X-ray photoelectron spectroscopy. The Ru/TiC electrocatalyst exhibited excellent HER activity, demonstrating low overpotentials, rapid reaction kinetics, and high stability in both alkaline and acidic environments. The results highlight the remarkable electrocatalytic performance of Ru/TiC and will generate interest in the future development of cost-effective nanomaterials for energy and environmental applications.

Biography:

Chanyong Yu is working as a Ph.D student in the group of Professor Kang-Hyun Park under Intelligent OrganoMetallic Chemistry Lab (IOM group), Department of Chemistry, Chemistry Institute for Functional Materials, Pusan National University, Republic of Korea. His research includes the synthesis and fabrication of various organic–inorganic hybrid nanomaterials, polymer-based materials for multiple applications.

Cage-Like Sodalite-Type Porous Organic Salts Enabling Luminescent Molecule's Incorporation and Room-temperature Phosphorescence Induction in Air

Hiroi Sei[1]*, Kouki Oka[1], Norimitsu Tohnai[1]

[1]*Graduate School of Engineering, Osaka University, Japan*

Abstract:

Room-temperature phosphorescent (RTP) materials show emission with a long lifetime at room temperature. However, RTP materials require complicated molecular design and specific intermolecular interactions, and therefore types of RTP materials have been restricted. In this work, tetrasulfonic acid with an adamantane core and triphenylmethylamines that are modified with substituents in the para-positions of benzene rings (TPMA-X [X= Cl, Br, I]) were combined to create cage-like porous materials. We incorporated luminescent molecules into them, and aimed to achieve RTP without molecular design. Adding a representative luminescent molecule (pyrene) to a reaction solution during the construction enabled the incorporation of pyrene in a facile manner. The cage-like porous material with iodine (X = I) on the pore surface did not adsorb oxygen (a quencher of phosphorescence) at room temperature, and induced RTP of the incorporated pyrene even in air. This strategy can be applied to various luminescent molecules, which may lead to the achievement of RTP of various colors.

Biography:

Hiroi Sei is a doctoral student at the Graduate School of Engineering, Osaka University (Supervisor: Prof. Norimitsu Tohnai). He is supported by Japan Science and Technology

Agency (JST), the establishment of university fellowships towards the creation of science technology innovation, and a travel grant from Yoshida Foundation for Science and Technology. His research focuses on the design and properties (gas adsorption and photophysical properties) of organic porous materials.

Precise Control of the Molecular Arrangement of Organic Semiconductors for High Charge Carrier Mobility

Ryota Akai[1]*, Kouki Oka[1], Norimitsu Tohnai[1]

[1]*Graduate School of Engineering, Osaka University, Japan*

Abstract:

The charge carrier mobility of organic semiconductors heavily depends on the overlap of πconjugation between neighboring molecules. In the current study, organic salts composed of disulfonic acid with [1]benzothieno[3,2-b][1]benzothiophene (BTBT) and alkylamines were prepared. As shown in Figure, based on the bulkiness of combined alkylamines, we precisely controlled only BTBT's arrangement without any chemical modifications. Flash-photolysis timeresolved microwave conductivity and quantum chemical calculations elucidated the effect of the subtle difference of the overlap of π-conjugation on charge carrier mobility. Figure. Molecular arrangement control based on a highly ionic hydrogen bond.

Biography:

Ryota Akai is a doctoral student at the Graduate School of Engineering, Osaka University (Supervisor: Prof. Norimitsu Tohnai). He is supported by Japan Science and Technology Agency (JST) SPRING, Grant Number JPMJSP2138, Kato Foundation for Promotion of Science (KS-3514), a travel grant from Yoshida Foundation for Science and Technology. He has already won four poster presentation awards in the field of crystals. His research focuses on organic materials science, organic crystals, and supramolecular chemistry.

Hydrogenation of CO_2 to Dimethyl Ether over WOx-ZrO_2/Cu-ZnO-ZrO_2 Nanocatalysts

Ching-Hui Peng[2], Kuen-Song Lin[1*], Abrar Hussain[1], Yung-Chen Hsieh[1], Yun Ko[1]

[1]*Department of Chemical Engineering and Materials Science/Environmental Technology Research Centre, Yuan Ze University, Chung–Li District, Taoyuan City 32003, Taiwan*

[2]*Research Centre for Energy Technology and Strategy, National Cheng Kung University, Tainan City 70101, Taiwan*

Abstract:

In this study, tungsten-zirconia (WOx/ZrO2) catalysts were synthesized by the impregnation method and combined with the CuO-ZnO-ZrO2 catalyst of methanol synthesis for dimethyl ether (DME) by direct hydrogenation of CO2. The calcination temperature of the WOx/ZrO2 catalysts played a vital role in determining their physicochemical properties. The synthesized catalysts were characterized by XRD, FE-SEM, BET, TPD, and XANES/EXAFS to elucidate their composition, morphology, and acidity. At calcination temperatures between 600 and 700 °C, the WOx/ZrO2 catalysts changed slightly in textural properties, while at 800 to 900 °C, the catalysts specific surface area was lost significantly. The highest surface density and catalytic activity observed for the WOx/ZrO2 catalyst calcined at 800 °C. Moreover, the catalytic performances of CuO-ZnO-ZrO2 combined with a WOx/ZrO2 catalysts were also calculated on the basis of obtained online FTIR and GC spectra. It can be seen that DME selectivity and yield at 240 °C and 30 bar increased after several hours, owing to the gas diffusion lag in the fixed–bed reactor. The combination of CuO/ZnO/ZrO2 and WOx/ZrO2 catalysts, calcination was conducted at 800 °C provided the highest DME selectivity (63.3%), DME yield (9.3%), and CO2 conversion (18.5%) at 240 °C and 30 bar. Cost/benefit analysis estimates a payback period of approximately 3.13 or 1.84 years for a plant design of CO2 catalytic conversion to DME with a capacity of 10– or 20–TPD production.

Biography:

Dr. Kuen-Song Lin, a senior distinguished professor of Department of Chemical Engineering and Materials Science, Yuan Ze University in Taiwan. He is also the director of Environmental Technology Research Centre (ETRC) in Yuan Ze University. His research topics include carbon capture utilization/storage (CCUS), hydrogen storage/PEMFC, waste recycling/utilization of circular economy, on-site soil/water pollution remediation, environmental photocatalysis, and sustainable energy generation. He is also the Associate Editor of Journal of the Taiwan Institute of Chemical Engineers and has published more 165 SCI papers (citation > 5425 and H-index = 37) and three Book Chapters.

Photothermally Tunable Photoluminescence from Graphene Oxide Quantum Dots *via* Intense Pulsed Light

Imjeong Yang[1*], Jae-Won Lee[1], Ji Hye Kwak[2], Kyong-Soo Hong[3], Juhee Kim[4], Geon-Woong Lee[4], and Hee Jin Jeong[4]

[1]*Department of Physics, Pusan National University, Busan 46241, South Korea*

[2]*Electrical Environment Research Center, Power Grid Research Division, Korea Electrotechnology Research Institute (KERI), Changwon 51543, South Korea*

[3]*Busan Center, Korea Basic Science Institute (KBSI), Busan 46742, South Korea*

[4]*Nano Hybrid Technology Research Center, Creative and Fundamental Research Division, Korea Electrotechnology Research Institute (KERI), Changwon 51543, South Korea*

Abstract:

Graphene oxide quantum dots (GOQDs) are two-dimensional carbonic material, having a lateral size of a few nanometers and a one-atom-thickness. Due to their exceptional properties such as the stable photoluminescence (PL), pronounced quantum confinement effect, good chemical stability, and low toxicity, GQDs are considered as one of novel candidate materials for bioimaging, biomedicine, and optoelectronics. GOQDs was fabricated from single-walled carbon nanotubes through chlorate-based oxidation and separation after acoustic cavitation with an average lateral diameter of 3.37 nm and a size deviation of ±0.1 nm. Subsequently, photo-reduced GOQDs (P-rGOQDs) were obtained by liquid-phase photoreduction of the GOQD suspension under intense pulsed light irradiation. Liquid-phase photoreduction selectively reduced epoxy groups present on the basal plane of GOQDs, and hydrogenated the basal plane without removal of carbonyl and carboxyl groups at the edges of the GOQDs. Such selective removal of oxidative functional groups was used to control the reduction degree of GOQDs, closely related to their optical properties. The optimized P-rGOQDs were bright blue in color and showed quantum yields up to about 19.7%, which was 10 times the quantum yield of GOQDs, which reveals that the P-rGOQDs have the potential to be used in the fields of bioimaging, biomedicine, and optoelectronics.

Biography:

Imjeong Yang is a professor at department of physics, Pusan National University, South Korea. She got a Ph. D. in physics from University of Georgia, USA, and has been working on the size confinement and surface effect of nanomaterials.

Two-stage conversion of CO2 to Methanol and Dimethyl Ether Using CuO–ZnO–Al_2O_3/protonated Y-type zeolite Catalysts

Kuen-Song Lin[1*], Ching-Hui Peng[2], Abrar Hussain[1], Yung-Chen Hsieh[1], Yun Ko[1]

[1]*Department of Chemical Engineering and Materials Science/Environmental Technology Research Centre, Yuan Ze University, Chung–Li District, Taoyuan City 32003, Taiwan*

[2]*Research Centre for Energy Technology and Strategy, National Cheng Kung University, Tainan City 70101, Taiwan*

Abstract:

The CuO–ZnO–Al2O3/protonated Y-type zeolite (CZA/HYZ) catalysts were prepared by co-precipitation and used in a two-stage CO2 conversion process. Catalytic components of CZA/HYZ were copper species that have been identified with XPS. Remarkably, the fine structures of metal atoms in CZA/HYZ were confirmed with XANES and EXAFS spectra. Molecular configurations of catalytic species in CZA/HYZ catalyst simulated from the XANES/EXAFS spectra-analyzed fine structural parameters were schematically displayed. The optimal catalytic performances of CZA/HYZ (CH3OH conversion=78.0%, CH3OCH3/HCOOH selectivity=91.7%/8.3%, CH3OCH3/HCOOH yield=71.5%/6.5%) were achieved at 250 ºC. A pseudo-first-order/second-order model and the Arrhenius equation were used to evaluate the rate constants and activation energies of CH3OH and CH3OCH3 formations at various catalytic temperatures. The low activation energies (2.720 and 1.160 kJ mol-1) and Gibbs energies (3.26 and -40.00 kJ mol-1) of CH3OH and CH3OCH3 formations at 250 ºC, demonstrated that their spontaneities were remarkably improved via CZA/HYZ, respectively. The overall income from a 10-TPD (ton per day) waste gas utility process for a petrochemical refinery plant was USD $64,252 d-1 with a payback of 2.44 years, based on cost evaluation. The proposed process provides a continuous two-step process for manufacturing high-value-added chemicals using industrial CO2 emitted and syngas.

Biography:

Dr. Kuen-Song Lin, a senior distinguished professor of Department of Chemical Engineering and Materials Science, Yuan Ze University in Taiwan. He is also the director of Environmental Technology Research Centre (ETRC) in Yuan Ze University. His research topics include carbon capture utilization/storage (CCUS), hydrogen storage/PEMFC, waste recycling/utilization of circular economy, on-site soil/water pollution remediation, environmental photocatalysis, and sustainable energy generation. He is also the Associate Editor of Journal of the Taiwan Institute of Chemical Engineers and has published more 165 SCI papers (citation > 5425 and H-index = 37) and three Book Chapters.

The Simultaneous Production of Electricity and Hydrogen on Electrified Interfaces

André Galembeck[1*], Leandra P. Santos,[2,3] Diana Lermen,[3] Rafael G. Yoshimura,[2,3] Bruno L. da Silva,[3] Thiago A. L. Burgo,[4] Fernando Galembeck[2,3]

[1]*Federal University of Pernambuco, Brazil*

[2]*Galembetech Consultores e Tecnologia Ltda., Brazil*

[3]*University of Campinas, Brazil; São Paulo State University, Brazil*

Abstract:

The spontaneous electrification of solid/moist air interfaces generates electric energy. Many authors confirmed this observation and explored it by building different devices that harvest energy from ambient moisture using different materials, including nanocarbons. Our working hypothesis to explain the operation of these hygroelectric cells involves two consecutive steps: (i) ion partition during water adsorption from humid air and; (ii) H+ reduction and OHoxidation. It has been demonstrated that the selective adsorption of the water ions occurs as described in the following: acid surfaces acquire an excess negative charge, and Bronsted-bases become positive under increased air relative humidity. So, it was hypothesized that the adsorbed chemical species combine to give reaction products plus electrical energy. This was tested by assembling different setups, and the strategy has proven successful. This talk will show that the simultaneous delivery of electric energy and hydrogen from water harvesting at room temperature can be obtained independently from any additional (light, electricity, mechanical, radiation) energy source. The hygroelectric cells are based on exfoliated and reassembled graphite and aluminum electrodes. Different setups allowed the construction and operation of hygroelectric cells, measuring their electrical output and detecting the simultaneous formation of hydrogen plus hydrogen peroxide.

Biography:

André Galembeck Background in Chemistry (D.Sc.), Full Professor at the Fundamental Chemistry Department of the Federal University of Pernambuco (UFPE), in Recife, Brazil. 25-year research experience in Materials Chemistry, Polymers, and Nanostructures. Published more than 80 peerreviewed papers and deposited ten patents. Formerly Director of a Research Institute of the Brazilian Ministry of Science and Technology (2011-18) and member of the National Nanotechnology Advisory Board (2014-2018).

Tailoring the Properties of Carbon Microfiber-based Electrodes Through Covalent Chemical Modification

Myriam Barrejón[1*], Hugo Vara[2], Fernando Langa[1] and Jorge Eduardo Collazos-Castro[2]

[1]*Castilla La-Mancha University, Spain*

[2]National Hospital for Paraplegics, Spain

Abstract:

Much research has been dedicated to the repairing and regeneration of neural tissues after spinal cord injury (SCI). In this line, neuroprosthetic devices (NPDs) are implantable electrodes that have been designed to evoke specific responses in neurons by applying electrical stimulation or alternately record neuronal electrical activity; however, the existing NPDs still show limitations that hinder the long-term performance of implantable neuroprostheses. The work here presented aimed to develop novel strategies for the design of advanced NPDs based on electro-conducting carbon microfibers (CMFs), that might be used to promote guided neural regeneration across the lesion and restore the function of the spine after injury. Concretely, novel hybrid nanoarchitectures with tunable properties have been synthesized by combining poly(ethylenedioxythiophene) (PEDOT)-based polymers with CMFs via covalent approaches through different organic linkers (Figure 1). The electrochemical and mechanical properties of the new hybrid materials have further been studied to assess their promise to be used in providing both electrical stimulation to neural cells and biocompatible scaffolds for directing neural cell growth.

Biography:

Myriam Barrejón obtained her PhD in Nanoscience and Nanotechnology (2015) at Castilla La-Mancha University (UCLM) (Spain), under the supervision of Prof. Fernando Langa. During her PhD, she worked on the functionalization and characterization of carbon nanostructures for optoelectronic applications, and she received the prize to the best doctoral thesis from the RSEQ-CLM. Then, she joined Prof. Prato's group as a post-doctoral researcher, where she worked on the synthesis of carbon nanostructure-based 3D networks for biomedical applications for two years. Currently, she is a Ramon y Cajal Fellow at UCLM, where she is working on the functionalization of carbon-based materials for biomedical and energy applications.

A New, Facile Synthesis of High-quality CMK-type Carbon Replicas

Rafał Janus[1*], Piotr Natkański[2], Mariusz Wądrzyk[1], Marek Lewandowski[1], Marek Michalik[3], Piotr Kuśtrowski[2]

[1]AGH University of Science and Technology, Faculty of Energy and Fuels, al. A. Mickiewicza 30, 30-059, Kraków, Poland

[2]Jagiellonian University, Faculty of Chemistry, ul. Gronostajowa 2, 30-387, Kraków, Poland

[3]Jagiellonian University, Institute of Geological Sciences, ul. Gronostajowa 3a, 30-387, Kraków, Poland

Abstract:

Carbon replicas (or mesostructured carbons), a class of porous carbons reported for the first time in 1999, pose an interesting alternative to conventional microporous activated carbons. They are basically mesoporous bodies, and although atomically disordered, they feature a long-range spatial ordering of channel networks.

Mesostructured carbons are chemically inactive, featuring tunable surface chemistry, good mechanical rigidity, and thermal stability as well as interesting electrical properties. Owing to these features, they have found a variety of applications, e.g. in adsorption and catalysis, medicine, and electrochemistry.

Carbon replicas can be synthesized by nanocasting of suitable hard templates, mostly porous silicas. Though, the majority of the developed recipes are laborious and energy-consuming, and usually require the use of advanced apparatus. These inconveniences, accompanied additionally by poor reproducibility and limited scalability have been a barrier that hindered the manufacturing and application of mesostructured carbons on a technological scale.

Herein, we proposed a novel variant of the nanocasting route, versatile for the synthesis of both hollow- and rod-type structures. The concept relies on a solvent polarity-controlled selective deposition of a carbon precursor (furfuryl alcohol) on a silica matrix in a non-polar medium (toluene). The process is driven by the adsorptive attraction between polar monomer and free silanols. Meanwhile, toluene serves only as the monomer-supplying carrier. By employing this procedure, we obtained six CMK-n structures (n = 3, 5–9) featuring excellent structural and textural parameters while maintaining the morphology of the mother silica particle. Furthermore, we have proven the satisfactory repeatability and scalability of this synthesis pathway.

Biography:

Rafał Janus achieved his PhD in chemistry at the Faculty of Chemistry, Jagiellonian University in 2013. During his doctoral studies, he did scholarships at the University of Antwerp (Belgium) and the University of Alicante (Spain). In 2011, he defended his engineering thesis in chemical technology at the Faculty of Energy and Fuels, AGH University of Science and Technology (AGH-UST). Since 2013, he has been an assistant professor at the Department of Fuel Technology at the AGH-UST. His scientific interests concern the synthesis and characterization of ordered mesoporous materials for the purposes of manufacturing and catalytic refining of liquid (bio)fuels.

Liquid Phase NMR for Characterization Solid Porous Carbon Materials

István Bányai*, Mónika Kéri, Dávid Nyul

Department of Physical Chemistry, University of Debrecen, Hungary

Abstract:

Nuclear Magnetic Resonance (NMR) provides information about the pore size and shape, pore wall structure and the mechanism of wetting processes. The combined use of NMR cryoporometry, low-field relaxometry and NMR diffusiometry complete each other and provide information on the behavior porous carbons under the condition of applications. From cryoporometry the size distribution and in certain cases the shape of pores are deduced. Low-field relaxometry beyond the size distribution refers to the wetting mechanism and hydrophilicity of the pore wall through the surface relaxivity. NMR diffusiometry shows the mobility of the liquid in the porous media and taking into account the vapor diffusion the filling factor can be determined for separate pores. Carbon aerogels prepared from resorcinol-formaldehyde aerogels are promising platforms for electrodes, catalysts, adsorbents in environmental chemistry and as electric conductors. For these applications the knowledge of their structure and behavior in aqueous (liquid) medium is essential. By means of NMR methods we could show the presence of water clusters formed at low hydration level on and around the hydrophilic functional groups of the surface. With increasing water content, spherical water drops formed inside the pore system, and vapor phase diffusion was observed in the partially filled pores. The determined wet structure was compared to low temperature nitrogen gas adsorption results and scanning electron microscopy images and we could present the strength of NMR for characterizing porous materials evaluating its advantages and some disadvantages compared to the classical surface analytical methods.

Biography:

István Bányai was born in Debrecen (Hungary) in 1953. He studied chemistry at the Lajos Kossuth University (at present University of Debrecen, UD) where he received his master degree in 1977. Then he worked for the Department of Physical Chemistry and received his degree on kinetics of redoxi reactions. Between 1986 and 1998 he spent 5 years in Stockholm (Sweden) at the Royal Institute of Technology (KTH) working with NMR. From 2005 to 2016 he was the head of the Department of Colloid and Environmental Chemistry at the University of Debrecen. His research focuses on dynamic aspects of NMR spectroscopy.

Hierarchical Porosity of Hybrid Carbon Nanomaterials Based on a Covalent Triazine Framework for Electrochemical and Electrocatalytic Application

Marta E. Plonska-Brzezinska[1*], Agnieszka Hryniewicka[1] , Joanna Breczko[1,2] , Anthony N. Papathanassiou[3] , Krzysztof Brzezinski[4] , Anna Ilnicka[5] , Artur P. Terzyk[5] and Luis Echegoyen[6]

[1]*Medical University of Bialystok, Poland*

[2]*University of Bialystok, Poland*

[3]National and Kapodistrian University of Athens, Greece

[4]Institute of Bioorganic Chemistry, Polish Academy of Sciences, Poland

[5]Nicolaus Copernicus University in Torun, Poland

[6]University of Texas at El Paso, USA

Abstract:

Covalent triazine frameworks (CTFs) constitute an emerging class of high-performance materials due to their porosity and the possibility of structural control at the molecular or atomic level. However, the use of CTFs as electrodes in supercapacitors is hampered by their low electrical conductivity and a strong stacking effect between adjacent CTF sheets. The study shows that covalently immobilizing triazinebased structures on spherical carbon nanostructures results in the organization of micro- and mesopores in a three-dimensional manner. We selected the nitrile-functionalized pyrrolo[3,2-b]pyrrole unit to form triazine rings to construct a covalent organic framework. Combining spherical carbon nanostructures with the triazine framework produced a material with unique physicochemical properties, exhibiting the highest specific capacitance value of 638 F g-1 in aqueous acidic solutions. It should be emphasized that the specific capacitance value for hybrids was 1.5-2 times higher than that for the CTF reference. We examined the factors responsible for such a large increase in electrochemical efficiency. This phenomenon is attributed to many factors. The material exhibits a large surface area, a high content of micropores, a high content of graphitic N, and N-sites with basicity and semi-crystalline character. Thanks to the high structural organization and reproducibility, and remarkably high specific capacitance, these systems are promising materials for use in electrochemistry. For the first time, hybrid systems containing triazine-based frameworks and carbon nano-onions were used as electrodes for supercapacitors. We gratefully acknowledge the financial support of the National Science Centre, Poland, grant #2019/35/B/ST5/00572 to M.E.P-B.

Biography:

Marta Eliza Plonska-Brzezinska received her Ph.D. in Chemistry in 2005. She is working at the Medical University of Bialystok since 2018, as a Head of Organic Chemistry Department. Marta maintains active research collaborations with USA, Ukraine, Greece, Spain, Iran, Columbia and Poland researchers. She holds a very active research program with interests in carbon nanostructures and materials chemistry, focusing on porous structures and their applications in electrochemistry, electrocatalysis and biomedical fields. She has published around 85 research articles. She was awarded by Stefan Batory Fellowship (2003), by the Polish Ministry of Science and Higher Education (2015) and the Polish Academy of Sciences (2018).

Organic Radicals and Proton Coupled Redox Reactions

Prasanta Ghosh*, Debasish Samanta and Souvik Mukherjee

Ramakrishna Mission Residential College (Autonomous), India

Abstract:

Metal centered electron transfer reactions are common in chemical science. Electron transfer reactions involving organic molecules are limited in scope. Thus modeling of redox reactions based on organic molecules is a subject of current investigation. In this context π-electron rich/deficient aromatic molecules which undergo oxidation and reduction reactions affording reactive organic radicals and the proton-coupled electron transfer avenue are significant. Redox reactions where the e− /H+ donor orbitals and e− / H+ acceptor orbitals validate a simultaneous transfer of proton and electron are defined by concerted proton-electron transfer (CPET).1 Hydrogen atom transfer (HAT) has been considered as proton-coupled redox processes, in which the proton and the electron move together, sharing the starting and the final orbitals. In this presentation, proton-coupled oxidation of a diarylamido to aminyl by a CPET path will be discussed.2 The effect of H-bonds to the proton coupled oxidation of phenolato to phenoxyls relevant to tyrosyl radical in biology has been analyzed.3 Also, activation of O2 by a coordinated -NH- function4 and turning the condensation reaction of the 1,2-diketones with amines to redox reactions5 involving HAT and methoxylation promoted CPET reaction6 will be delineated.

References: 1. Huynh, M. H. V.; Meyer, T. J., Chem. Rev. 2007, 107, 5004. 2. Kundu, S.; Dutta, D.; Maity, S.; Weyhermueller, T.; Ghosh, P. Inorg. Chem. 2018, 57, 11948. 3. Samanta D., Saha P., Ghosh P., Inorg. Chem. 2019, 58, 15060. 4. Mukherjee, S.; Ghosh, P. unpublished results. 5. Samanta D., Saha P., Ghosh P., Unpublished results. 6. Mukherjee, S.; Ghosh, P. unpublished results.

Biography: Dr. Prasanta Ghosh, Associate Professor, Department of Chemistry, Ramakrishna Mission Residential College, Narendrapur, Kolkata, Homepage: https://pghosh.in/

Research Interest: Modeling of functional metal-organic fragments, particularly stabilization of organic radicals and study of their role in multi-component electron transfer, aromatic ring cleavage, C-H activation, redox cascade, CPET reactions, mixed valence species and catalysis

Awarded: Alexander von Humboldt, Max-Planck-Society, Senior Alexander von Humboldt Research Fellowships. Prof. D. Nasipuri Memorial Award from Chemical Society of India and elected as a Fellow of WAST

Publications: Published more than 140 articles in the journals of international repute.

New Nanoporous Carbon Materials and Composites Applied for CO_2 Uptake and Hydrogen Fuel

Boyko Tsyntsarski[1*] and Eli Grigorova[2], Momchil Dimitrov[1], Ivanka Stoycheva[1], Bilyana Petrova[1], Angelina Kosateva[1], Georgi Georgiev[1], Urszula Szeluga[3], Alexandro Erto[4], Nartzislav Petrov[1]

[1] *Institute of Organic Chemistry, Bulgarian Academy of Science, Sofia, Bulgaria*

[2] *Institute of General and Inorganic Chemistry, Sofia, Bulgaria*

[3] *Centre of Polymer and Carbon Materials, Polish Academy of Sciences, Zabrze, Poland*

[4] *Università degli Studi di Napoli Federico II, Napoli, Italy*

Abstract:

Hydrogen is a prospective renewable and clean energy source. One of the methods of solid-state hydrogen storage is in the form of metal hydrides, which provides safe storage in small volume tanks. Mg based materials are promising for hydrogen storage, despite their slow kinetics and high desorption temperature. Hydrogen production from methanol is also promising eco-friendly method.

In this investigation nanoporous carbons with different textural and chemical surface propertied are synthesized after thermo-chemical treatment of various precursors. The resulting solid product is subjected to high-temperature hydro-carbonization at 800oC. The obtained nanoporous carbons and metal containg samples are characterized by set of physicochemical methods.

Nanoporous carbons and carbon-metal composites are tested as catalysts in methanol decomposition, leading to production of CO and hydrogen. Hydrogen absorption-desorption propertied of carbon-magnesium composites during prolonged cycling are also studied. The absorption-desorption characteristics during prolonged cycling towards hydrogen of Mg-C composite obtained by ball milling under Ar atmosphere are studied.

Further CO2 adsorption experiments are performed. Adsorption tests have been carried out in lab-scale fixed-bed column, at different temperatures and CO2 concentrations, in order to investigate both kinetic and thermodynamic aspects. It was established that the synthesized nanoporous carbons have very good CO2 adsorption capacity. Experimental results confirm that CO2 adsorption is a reversible process.

Acknowledgements: The authors are grateful for the funding provided by the Project DMC No 206/07.04.2022, Project KP-06-27/9 and Polish-Bulgarian Joint Project IC-PL/05/2022-2023.

Biography:

Prof. Dr. Boyko Tsyntsarski (born 1974) is a Head of Lab. Chemistry of Solid Fuels in the Institute of Organic Chemistry with Centre of Phytochemistry, Bulgarian Academy of Sciences. Main research area and subareas: New nano-structured carbon materials, Technology and chemistry of natural and synthetic fuels, Adsorption, Catalysis, Ecology, IR spectroscopy More than 100 scientific papers more than 1000 citation, h-index 18 (Scopus). Coordinator of a project with Bulgarian National Science Fund, Polish-Bulgarian joint project and Romanian-Bulgarian Project.

Carbon Dioxide Reduction Catalyzed by Silicon-based 2D Material.

Wilmer Esteban Vallejo Narváez[1*] and Serguei Fomine[1]

Materials Research Institute, National Autonomous University of Mexico (IIM-UNAM), Circuito Exterior S/N, Circuito de la Investigación Científica, Ciudad Universitaria, Mexico City.

Abstract:

The excessive emission of CO2 is an environmental challenge, and the development of 2D materials has become a promising alternative to capture and transform CO2 into value-added chemicals. In this work, a theoretical exploration of the catalytic activity of CO2 reduction mediated by three allotropic forms of silicon—monolayer, bilayer, and haeckelite bilayer—was carried out. The calculations were made with density functional theory. Our results show that the reaction pathway involves the adsorption of CO2 on the silicon surface, followed by the addition of hydrogen molecules to form products such as formic acid, methanol, methane, carbon monoxide, and formaldehyde. Our proposed mechanism indicates that the silicon haeckelite bilayer exhibits a higher affinity for CO2 than honeycomb silicene structures. Hydrogenation with H2 occurs by adding one hydrogen atom to the absorbed CO2 and another to the surface of the material. Intermediate species are reduced by systematically adding hydrogen atoms and removing water molecules, forming formic acid as the most favored product. Our study provides important insights into the fundamental mechanisms underlying silicon-mediated CO2 reduction and could facilitate the development of more efficient catalysts for this process.

Biography:

Wilmer E. Vallejo Narváez is a Chemist from University of Nariño, Colombia. He received his Ph.D. in Chemical Science from the National Autonomous University of Mexico (UNAM) in 2018 under the supervision of Prof. Tomás Rocha. Now, he is working as a postdoc under the supervision of Prof. Serguei Fomine at the Research Materials Institute of UNAM. He has investigated non-covalent interactions and reaction mechanisms from an experimental and theoretical perspective. Currently, his research focuses on studying 2D materials and the theoretical exploration of their catalytic activity in CO2 reduction

Electrical Energy Harvester from Carbon Nanotube Yarns

Seon Jeong Kim*

Center for Self-Powered Actuation, Department of Biomedical Engineering, Hanyang University, Seoul 04763, Korea

Abstract:

Energy harvesters are needed for such diverse applications as self-powered wireless sensors, structural and human health monitoring systems, and cheaply harvesting energy from ocean waves. We reported carbon nanotube (CNT) yarn harvesters that electrochemically convert tensile or torsional mechanical energy into electrical energy. Stretching coiled yarns generated peak electrical power when cycled up to Hz. Unlike for other harvesters, torsional rotation produces both tensile and torsional energy harvesting and no bias voltage is required, even when electrochemically operating in salt water. Since homochiral and heterochiral coiled energy harvester yarns provide oppositely directed potential changes when stretched, both contribute to output power in a dual-electrode yarn. These energy harvesters were used in the ocean to harvest wave energy, combined with thermally-driven artificial muscles to convert temperature fluctuations to electrical energy, sewn into textiles for use as self-powered respiration sensors, and used to power a LED and to charge a storage capacitance (1). Stretching a coiled CNT yarn can provide large, reversible electrochemical capacitance changes, which convert mechanical energy to electricity. The performance of these coiled energy harvesters was increased by optimizing the alignment of precursor CNT forests, plastically stretching the precursor twisted yarn, applying much higher tensile loads during pre-coiling twist than for coiling. The peak output power for 1 ~ 30 Hz sinusoidal stretch were over 10-fold that of previous Twistron energy harvesters at these respective frequencies (2).

References:

(1) Kim et al., Science 357, 773 (2017)

(2) Wang et al., Advanced Materials 34, 2201826 (2022)

Hot Electron Injection into Aqueous Electrolyte Solutions from Carbon Particle-doped Polymer Electrodes

Sakari Kulmala* and Kalle Salminen

Aalto University, School of Chemical Engineering, Department of Chemistry and Materials Science, Finland

Abstract:

This contribution reports utilization of printed and otherwise manufactured hot electron

emission electrodes for hot electron-induced electrochemiluminescence (HECL) and other hot electron electrochemistry applications. HECL is typically a method utilizing luminophores as labels in sensitive bioaffinity assays such as in immunoassays. Method normally applies hot electrons generated by tunnel emission from thin insulating film-coated cathodes such as oxide-coated silicon electrodes or coated with organic polymers doped with conductive particles. All the electrode types discussed presently are composed of a metal or printed silver base that is coated with a carbon particle-coated polymer film. If the energy of tunnel-emitted hot electrons is above the conduction band edge of water, electrons may enter the conduction band of water and are likely to become hydrated (eaq-) after thermalization and solvation likewise in the photoemission of electrons. When these hot or hydrated electrons react with dissolved oxygen and added co-reactants, such as electron scavengers producing highly oxidizing radicals (peroxodisulphate, peroxodiphosphate or hydrogen peroxide), both extremely strong oxidants and reductants are simultaneously available, and many kind of difficult redox reactions e.g. excitation of label compounds are enabled.

Biography:

Sakari Kulmala, PhD, Professor of Analytical Chemistry, Aalto University, since year 2000. Pioneer of analytical applications of hot electron electrochemistry. Acted as the director of national graduate school of Chemical Sensors and Microanalytical Systems 2002-2010.

Development of an Online Monitor for Ambient Total and Water-soluble Organic Carbon (TOC and WSOC) Measurements

Constantinos Sioutas*, Ramin Tohidi, Mohammad Aldekheel, Mohammad Mehdi Badami, Vahid Jalali Farahani

University of Southern California, Department of Civil and Environmental Engineering, Los Angeles, California, USA

Abstract:

Organic carbons (OC) have been linked to numerous adverse health risks by triggering inflammatory responses in respiratory system. Organic carbon compounds that are highly water-soluble can easily dissolve in water and be inhaled and absorbed into the bloodstream, which increases the risk of cardiovascular diseases. OCs are one of the major contributors to total particulate matter (PM) with higher concentrations in PM2.5 ($dp < 2.5\mu m$) compared to coarse PM ($2.5\mu m < dp < 10\ \mu m$). In this study, two novel setups were proposed for measurements of OC in PM2.5 and coarse PM and their performance has been investigated to test the feasibility of using them to measure the real time concentrations of water-soluble organic carbon in ambient. Few studies have investigated the measurements of OCs in ambient environments with high time resolution, which can provide a better insight into potential short-lived sources of these particles. A Sievers M9

TOC analyzer was utilized in a setup with an aerosol-into-liquid sampler to collect PM2.5, and a setup with Biosampler to ambient coarse PM, to read total OC levels on an hourly basis. The measurements were compared with an EC/OC sunset lab monitor running in parallel to measure OC concentrations in both coarse and PM2.5. Our results showed that, the hourly TOC levels measured by the TOC analyzer in our setups were in good agreement with those quantified by the EC/OC monitor in PM2.5 (R2=0.81) and coarse PM (R2=0.85). The diurnal trend of WSOC was investigated to gain a better insight into the nighttime chemistry of these particles.

Modulation of Optoelectronic Properties of Transition Metal Dichalcogenides (TMDCs) By Substrate Engineering

Atomically thin layers (with thicknesses <1nm) of monolayer (ML) thick transition metal dichalcogenides (TMDCs) showed exciting electrical and optical properties. Growth of these materials as well as electrical, optical, vibrational, and other properties of these materials largely depend on which TMDCs are deposited or transferred. Many interesting substrate/underlying layer-TMDC interactions such as interface strain, charge transfer, dielectric screening, and optical interference and others had been studied. Thus, a variety of substrates and other intermediate thin film layers have been employed to modulate the properties of TMDCs. These approaches resulted in numerous exciting phenomena that differ from those observed in their bulk counterparts. Using these properties low power, ultra-thin tunable opto-electronic devices, non-volatile memories, and devices were made. In this talk, I will present the some of the novel and interesting electrical, optical, and other properties of TMDCs utilizing substrate engineering.

Biochar as a multifunctional amendment to agriculture and climate change.

Sara de Jesus Duarte

The Next 150, Mexico

Abstract Not Available!!!!

Biomaterials Innovations for the Future: Unveiling the Ten Most Captivating Areas for Advancement

Gilles Georges, Angela Zhou.

CAS, a Division of the American Chemical Society.

Abstract:

Owing to the excellent applicability of biomaterials, a rapid and diversified expansion of the biomaterial repertoire has been observed over the last few decades. Biomaterials refer to materials that are designed to interact with biological systems without significant adverse effects. Because of this excellent biocompatibility, biomaterials are commonly engineered to perform therapeutic or diagnostic functions within the body.

Our work employed over half million publications related to biomaterials from CAS Content Collection. By integrating big data analytical approach, such as Natural Language Toolkit (NLTK), and expertise knowledge, we identified the ten most promising research areas in biomaterials. We then present their publication trends in journals and patents, highlight their diverse applications, and shed light on the rapid development of specific properties or substances. Our objective is to provide a comprehensive overview of the evolving landscape in this field and offer valuable insights for future directions. We hope our work will serve as a valuable resource for researchers, agencies, and perhaps entrepreneurs and investors as well, empowering them in strategic planning and furthering their endeavors in this domain.

Biography:

Dr. Gilles Georges, Vice President and Chief Scientific Officer at CAS. Prior to joiningCAS, Gilles held various executive, P&L management positions with Milacron, DowDuPont, Axalta, and 3M, representing Aerospace, Oil & Gas, Materials, Optical & Electronics industries. Gilles has a Ph.D. in Chemistry from the University of Montreal, Canada, as well as Masters and Bachelor's degrees in chemistry and Material Sciences from Université de Pau, France. Gilles also holds a Diploma in Management from McGill University and an MBA from HEC School of Commerce in Montreal, Canada.

Laser-Induced Graphene Electrode: Advances in Foodborne Illness Detection and Point-of-Care Ion Analysis

Nipapan Ruecha[1*], Pattarachaya Preechakasedkit[1], Kanyapat Teekayupak[2], Atchara Lomae[1], Orawon Chailapakul[2], Tugba Ozer[3], Daniel Citterio[4]

[1]Metallurgy and Materials Science Research Institute, Chulalongkorn University, Thailand;

[2]Electrochemistry and Optical Spectroscopy Center of Excellence (EOSCE), Chulalongkorn University, Thailand

[3]Yildiz Technical University, Turkey

[4]Department of Applied Chemistry, Faculty of Science and Technology, Keio University, Japan

Abstract:

The cost-effective and readily producible laser-induced graphene electrode (LIGE), fabricated through carbon dioxide (CO2) laser pyrolysis of a carbon-rich precursor polyimide (PI) in an ambient atmosphere without the need for wet chemical steps, encompasses all the essential characteristics necessary for an electrochemical biosensor. In this work, the LIGE has been developed as an alternative sensor with two advanced approaches: 1) integrated electrochemical lateral flow immunosensor for foodborne illness detection and 2) potentiometric sensor for point-of-care ion analysis. The integrated electrochemical lateral flow immunosensor for foodborne illness detection demonstrates high selectivity and sensitivity for detecting a small amount of pathogen contaminated in food samples by the combination of the specific binding pathogen-antibody interaction and signal-on electrochemical response of gold-bound gold nanoparticles complex labeled antibody. For potentiometric sensor of point-of-care ion analysis, an ion-selective electrode based on carbon black-modified LIGE has been introduced to simultaneously detect multiplex ions in real urine and simulated sweat samples, facilitating point-of-care analysis for early and rapid diagnosis. Regarding advanced applications, the LIGE could be a high potential as a promising tool for the further development of various biosensors due to its numerous advantages of low cost, fast and easy fabrication, and environmentally friendly method.

Biography:

Dr. Nipapan Ruecha received her Ph.D. (Macromolecular Science) in 2015 from Chulalongkorn University, Bangkok, Thailand. Currently, she is a research researcher at Metallurgy and Materials Science Research Institute, Chulalongkorn University in Thailand. Her areas of interest include the preparation of nanomaterials for biosensors, miniaturized analytical systems such as paper-based analytical devices and microfluidics, lateral flow immunoassay test strips, colorimetric and electrochemical sensors for applications in food safety and biomedical diagnosis.

Techno- economic and Ecological Assessment of Synthetic Fuels Production Using Sustainable Carbon and Hydrogen

Sandra Adelung[1], Felix Habermeyer[1], Simon Maier[1], Moritz Raab[1], Yoga Rahmat[1], Julia Weyand[1], Ralph-Uwe Dietrich[1*]

[1]German Aerospace Center (Deutsches Zentrum für Luft- und Raumfahrt e. V., DLR) Institute of Engineering Thermodynamics Stuttgart, Germany

Abstract:

Around ¼ of the global CO2 emissions can be attributed to the transport sector. The EU-wide CO2 reduction target of 30 % from 2005 level is out of reach without massive efforts even in the transport sector. The use of synthetic fuels is an attractive solution to reduce greenhouse gas (GHG) emissions where electrification proves to be challenging or too cost intensive. Combining the use of renewable electricity to produce electrolytic hydrogen and sustainable carbon (e.g. from non-crop-based biomass) offers a promising route for large-scale, low carbon power-to-X-products (PtX). While the process technology is pretty mature, the energy efficiency, the production costs, the GHG savings and the

possible production capacity is a part of the political debate.

Rigorous chemical process simulation using standard software like Aspen Plus® with experimentally validated unit performance data is the basis to get an exact representation of the entire process. Chemical engineering cost estimation is applied to predict net production costs (NPC) of PtX-products for transport fuels. A life cycle assessment (LCA) is performed with the open source framework Brightway21 using the same data set of rigorous process simulation. Costs and GWP where calculated using the in-house tool Techno-Economic Process Evaluation Tool (TEPET)2,3.

Biography:

Dr. Ralph-Uwe Dietrich has led a research group on techno economic and ecological assessment at the DLR since 2015. There he applies his knowledge of chemical engineering process design and simulation to the assessment of new production routes for chemicals and fuels. He provided 10 years of research and a PhD in high temperature fuel cells. Dr. Dietrich worked for 15 years in project development and management in the process and automation industry.

Synthesis of SGLT2 Inhibitors by Means of Metal-Mediated Coupling Reaction with Grignard Reagent

Masahiko Seki,[*, 1, 2] Shaheen Kasim Mulani,[2] Subarna Jyoti Kalita,[2] Tapkir Sandeep Rameshrao,[2] Maheshwara Reddy Nadiveedhi[2] and Kazushi Mashima[2]

[1]*R&D Planning Department, Tokuyama Corporation, Japan*

[2]*Graduate School of Pharmaceutical Science, Osaka University, Japan*

Abstract:

Sodium dependent glucose transporter2 (SGLT2) inhibitors 1 have received keen attention as a diabetes drug due to high efficacy and safety.1 Recent discoveries on additional potency of those drugs for nephritis and heart failure have enhanced the importance as a therapeutic agent significantly.2 SGLT2 inhibitors have β-C glycoside motif as a common structure where sugar unit is combined with aromatic group by β orientation.3 Previous synthetic methods have a serious issue of need of cryogenic conditions (78 oC) to install the characteristic structure itself. To address the drawbacks, we have developed new synthesis which can be undertaken at ambient temperature for the key step.4 The method consists of a new ketone synthesis from 2 to 3 through metal-mediated coupling reaction with Grignard reagent. The mild reaction conditions enable use of labile acetyl protecting group.

1.Marsenic, O. Am. J. Kidney Dis. 2009, 53, 875.

2.Bruce Neal, M. B. et al. N. Eng. J. Med. 2017, 377, 644.

3.Aguillón, A. R. et al. Org. Process Res. Dev. 2018, 22, 467.

4.(a) Kato, D.; Murase, T.; Nagae, H.; Tsurugi, H.; Seki, M.; Mashima, K. Chem. Eur. J., 2022, Early View, (b) Seki, M.; Tapkir, S. R.; Reddy, M. N.; Mulani, S. K. ACS Omega, 2023, 8, 17288, (c) This work has been awarded CPhI Pharma Awards 2022 on Excellence in Pharma: API Development.

Biography:

Masahiko Seki received his Ph.D. degree in 1988 from Kyoto University. He has been working for research laboratories of Mitsubishi Tanabe Pharma Corporation since 1982. As of 1993, he spent a year as a postdoc at CSU (Prof. Albert I. Meyers). He received 1996 Incentive Award in Synthetic Organic Chemistry, Japan in 1997, and CPhI Pharma Awards in 2013 and 2022. He is the author of 100 scientific papers and an inventor on 200+ patents. As of 2016, he relocated to Tokuyama Corporation, where he became Fellow in 2020. He has been a Guest Professor at Osaka University since 2018.

Reaction Mechanisms of Acid-catalyzed Cracking and Alkylation in the Upcycling of Polyethylene: AIMD study

Mal-Soon Lee[1*], Debmalya Ray[1], Rachit Khare[2], Wei Zhang[2], Donald M Camaioni[1], Oliver Y. Gutiérrez[1], Johannes A. Lercher[1,2]

[1]Pacific Northwest National Laboratory, USA; 2TU München, Germany

Abstract:

Material made of plastic is ubiquitous in products ranging from packaging and textiles to medical equipment and vehicle components. However, most of the disposed plastic is accumulated in landfills and dispersed into water bodies. In the US, discarded polyolefins can provide about 30 MT per year of hydrocarbon-based waste carbon. This engenders unprecedented attention to catalytically upgrade polyolefin waste into fuels and value-added chemicals. However, the conversion of waste polyolefins is particularly challenging due to the stable C(sp3)-C(sp3) bonds compared with the chemical bonds of functionalized polymers. There have been efforts to develop strategies for the conversion such as aromatization, hydrogenolysis, and hydrocracking. However, these strategies still require temperatures above 200 C. Although low-temperature operation would empower significant energy savings, the endothermic cleavage of the C-C bonds makes processes thermodynamically unfavorable at low temperatures. As a consequence, converting polyolefins requires severe reaction conditions to overcome the kinetic and thermodynamic constraints at low temperatures. Recently our group proposed a new approach where endothermic process of cracking is combined with exothermic alkylation.

We experimentally observed low-temperature conversion of polyethylene to liquid isoalkanes (C6-C10) at temperatures below 70 °C from a tandem cracking-alkylation process, i.e., acid-catalyzed cracking and alkylation of polyolefins with isoalkanes, catalyzed by a Lewis acidic chloroaluminate ionic liquid. In this talk, I am going to present our computational study of the reaction mechanisms of these reactions at the atomic scale from ab initio molecular dynamics simulations in aid of a Blue Moon ensemble method.

Biography:

Dr. Mal-Soon Lee is a senior scientist at Pacific Northwest National Laboratory, USA. She has been working in the field of computational physics/chemistry with an emphasis on studying dynamics and reactions at complex interfaces, confined systems, and liquid phases. Her areas of application include catalysis, battery materials, surface science, and polymer upcycling. To understand the reactivity of homo- and hetero-phase materials, large-scale high-performance computing techniques such as ab initio molecular dynamics combined with enhanced sampling techniques are employed. With obtained data, various statistical mechanics techniques are applied to calculate reaction enthalpies/entropies, spectroscopies, which can be directly compared with experimental observations.

Optical Modulation of Linear π-Conjugated Systems with Molecular Actuators

Giuseppe Sforazzini[1,2*], Augustina Jozeliunaitè[2] , Edvinas Orentas[3] and Daniele Fazzi[4]

[1]*Department of Chemical and Geological Sciences, University degli Studi di Cagliari, 09042 Monserrato, Cagliari, Italy*

[2] *Institute of Material Science and Engineering, Ecole Polytechnique Federale de Lausanne (EPFL), 1015 Lausanne, Switzerland*

[3] *Department of Organic Chemistry Faculty of Chemistry and Geosciences, Vilnius University Naugarduko24, LT-0325 Vilnius, Lithuania*

[4] *Dipartimento di Chimica "Giacomo Ciamician", Università di Bologna Via F. Selmi 2, 40126 Bologna, Italy.*

Abstract:

The geometric arrangement of π-orbitals in organic semiconductors significantly impacts the optoelectronic properties of bulk materials. Adjusting the π-bond geometry, such as planarity, within an extended conjugated system offers the chance to tailor the effective conjugation length, thereby tuning its optical and electronic properties. An effective strategy to modulate the π-orbital orientation in a conjugated structure is by incorporating photochromic segments into the π-system's 'backbone'. Integrating photochromic molecules as monomer units within a conjugated chain has revealed diminishing photo-reversibility efficiency as π-conjugation strengthens. In this study, we introduce a novel 'photochromic torsional switch' (PTS) molecular structure designed to

overcome limitations faced by current photochromic dyes. This arrangement includes a polymerizable bithiophene unit that adjusts its π-system planarity through photochromic isomerization of an azobenzene unit attached orthogonally to the backbone. In darkness and under visible light, the azobenzene adopts its elongated trans shape, causing the bithiophene backbone to deviate from coplanarity, resulting in a 60° dihedral angle. Conversely, exposure to UV light triggers isomerization of the azobenzene, transitioning it to the cis shape. This change enables the bithiophene segment to adopt a flat, π-conjugated configuration with dihedral angles of 152°. The PTS designs introduced here present a novel category of light-responsive actuators, potentially enabling the creation of 'conjugated photochromic semiconductors' and deepening our understanding of the interplay between molecular structure and optoelectronic properties in π-conjugated macromolecules.

Biography:

Giuseppe Sforazzini completed his Ph.D. at the University of Oxford in 2010 under the guidance of Prof. Harry Anderson, focusing on supramolecular wires for organic electronics. Afterward, he worked as a research scientist at the Italian Institute of Technology's Center for Nano Science and Technology, led by Prof. Guglielmo Lanzani. In 2011, he was awarded a Marie-Curie Fellowship to research supramolecular artificial photosystems under Prof. Stefan Matile at the University of Geneva. Joining EPFL's Institute of Materials in 2013, he held a Swiss National Science Foundation (SNSF) Ambizione grant in collaboration with Prof. Holger Frauenrath. He currently serves as an Associate Professor at the University of Cagliari's Department of Chemical and Geological Science since 2020.

Advanced Synthetic Hydrogels for Life Science Research and Applications

Xiuzhi Susan Sun*

Kansas State University, USA

Abstract:

Life Science research and development have been limited by two-dimensional monolayer cell culture (2D). Thus, a variety of three-dimensional (3D) technologies have been developed and commercially available. The advanced synthetic peptide hydrogel (PepGel) technology, crafted from human muscle and spider silk protein domains, offers unique properties for a broad-spectrum application in medical and life science area. PepGel not only promotes biocompatibility and presents no immunogenic effects but its unique properties have been proven beneficial for various applications in 3D culture of various cancer cells and stem cells, 3D DNA transfection, and in vivo delivery of cells, drugs, antigens, and virus. Particularly, PepGel system is scalable and produces physiological relevant 3D cell colonies (spheroids) that can be easily retrieved and the spheroids show superior integrity for drug screening, disease modeling, tissue engineering, and

therapeutics. Specific use examples will be presented in this presentation.

Biography:

Xiuzhi Susan Sun is a University Distinguished Professor of Kansas State University (KSU). Dr. Sun's research interests include biopolymer design, synthesis, and manufacturing for environmental and biomedical applications. She is specialized in protein and lipids structure and functional properties for hydrogels, biobased adhesives, resins for coatings, and biodegradable plastics and composites. Dr. Sun has published 220 SCI referee articles and holds 17 patents. Dr. Sun is the Fellow of National Academy of Inventors; and the Fellow of American Society of Agricultural and Biological Engineers. Dr. Sun earned her PhD from the University of Illinois, Urbana, IL. USA.

Carbon Dots Hybrid Nanostructures: Applications in the Electrochemical Sensors and Nano Filter Development.

Thiago C Canevari*,Joao A. Ferreira, Luccas L. Name, Laura C Lieb, Daniel Y Tiba, Mariana M da Silva, Aprys C Oliveira, Ana Assed and Otávio P L de Sousa

LabNaHm: Multifunctional hybrid nanomaterials laboratory. Engineering School, Mackenzie Presbyterian University, 01302-907 São Paulo, SP, Brazil.

Abstract:

This work describes the synthesis, characterization, and application of different carbon dots hybrid nanostructures obtained by chemical interaction between nanomaterials or nanomaterials bonded to another material employed in developing electrochemical (bio)sensors and nano filters. -The hybrid nanostructures have been prepared without external catalysts, where the Cdots have been employed as catalysts and templates. The formation of different carbon dots hybrid nanostructures has been characterized by X-ray diffraction (XRD), Raman and ultraviolet-visible spectroscopy, atomic force microscopy (AFM), high-resolution transmission electron microscopy (HR-TEM), and electrochemical techniques. These carbon dots hybrid nanostructures have been used to modify the surface of glassy carbon and screen-printed electrode. Besides that, it has been used as support in the nano filter constructions onto nylon and PES support. The electrodes have been employed to determine distinct analytes, i.e., dopamine, uric acid, paracetamol, ephynefrine, dihydroxybenzenes, pesticides, disruptor endocrines, NADH, and other substances in real samples. The nano filter has been employed to retain different dyes and endocrine disruptors. Funding by FINEP and MAckpesquisa.

Biography:

Graduated in Chemistry, Bachelor's degree with Technological option from the State University of Londrina, Master's in Inorganic Chemistry, and Doctorate in Materials

Chemistry from the State University of Campinas. He has two postdoctoral internships at the University of São Paulo in nanotechnology. Leader of the research group, consolidated by CNPq, called Multifunctional Hybrid Nanomaterials (NaHM). He works mainly on the following topics: electrocatalysis, (Bio) electrochemical sensors, multifunctional hybrid nanomaterials, filtering nanomembranes, and the sol-gel process. He is currently a professor in the chemistry course and the postgraduate program in Materials and Nanotechnology Engineering at Universidade Presbiteriana Mackenzie.

Nanomechanical Performance of Ultrathin Carbon Nanomembranes for Water Separation

Marinos Dimitropoulos[1], Christos Pavlou[1,2,] Nikolaus Meyerbröker[3], Raphael Dalpke[3,] Albert Schnieders[3], Costas Galiotis[1,2] and Konstantinos Dassios[1*]

[1]Department of Chemical Engineering, University of Patras, Patras, Greece

[2]Institute of Chemical Engineering Sciences, Foundation for Research and Technology Hellas, Patras, Greece

[3]CNM Technologies GmbH, Morgenbreede 1, Bielefeld, Germany

Abstract:

Intended for purifying water, water separation technologies are widely employed in a variety of contemporary househouse and industrial applications. Ultrathin Carbon Nanomembranes (CNMs) offer a highly selective, fast-flow, energy-efficient water separation technology intended for demanding water treatment applications as a technological replacement for biological filtration membranes. The membranes are two-dimensional (2D) materials with sub-nm functional pores and a thickness of roughly 1 nm; they may be generated in large quantities on porous supporting substrates and have customizable properties. The purpose of this work was to investigate and analyze the mechanical characteristics of CNMs and their substrates in order to ensure the structural stability of the membrane during operation. Contrary to macro-materials, it is difficult to measure the mechanical properties of membranes that are only a few nanometers thick. The membranes were supported on atomically flat substrates as well as suspended over patterned substrates and their inherent mechanical properties tested with atomic force microscopy. Quantitative experiments under nanomechanical loading, nanoindentation, and nanofatigue demonstrated the membranes' potential for usage in water separation applications.

Biography:

Konstantinos Dassios is Associate Professor in the Department of Chemical Engineering of the University of Patras, Greece. He holds a Dipl.Eng. in Chemical Engineering from the same department, MSc in Chemical Engineering from Carnegie Mellon University, Pittsburgh, USA and a PhD on the Fracture Mechanics of Ceramic Matrix Composites carried out at the Joint Research Center of the European Commission, The Netherlands. He has more than 20 years of academic and scientific experience on composite materials, nanotechnology and NDE. He has participated in US, European and national research projects and has lead, as Principal Investigator, National and European Commission projects.

Amphiphilic Carbon Dots

Elena V. Ushakova[1]*, Sergei A. Cherevkov[1], Evgeniia A. Stepanidenko[1], Anna A. Vedernikova[1], Mikhail D. Miruschenko[1], Irina A. Arefina[1], Denis V. Danilov[2], Aleksandra V. Koroleva[2], Evgeniy V. Zhizhin[2], and Andrey L. Rogach[3]

[1]ITMO University, Russia

[2]Research Park, Saint Petersburg State University, Russia

[3]Department of Materials Science and Engineering, and Centre for Functional Photonics (CFP), City University of Hong Kong, Hong Kong SAR, China

Abstract:

Carbon dots are emissive nanoparticles promising for a wide range of applications due to the ease of fabrication, low toxicity, and attractive optical properties. We have developed the synthesis method for amphiphilic carbon dots via solvothermal treatment of amines and organic acids as precursors dissolved in acetylacetone. In this case, the solvent not only facilitates the reaction of the precursors as media, but also participates in the formation of carbon dots. These nanoparticles can be efficiently redissolved in a set of polar and nonpolar solvents (with relative polarity from 0.002 to 1) such as tetrachloromethane, chloroform, isopropanol, and water. The energy of optical transitions while changing the solvent is almost the same; moreover, the photoluminescence quantum yield is largest for nonpolar solvents and reaches 36%. The amphiphilicity makes it possible to use these carbon dots for fabrication of photoactive functional films in optoelectronic devices. This work was financially supported by the Russian Science Foundation (RSF22-13-00294).

Biography:

Elena V. Ushakova received her Ph.D. in Optics from ITMO University (St. Petersburg, Russia) in 2013. She is now a leading researcher and head of laboratory "Light-emissive carbon quantum nanostructures" at ITMO University. Her research interests are focused on the optical properties of carbon dots, colloidal semiconductor quantum dots, metal nanoparticles, perovskite nanocrystals, and composite nanostructured materials with optical transitions in the visible and near infrared region.

Enhancing Peroxidase-Like Activity Through Heteroatom-Doped Carbon Materials

Sadaf Saeedi Garakani[1*] and Jiayin Yuan[1]

[1]*Department of Materials and Environmental Chemistry, Stockholm University, Stockholm 10691, Sweden*

Abstract:

Peroxidase enzymes, known for their specificity and reliability, are widely used in various applications, yet face challenges of stability, cost, and scalability. Carbon-based materials offer cost-effective, easily synthesized alternatives due to their tunable properties and chemical stability. However, their intrinsic low catalytic activity limits practical use.

To overcome this limitation, heteroatom doping has been explored to transform carbon materials into artificial enzymes. This study presents hierarchically porous heteroatom co-doped carbon materials synthesized using polymeric ionic liquids (PILs) as precursors. Sacrificial template pore-inducing agents create abundant edge defects, increasing active sites for catalytic activities, including peroxidase-like activity. Co-doped carbon materials outperform single-doped counterparts, with hierarchically porous B/N co-doped nanozymes exhibiting excellent peroxidase-like activity.

Additionally, the study explores ultrafine Fe3C nanoparticles dispersed within heteroatom-doped porous carbon matrices. Fe3C nanoparticles offer excellent peroxidase-like catalytic activity but tend to aggregate. Incorporating them into a heteroatom-doped porous conductive carbon matrix mitigates aggregation, maintaining a high catalytically active surface area. This composite catalyst combines Fe3C's active sites with carbon matrix conductivity and stability, promising exceptional peroxidase-like activity.

In summary, this research showcases the efficacy of heteroatom doping and hierarchically porous structures in enhancing the catalytic performance of carbon materials, opening avenues for diverse applications, including catalysis, sensing, and environmental remediation.

Biography:

Sadaf Saeedi Garakani, originally from Tehran, Iran, is an accomplished researcher with over 7 years of academic and professional experience. She holds a Bachelor's degree in Polymer Engineering and a Master's degree in Chemical Engineering, both earned at the University of Tehran. Throughout her academic journey, Sadaf actively contributed to 9 diverse research projects, showcasing her versatility and commitment. In September 2019, she embarked on a Ph.D. in materials chemistry under the guidance of Prof. Jiayin Yuan at Stockholm University. Her research focuses on porous carbon materials synthesis and characterization.

Magneto-spectroscopy of Excitons in Atomically Thin Semiconductors

Dmitry Smirnov

National High Magnetic Field Laboratory, Tallahassee, FL 32310, USA

Abstract:

Atomically thin semiconducting transition metal dichalcogenides (TMDC), such as MoSe2 and WSe2, are two-dimensional (2D) semiconductors featuring direct bandgap electronic structure and strong Coulomb interactions. As a result, their optical properties are dominated by strongly bound electron-hole states (excitons). The remarkable spin-valley coupling results in specific rules for optical interband transitions in TMDCs, based on various combination of valley and spin indices. Optical spectroscopy studies at high magnetic fields provide unique ways for better understanding of excitonic physics in atomically-thin TMDC based semiconductors. First, I will briefly discuss the electronic properties of TMDC monolayers and show how the energy of neutral valley excitons shifts linearly with the magnetic field through the valley-dependent Zeeman effect. More exotic excitonic complexes, such as neutral and charged bi-excitons, optically inactive "dark" excitons, dark trions and their chiral phonon replicas, were found and studied using high-field magneto-spectroscopy. Finally, I will discuss the most recent studies of TMDC hetero-structures including moire systems.

Biography:

Dmitry Smirnov is a senior research faculty at the National High Magnetic Field Laboratory operated by Florida State University in Tallahassee, FL. His research belongs to a broadly defined field of experimental condensed matter physics with a focus on high-field optical magneto-spectroscopy probes. He received his Ph.D. in Physics & Mathematics in 1996 from Ioffe Institute in St. Petersburg, Russia. Before joining the US National Magnet Lab in 2003, he was a post-doctoral associate and a CNRS research fellow at the French National High Magnetic Field Laboratory in Toulouse, France.

Impact of the Surface Area of Simulated Graphite Surfaces on the Adsorption of Carbon dioxide

Octavio Castano Plaza[1], Quang K Loi[2], Luis F Herrera Diaz[1] , and D.D.Do[3]

[1]Energy and Resources Institute, Charles Darwin University, Darwin, NT 0909, Australia

[2]Centre for Theoretical and Computer Molecular Science, Australian Institute for Bioengineering and Nanotechnology

[3]School of Chemical Engineering, The University of Queensland, St Lucia, QLD, 4072, Australia

Abstract:

As the effect of climate change becomes increasingly apparent, there are considerable interests from the energy industry to develop new processes for the purpose of CO2 separation and sequestration. In that respect, molecular simulation has been a valuable tool for screening or tailoring the design of materials. In the case of graphitized carbon adsorbents, common simulation practice invokes periodic boundary conditions (PBCs) and mirror image (MI) convention to mimic the infinite extent of real surfaces due to the current limit of computer power. However, the use of PBCs and MI failed to describe experimental data at low temperatures because it does not account for the free boundary of the adsorbed phase as evident by the unphysical sub steps in the isotherms. This study investigates the effect of free boundary to the gas-to-solid transition of CO2 adsorption by using a finite 2D-surface to simulate graphitized carbon. The finite surface is shown to outperform the infinite surface and the unphysical substeps are absent, in agreement with experimental measurements at low temperatures. The free boundary allows CO2 molecules to achieve their optimal packing, without the constraints imposed by their neighbours in the mirror images. This research studies the size of the 2D-surface that best simulate the CO2 adsorption with minimum impact in the simulation time. The insights gained from this study improves the understanding of CO2 adsorption for the purpose of separation.

Biography:

Octavio Andres Castano Plaza is a PhD student at Charles Darwin University who is researching the adsorption of gases on carbon materials—his work centres around the structure of adsorbates at low temperatures on graphitic surfaces. Octavio's research is developed with the help of Monte Carlo simulation methods.

Carbon Nanorod Arrays (CNAs) as Promising Electrode Materials: Synthesis and Characterization

Brijmohan Paramanik* and Debajyoti Das

Energy Research Unit, School of Materials Sciences, Indian Association for the Cultivation of Science, Jadavpur, Kolkata – 700 032, India.

Abstract:

The growth of three-dimensional carbon nanostructures without the use of templates remains a formidable challenge. We have ingeniously succeeded in fabricating horizontally aligned carbon nanorod arrays (CNAs) through Microwave Plasma Enhanced Chemical Vapor Deposition (MWPECVD) on glass substrates coated with a cobalt catalyst. In this process, a gas mixture of C_2H_2, H_2, and CO_2 was utilized for CNA development at a relatively low substrate temperature of ~300 °C. Electron microscope analysis provides

evidence of both the independent growth of individual carbon nanorods and the fusion of two or more nanorods. Moreover, it reveals that the inner region of the carbon nanorod is hollow. To optimize the uniform arrangement of crystalline carbon nanorods, we conducted comparative studies on CNA films grown on cobalt-coated substrate pretreated at varying annealing temperatures. We observed a characteristic peak at 1337 cm-1 (C-C stretching vibration) and a G band peak at 1593 cm-1 , along with a 2684 cm-1 peak (2D band), identifying a well-graphitized carbon nanorods feature. Additionally, the presence of characteristic graphite peaks in the (002) plane at around 26° is identified. In optimally fabricated films, we observed a homogeneous microstructure of nanorods, each with an average diameter of approximately 300 ± 10 nm. The C 1s spectra showed a peak at 284 eV, signifying the presence of crystalline sp2 nanorods. These horizontally aligned CNAs hold promise as electrode materials in energy storage applications, especially in batteries and electrochemical capacitors, due to their tuneable size and shape, along with favourable architectural properties.

Biography:

Mr. Brijmohan Paramanik is a fifth year Ph.D. student working under the guidance of Prof. Dr. Debajyoti Das at the Indian Association for the Cultivation of Science, Kolkata, INDIA.

Graphyne-based Membrane as a Promising Candidate for Li-battery Electrodes Protection: Insight from Atomistic Simulations.

Philippe Carbonnière [1*], Nabil Khossossi[2], Mohammed Lemaalem[1]

[1]*Université de Pau et des Pays de l'Adour, E2S UPPA, CNRS, IPREM UMR5254, Institut des Sciences Analytiques et de Physico-chimie pour l'Environnement et les Matériaux, Helioparc, Pau, France*

[2]*Department of Materials Science and Engineering, Delft University of Technology, 2628*

Abstract:

All-solid electrolytes could lead to a technological breakthrough in the performance of all-solidstate batteries when combined with a lithium-metal anode. However, the use of a lithium-metal anode presents several challenges, such as dendrite growth, interface electrochemical stability, formation and propagation of cracks, and delamination of the electrode/electrolyte interfaces [1]. This talk deals with the exploration of the effectiveness of using newly synthesized 2D graphynebased membranes for electrode protection in a solid polymer electrolyte battery through first-principle calculations and classical molecular dynamics simulation [2]. Specifically, we aim to investigate the effectiveness of these membranes in mitigating the aforementioned challenges. A high external electric field was applied to accelerate the ions diffusion process. The adsorption energies, charge transfer, and in-plane/out-plane diffusion of single lithium on graphyne-based surfaces were investigated. Afterward, we calculated and compared the Li+ permeability,

the electrolyte molecules' rejection efficiency, and the intrinsic properties of graphyne-based nanoporous membranes. Our findings show that such a material can permit Li+ intercalation while preventing other electrolyte molecules from reaching the electrodes.

Biography:

[1] Y. Y. Sun et al., A review of interfaces within solid-state electrolytes: fundamentals, issues and advancements, Chemical Engineering Journal (2022) 135179.

[2] M. Lemaalem et al., Graphyne-based membrane as a promising candidate for Li-battery electrodes protection: insight from atomistic simulations, Journal of Power Sources (2023), under review.

Catalytic Conversion of CO_2 selective for C_4 on Ir-Ru/MCM-41 Catalyst

Hajime Kawanami[1*], **Maya Chatterjee**[1]

[1]*National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Japan*

Abstract:

The development of an effective method to produce petroleum-derived compounds using CO2, is emerging as an increasingly important strategy for the synthesis of value-added chemicals because of its abundancy, nontoxicity and nonflammability. With the use of compressed CO2, it is possible to avoid the catalytic deactivation and to prevent the destruction of reactor system, still compressed CO2 (scCO2) is rarely explored as a reactant. To develop a strategy utilizing compressed CO2 as a prospective reactant with laboratory scale verification and validation of predicted performance is important for securing access to CO2 economy. We examined the direct PGME synthesis from CO2 and H2 with high-selectivity using a simple and efficient catalytic strategy comprised of ruthenium (Ru) and iridium (Ir) particles supported on MCM-41 with large surface area to increase the effectiveness of active atoms as catalysts. These catalysts effectively work for hydrogenation followed by C-C coupling of CO2. Our experimental approach was to assess the viability of the single-metal Ru/MCM-41 and Ir/MCM-41 catalysts individually, and we found that both of the catalysts successfully converted scCO2 into methanol, ethanol, 2-propanol, and PGME. The implementation of the individual single-metal Ru/MCM41 and Ir/MCM-41 catalysts resulted in a mixture of compounds rather than a single targeted product; thus, we applied a physical mixture of the Ru/MCM-41 and Ir/MCM-41 (Ru–Ir-PM) as a catalyst for the conversion of scCO2. In the presentation, we will show more detail and discuss about the catalytic performance as well as the plausible reaction mechanisms.

Biography:

Hajime Kawanami is Chief Senior Researcher at National Institute of Advanced Industrial Science and Technology (AIST), and Professor of University of Tsukuba, Collaborative Graduate School Program. He graduated from Tohoku University and received a Ph.D. from Tohoku University in 1997. After then he was Research Associate at Kindai University, and from 2001, he joined AIST. He is studying organic chemistry under high-pressure and supercritical fluid conditions, and one of his present interests is CO2 utilization using high-pressure technology. He recently received The Ichimura Prize in Science against Global Warming for Distinguished Achievement, in 2019.

Carbon-based Materials Obtained from Biomass for Li-ion, Na-ion, and Al-ion Batteries

Nonglak Meethong[1,2*], Nattapong Kamma[1], Komsak Aranmala[1], Yutthanakon Kanaphan[1], Panya Thanwisai1, Pimpa Limthongkul[3], Annop Klamchuen[4], Monrudee Liangruksa[4], and Songyoot Kaewmala[2]

[1]*Department of Physics, Faculty of Science, Khon Kaen University, Khon Kaen 40002, Thailand*

[2]*Institute of Nanomaterials Research and Innovation for Energy (IN-RIE), Khon Kaen University, Khon Kaen, 40002, Thailand*

[3]*National Energy Technology Center, National Science and Technology Development Agency (NSTDA), Khlong Luang, Pathum Thani 12120, Thailand*

[4]*National Nanotechnology Technology Center, National Science and Technology Development Agency (NSTDA), Khlong Luang, Pathum Thani 12120, Thailand*

Abstract:

Carbon-based materials from biomass resources have gathered huge interest for use as electrode materials for alkali-ion batteries due to its high specific capacity, sustainability, wide availability, stable physicochemical, and good electrochemical properties. Developing advanced sustainable electrode materials is becoming increasingly urgent, but also challenging. Electrochemical performance of the planted-derived carbon significantly depends on its microstructure, morphology, and pore size distribution. Understanding the correlation of structural features with electrochemical performance and specific mechanisms of differing ion storage can pave the way to realize large-scale production to meet the requirements for industrialization or commercialization. In this work, various forms of carbon-based materials including activated carbon, laser induced graphene oxide, hard carbon derived from plants for use in Li-ion, Na-ion, and Al-ion batteries will be present.

Biography:

Dr. Nonglak Meethong received her Ph.D. in Materials Science and Engineering from Massachusetts Institute of Technology (MIT) in 2009. Currently, she is a Professor in the Department of Physics, Faculty of Science, Khon Kaen University (KKU), Thailand. Her research focuses on energy storage materials and implementation into commercial Li-ion and Sodium-ion battery products. She has co-authored over 70 scientific articles and holds about 20 International and national patents. She is also the Director of KKU Battery and New Energy Factory (UVOLT), the nation's leading battery R&D facility, product developments, and battery safety and performance testing center. She has served as a member of several national level committees for the Thai government and advisory boards of several leading energy related companies in Thailand.

Integration of Organic Photodetector with Spin-Valve: Development of Novel Spin Controlled Organic Optoelectronic Eco-friendly and Energy Efficient Device

P. Dey[1, 2*] Apurba Pal[1] and S. M. Yusuf [3,4]

[1]Department of Physics, Kazi Nazrul University, Asansol, 713340, W.B., India

[2]Centre for Organic Spintronics and Optoelectronics Devices, Kazi Nazrul University, Asansol, 713340, W.B., India

[3] Solid State Physics Division, Bhabha Atomic Research Centre, Mumbai 400085, India

[4]Homi Bhabha National Institute, Anushaktinagar, Mumbai 400094, India

Abstract:

Carbon-based Opto-Spintronics is a promising field of research that explore the integration of high-speed operation of Optoelectronics and data storage capability of Spintronics in a single device to achieve future demands of Multifunctional, fast and Energy Efficient integrated memory-logic devices. Incorporation of Carbon-based materials addresses the problem of spin relaxation and poor spin injection, and promises Eco-friendly and Energy efficient devices. In recent years, Organic SpinValves derived from Carbon-based materials, combined with the properties of light emission, photovoltaic, electrical memory etc. have gained considerable research interest as spin-based multifunctional devices. Our work in the field of Carbon-based Opto-Spintronics is on the demonstration of coupling between optical response and spin valve property in a coupled organic photodetector and organic spin valve, i.e., in a single Magnetic Organic Photodetector (MOPD) heterostructure device for the first time, at room temperature. According to our experimental evidences, this MOPD shows photocurrent generation with 40% photocurrent to dark current ratio under illumination of 660 nm red laser light. Also, it exhibits negative magnetoresistance as high as -25.85% under dark. Moreover, spin valve effect with peak up to 3% spin valve magnetoresistance is shown. Thus, this device can operate as an individual spin valve, and a photodetector. Importantly, coupling between spin valve and photodetector characteristics is observed in this MOPD device. Such "cross-talk" between optical 2 response and spin valve property in a single Carbon-based device are highly significant for future development of novel optically controlled integrated memory logic devices, such as LiFi and ElectroOptical Hybrid Computing technologies.

Biography:

Dr. PUJA DEY is an Associate Professor in the Department of Physics and Joint-Coordinator of Centre for Organic Spintronics and Optoelectronic Devices at Kazi Nazrul University, Asansol, India. Dr. Dey received Ph D degree in Physics from Indian Institute of Technology Kharagpur, India. She has also received CNRS Post-Doctoral Fellowship from CNRS, Strasbourg, France. She has already published more than 60 research papers and three books. Dr. Dey received two research grants from Department of Science and Technology India and Board of Research in Nuclear Sciences, Department of Atomic Energy, India. Dr. Dey is involved in research activities in Multifunctional Materials and Opto-Spintronics.

A Comprehensive Chemical Kinetics Framework for Carbon Materials and Hydrogen Production from Hydrocarbons Pyrolysis

Matteo Pelucchi[*1]

Department of Chemistry, Materials and Chemical Engineering, Politecnico di Milano, Italy

Abstract:

Hydrogen (H2) is highlighted as a key energy vector in the context of sustainable development and circular economy. The CO2 emissions that accompany the most widely used process for its production today (steam methane reforming, SMR) highlights the need for efficient CO2 capture technologies that are presently struggling for large scale implementation. Pyrolysis of fossil or biogenic hydrocarbons (e.g. methane, biomethane, natural gas) is one of the most promising solutions in a short- to mid-term perspective. Indeed, thanks to the concomitant carbon fixation in value-added carbon materials (VACs), the produced “turquoise” H2 can be sold at a price comparable to that from SMR.

The key points to scale-up pyrolysis processes to produce H2 and VACs are to accelerate deposition efficiency, minimize the formation of amorphous carbon (i.e., particulate matter) and improve the quality of carbon material by-products. Therefore, it is of primary importance to control both homogeneous reactions in the gas phase, including particulate matter formation, and heterogeneous reactions occurring at the gas-solid interface. Detailed and semi-detailed chemistry models coupled with computational fluid dynamics models support the design of innovative reactor technologies by providing tools for process conditions optimization.

This work showcases recent research efforts in the development of a comprehensive chemical kinetic framework capable to contextually describe amorphous carbon formation in the gas phase (i.e. particulate matter), structured pyrocarbon production in CVD/CVI processes, carbon nanotubes synthesis in floating catalyst CVD reactors and turquoise hydrogen production.

Biography:

Matteo Pelucchi is currently a Tenure Track Assistant Professor of Chemical Engineering at Politecnico di Milano. He received from the same institution a Master of Science in Chemical Engineering in 2013, and a PhD in Industrial Chemistry and Chemical Engineering in 2017. Within others, his research interests cover the development of chemical kinetic models for the pyrolysis of different feedstock (e.g. natural gas, biomass and plastic wastes) and the development of theoretical protocols (e.g. ab initio, DFT, molecular dynamics) for the estimation of thermochemical kinetic model parameters for homogeneous gas-phase and heterogeneous gas/solid systems.

Solid Oxide Fuel Cell: Effect of Dimensionality, Interface and Strain

Chandrani Nath[1*,] Avinash Patel[1], Roshan Patel[2], A.K. Pramanik[2] and Satyendra Singh[1]

[1]*Special Centre for Nanoscience, Jawaharlal Nehru University, New Delhi, India*

[2]*School of Physical Sciences, Jawaharlal Nehru University, New Delhi, India*

Abstract:

The combined effect of increasing population, expanding economy and excessive emission of greenhouse gasses has necessitated to explore carbon neutral alternate source of energy. Solid oxide fuel cell (SOFC) which converts chemical energy of fuel into electrical energy, offers promising solution to address these issues as this process is quite efficient and involves no combustion of hydrocarbon. Compared to other types, SOFC has advantage of oxidizing any types of fuel, from hydrogen to diverse hydrocarbons, because the electrolyte here transports an oxygen ion. However, the key drawback which has limited the development and deployment of this transformative technology is its high operating temperature (800 - 1000 oC), resulting in higher systems costs and performance degradation rates. The intermediate operating temperature (350 - 600 oC) has potential to reduce the system cost significantly by allowing the use of less expensive components However, lowering the operating temperature has adverse effect on electrolyte conductance which will eventually lower the efficiency of the fuel cell. This suggests for development of electrolytes with enhanced ionic conductivity. Thin films and heterostructures have shown promising oxygen-ionic conductivity due to short ion-path and interface effect. In my talk, I will discuss the ionic conductivity of thin films and heterostructures of CeO2 and La2Mo2O9 electrolytes deposited on different substrates by pulsed layer deposition. Our results show promising enhancement in ionic conductivity which is believed to be due to the combined effect of nanostructuring and interfacial strain.

Biography:

Dr. Chandrani Nath has obtained Ph.D. degree in Physics in 2014 from Tezpur University, Assam, India. During her Ph.D. she worked in investigating the electrical, thermal and magnetic properties of polyaniline nanostructures. In 2016, she was awarded the National Post-Doctoral Fellowship by Science and Engineering Research Board, Department of Science and Technology, India. She executed her project on Oxide based nanostructured thermoelectrics at the Department of Physics, Indian Institute of Technology, Delhi. Later in 2018, she was awarded the prestigious DST INSPIRE Faculty Award, a tenure based faculty cum research grant award. She is currently a DST INSPIRE Faculty at the Special Centre for Nanoscience, Jawaharlal Nehru University, New Delhi, India, currently working on developing materials for solid oxide fuel cells that could operate at intermediate temperatures.

Recent Progress in Computational Studies of True Amorphous Carbon

Oleksiy Khavryuchenko[1,2*] and Gilles Peslherbe[3]

[1]*Shupyk National Healthcare University of Ukraine*

[2]*NVision Imaging Technologies GmbH, Germany*

[3]*Concordia University, Montréal, QC, Canada*

Abstract:

Absolute majority of carbon materials have undefined local structure, varying from highly-defective micro-crystalline to completely amorphous. True amorphous ones, i.e. having no translational symmetry even on sub-nanoscale level, are the most enigmatic of them. In order to explain their physical (optical, mechanical and magnetic) and chemical properties we have elaborated a 'two-domain' model, comprising 1) curved graphene sheets and 2) short chains of carbene atoms, connecting them. Model carbon nanoparticles representative of the graphene-like and amorphous domains of active carbon are investigated with density-functional theory (DFT), time-dependent DFT (TDDFT), and complete active space self-consistent field (CASSCF) with n-electron valence state perturbation theory (NEVPT2) methods, exhibiting a variety of local structures with different chemical, optical and magnetic properties. Interplay between singlet and triplet states in large models and its effect on chemistry of true amorphous carbon is discussed, along with limitations and perspectives of computational approaches in carbon chemistry.

Biography:

Graduated from Chemistry Department of Kyiv Taras Shevchenko National University in 2002. PhD in inorganic chemistry (2006). Working in computational chemistry of amorphous materials (silica, carbon, etc) and spin chemistry of carbon

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Self-Diagnostic Vitrimers

Roberta Pinalli[1*,] Alessandro Torri[1], Alessandro Pedrini[1], Enrico Dalcanale[1], Valentina Antonia Dini[2], Damiano Genovese[2]

[1]*University of Parma, Italy*

[2]*University of Bologna, Italy*

Abstract:

A powerful new strategy to produce reprocessable cross-linked polymers is the functionalization of the polymer matrix with cross-links able to reverse or exchange at elevated temperatures. These covalent adaptable networks (CANs) are able to shuffle chemical bonds through exchange reactions at high temperature, allowing for material

reprocessing. Vitrimers are a type of CANs that make use of associative bond exchanges between polymer chains, in which the original cross-link is only broken when a new covalent bond to another position has been formed. Vitrimers possess both the properties of thermosets and the reprocessability of thermoplastics. Self-diagnostic materials are polymers functionalized with mechanochromic dye able to change color upon mechanical solicitations. These probes enable the early detection of crack formation inside a polymer matrix. So far, most of the activity has been concentrated on mechanochromic thermoplastics realized by directly linking dyes into the polymer chains of elastomeric or on glassy cross-linked polymers. More recently a different damage-reporting strategy has been introduced, using aggregation-induced emission of fluorophores confined in core-shell microcapsules. Here, we present the preparation of self-diagnostic vitrimers designed with the aim to detect in a nondestructive way early-stage damage introducing a suitable probe inside the polymer matrix. The probe has been used as cross-linker or encapsulated inside microcapsules. The activation of the mechanophore off/on process allows for the identification of the microfracture, while dynamic nature of the vitrimers allows for the repairing of the damage by local heating.

Biography:

Roberta Pinalli received her scientific training at the University of Parma, graduating in Industrial Chemistry in 1998. After a two year stint in Antibioticos SpA as process chemist, in 2002 she obtained her PhD in Chemistry from the same University working on nanosize coordination cages. During her PhD tenure she spent a semester at the University of Twente, in the group of Prof. D.N. Reinhoudt. After a three year experience as senior researcher in Bracco Imaging SpA, she rejoined the Parma University where she is Associate Professor. Her research interests focus on supramolecular chemistry, sensors, polymers and advanced materials.

Observation of Franz-Keldysh modulation in a $CH_3NH_3PbBr_3$ Crystal as Revealed by Femtosecond Transient Absorption Microscopy

Tetsuro Katayama

[1]*Institute of post-LED photonics, Tokushima University, Japan*

Abstract:

Organic-inorganic lead halide perovskite materials have attractive properties for solar cells and LED because of their high performance and wavelength tunability. Such an efficient light-emitting and lasing nature are indispensable for their applications, and the essential needs are miniaturization and low lasing threshold. One material that satisfies these requirements is lead halide perovskite. To understand the time evolution of the interaction between light and matter in a perovskite crystal system, it is necessary to reveal the carrier dynamics in each crystal. In this study, the transient absorption spectra of $CH_3NH_3PbBr_3$ crystals were measured using a femtosecond transient absorption microscopy. Surprisingly, strong spectra modulation has been observed and these results indicate the charge separation on the surface of the crystal. Amplified spontaneous emission dynamics was also observed in the transient absorption spectra. We will also discuss lasing mechanism on the conference site.

Biography:

EDUCATION

4/2001～3/2005 Department of Chemistry, School of Engineering Science, Osaka University

4/2005～3/2007 Master course, Division of Frontier Materials Science, Graduate school of Engineering Science, Osaka University

4/2007～3/2010 Doctoral course, Division of Frontier Materials Science,Graduate school of Engineering Science, Osaka University

RESEARCH EXPERIENCE

4/2010～3/2013 Posdoc Fellow, Engineering science, Osaka University

4/2013～4/2014 JST PRESTO Researcher

5/2014～3/2015 Nano science design educational center, specially appointed assistant professor, Osaka University

4/2015～3/2019 Assistant professor, Department of chemistry, engineering science, Kwansei Gakuin University

7/2019～ Assistant professor, Institute of pLED photonics, Tokushima University

Selective Methane Oxidation to Acetic Acid using Molecular Oxygen over a Metal-Organic Framework Supported Mono-Copper Hydroxyl Catalyst

Kuntal Manna[1*], Manav Chauhan[1], Neha Antil[1]

[1]*Indian Institute of Technology Delhi, Department of Chemistry, Hauz Khas, New Delhi, India*

Abstract:

Acetic acid is an industrially important chemical, produced mainly via carbonylation of methanol using precious metal-based homogeneous catalysts. As a low-cost feedstock,

methane is commercially transformed to acetic acid via a multi-step process involving energy-intensive methane steam reforming, methanol synthesis, and subsequently, methanol carbonylation. We have developed a direct single-step conversion of methane to acetic acid using molecular oxygen (O2) as the oxidant under mild conditions over a mono-copper hydroxyl site confined in a porous metal-organic framework (MOF). The heterogeneous MOF-supported single-site copper hydroxyl catalyst gave exceptionally high acetic acid productivity of 335 mmolgcat-1 in 100% selectivity at 115 ℃ in water. The oxidation state and coordination environment of the copper ion within the MOF-catalyst and the catalyst's resting state were determined by X-ray absorption spectroscopy. Our spectroscopic and theoretical studies and controlled experiments reveal that the conversion of methane to acetic acid occurs via oxidative carbonylation, where methane is first activated at the copper-hydroxyl site via σ-bond metathesis to give Cu-methyl species followed by carbonylation with in-situ generated carbon monoxide and subsequent hydrolysis by water. We demonstrate that the confinement of an active mono-copper hydroxyl site within a porous MOF represents an efficient strategy to develop novel earth-abundant metal catalysts for the selective functionalization of methane and other light hydrocarbons. This work may guide the rational design of heterogeneous abundant-metal catalysts to activate and convert methane to acetic acid and other valuable chemicals under mild and environment-friendly reaction conditions.

Biography:

Kuntal Manna is an Associate Professor in the Department of Chemistry of Indian Institute of Technology Delhi (IIT Delhi), India. He completed his master's in Chemistry from IIT Kanpur in 2006. After receiving his PhD in Inorganic Chemistry from Iowa State University in 2012 under the guidance of Prof. Aaron D Sadow, Dr. Manna was a postdoctoral researcher at the University of Chicago (2013-2016). He joined the Department of Chemistry of IIT Delhi as an Assistant Professor in 2017. His research focuses on developing single-site heterogeneous catalysts for sustainable organic transformations, functionalization and upgradation of light hydrocarbons, and energy-related transformations.

Smart pH-responsive Nanocontainers Dual loaded with Oxaliplatin and Ylang Ylang Oil showed Boosted Cytotoxic and Apoptotic effects against Triple-Negative Breast Cancer

Sherif Ashraf Fahmy[*1], Nada K. Sedky[1], Nour M. Abdel-Kader [1,2#,] Marwa Y. Issa[3], Manal M. M. Abdelhady[4], Samir N. Shamma[5], Udo Bakowsky[6]

[1]*School of Life and Medical Sciences, University of Hertfordshire Hosted by Global Academic Foundation, Cairo, Egypt*

[2]*Department of Biochemistry, Faculty of Science, Ain Shams University, Cairo Egypt.*

[3]*Department of Pharmacognosy, Faculty of Pharmacy, Cairo University, Egypt*

[4]Clinical Pharmacy Department, Faculty of Pharmacy, Badr University, Cairo, Egypt

[5]Institute of Global Health and Human Ecology, School of Sciences & Engineering, The American University in Cairo, New Cairo, Egypt.

[6]Department of Pharmaceutics and Biopharmaceutics, University of Marburg, Marburg, Germany

Abstract:

Smart pH-sensitive niosomes loaded with either Oxaliplatin (Ox), Ylang ylang essential oil (Y-oil), or co-loaded with both compounds (Ox-Y) (Ox@NSs, Y@NSs, and Ox-Y@ NSs, respectively) were formulated utilizing the thin film method [1]. The developed nanocontainers had a spherical morphology with mean particle sizes lower than 170 nm and showed negative surface charges, high entrapment efficiencies, and a pH-dependent release over 24 h. The prepared pH-responsive niosomes' cytotoxicity was tested against the invasive triple-negative breast cancer (MDA-MB-231) cells, compared to free OX and Y-oil. All niosomal formulations loaded with Ox and/or Y-oil significantly improved cytotoxic activity relative to their free counterparts. The Ox-Y@NSs demonstrated the lowest IC50 (0.0002 µg/mL) when compared to Ox@NSs (0.006 µg/mL) and Y@NSs (18.39 µg/mL) or unloaded Ox (0.05 µg/mL) and Y-oil (29.01 µg/mL). In addition, the percentages of the MDA-MB-231 cell population in the late apoptotic and necrotic quartiles were profoundly higher in cells treated with the smart Ox-Y@NSs (8.38% and 5.06%) than those exposed to free Ox (7.33% and 1.93%) or Y-oil (2.3% and 2.13%) treatments. Gene expression analysis and protein assays were performed to elucidate the molecular mechanism by which the prepared pH-sensitive niosomes induce apoptosis. Ox-Y@NSs significantly induced the apoptotic markers Tp53, Bax, and Caspase-7 gene expression while downregulating the antiapoptotic Bcl2. As such, Ox-Y@NSs are shown to activate the intrinsic pathway of apoptosis. Our findings suggest that combining natural essential oil with synthetic platinum-based drugs in pH-responsive nanovesicles is a promising approach to breast cancer therapy.

References:

[1] Sedky, N.K.; et al. Int. J. Mol. Sci 24 8392. (2023)

Biography:

Dr. Sherif Ashraf Fahmy obtained his B. Pharm with honors from the Faculty of Pharmacy, Cairo University, Ph. D. (2020) in Chemistry from The American University in Cairo. His Ph. D. was conducted in collaboration with the Department of Pharmaceutics & Biopharmaceutics, Faculty of Pharmacy, Philipps-Universität Marburg, Germany. Dr. Fahmy was selected as one of the first recipients of the prestigious and very competitive fellowship offered by the Alfi Foundation for Ph.D. students. He has received several other awards and recognitions, most notably, the Royal Society of Chemistry (RSC, UK) Travel Grant for Ph.D. students & Early Career Scientists in 2019, the Fulbright Scholarship at

Ohio University in 2019, USA, and others. Dr. Fahmy is a full-time Assistant Professor of Chemistry, and Head of the Herbal Medicine & Nanotherapeutics research group at the University of Hertfordshire, Egypt Campus.

Plasma Modification of GO nanosheets for Hole Transport Layer-based Perovskite Solar Cells

M. Abdelhamid Shahat*

PV Unit, Solar and Space Research Department, National Research Institute of Astronomy and Geophysics (NRIAG), 11421 Helwan, Egypt.

Abstract:

The basic concept for the future development of human society has become to reduce emissions of greenhouse gases such as carbon dioxide that cause climate change. As a result, one of the best sustainable and environmentally acceptable solutions to this challenge is to use perovskite solar cells (PSCs), which may be used as an efficient alternative for fossil fuels.

The main objective of this work is to design and improve the performance of carbon quantum dot-based PSCs. We presented a simple method for modifying the physicochemical properties of hole transport layer (HTL) and electron transport layer (ETL) as the most efficient components in solar cells, using in-situ plasma surface treatment. Following that, the effects of the treatment on the microstructure, active sites, surface area, optical, and electrical characteristics of these nanolayers were examined. Whereas, these treatments resulted in a considerable improvement in the chemical functionalization of the nanolayers, as well as a rapid increase in surface roughness, which reduced photons reflection and therefore increased the generation of charge carriers.

Biography:

Dr. Mohamed Abdelhamid Mohamed Shahat is a Researcher at NRIAG, Egypt. He was born in April 1990. He holds a PhD in Physics of Material Science and Solar Energy, Feb. 2021. His expertise includes plasma applications in water treatment as well as photovoltaics (Perovskite, Dye-sensitized, and Organic cells).

Recently, Efficient CO2 capture and storage utilizing plasma modification of Carbon-based nanocomposite materials.

- Improved Thermophysical Properties of Nanocarbon-based Composite Clay Bricks for Sustainable Building and Construction Applications via Plasma Modification.

- A novel design for Energy, Hydrogen, and Water production utilizing Solar Energy for climate change mitigation.

Z-Scheme Heterojunction of Chemically Integrated COF-366-Co/UiO-66-NH2 MOFs Nanocomposites for Selective Production of CO *via* CO_2 Solar-Drive Photoreduction

Toan-Anh Quach*, Trong-On Do*

**Department of Chemical Engineering, Laval University, 1065 Avenue de la Médecine, Quebec, QC G1V0A6, Canada*

Abstract:

The increasing demand for energy in modern society has put various challenges to the environment and the ecosystem. Throughout the years, carbon dioxide, along with different greenhouse gases are recognized as the main reason for global warming and thus, many attempts have been made to reduce the emission of these greenhouse gases. Inspired by natural photosynthesis, the use of photocatalysts for various chemical reactions to produce the renewable energy from sunlight has become highly intriguing. The photocatalytic conversion of CO2 to renewable fuels using solar energy has recently become an interesting topic, owing to its potential to solve the riddle of reducing fossil fuels dependence and CO2 emission. However, the low efficiency and selectivity of photocatalysis prevent the development of this method from practical applications. The emergence of COF-based material is expected to maximize solar light absorption on the development of nanomaterials with high efficiency for photocatalytic CO2 reduction. Herein, a nanocomposite photocatalyst composed of UiO-66-NH2 and porphyrin-based COF-366-Co materials is developed using a facile synthetic route with different concentrations of UiO-66-NH2. Subsequently, the composites were investigated under various conditions, with the optimized result exhibiting a remarkable CO production rate, ~ 4092.16 µmol. g-1.h-1 at the end of 4 h, which is ~2.37 times higher than the bare COF, while maintaining a significant CO selectivity at 73.28%. Furthermore, different characterization techniques were conducted, confirming the performance of this type of material. This research could promote the development of porphyrin-based COF/MOF-based nanocomposites for selective CO2 photoconversion into valuable chemicals and fuels.

Biography:

My name is Toan-Anh Quach, I am a PhD student, working in the Chemical Engineering department at the Université Laval, Québec, Canada. As a research student, I work under the supervision of Professor Trong-On Do, in the field of nanomaterials and their application for green energy and environmental remediation, such as CO2 emission and water pollution. Our work focuses on the use of nanomaterials as photocatalysts for photo-chemical reactions like CO2 reduction and antibiotic treatment. For 4 years at Université Laval, I have published 7 papers as the first author and coauthor in various journals, targeting the use of composite nanomaterials for photocatalytic reactions.

From Graphene Oxide Liquid Crystal to Artificial Muscle

Sang Ouk Kim

National Creative Research Initiative Center for Multi-Dimensional Directed Nanoscale Assembly, Department of Materials Science & Engineering, KAIST Institute for NanCentury, KAIST, Daejon 34141, Republic of Korea

Abstract:

Graphene Oxide Liquid Crystal (GOLC) is an intriguing 2D carbon based soft material, which exhibits nematic type colloidal discotic liquid crystallinity with the orientational ordering of graphene oxide flakes in good solvents, including water. Since our first discovery of GOLC in aqueous dispersion at 2009, this interesting mesophase has been utilized over world-wide for many different application fields, such as liquid crystalline graphene fiber spinning, highly ordered graphene membrane/film production for water treatment, nanoporous graphene assembly for energy/environmental applications and so on. Interestingly, GOLC also allow us a valuable opportunity for the highly ordered molecular scale assembly of functional nanoscale structures. This presentation will introduce our current status of GOLC and other 2D material research particularly focusing on the nanoscale assembly of functional nanostructures, including highly oriented 1D fibers, 2D films and 3D nanoporous structures. In particular, human muscle inspired graphene based nanocomposite fiber actuators will be highlighted along with its interesting demonstration for biomimetic behaviors. Besides, relevant research works associated to the nanoscale assembly and chemical modification of various low dimensional materials, including 2D TMDs and MXene, will be presented particularly aiming at energy and environmental applications. In the last part of presentation, our first discovery of single atom catalyst will be introduced, including other relevant research efforts exploiting the customized heteroelement doping of graphene based structures.

Biography:

Prof. Sang Ouk Kim is the director of the National Creative Research Initiative Center for Multi-Dimensional Directed Nanoscale Assembly, and the director for the KAIST Institute for Nanocentury in KAIST. His main research interest is the directed self-assembly of soft materials, including block copolymers and low-dimensional materials such as graphene oxide aiming at electronics, energy, environmental and biomedical applications. His contribution in the materials research area has been widely recognized by prestigious honours, including the Highly Cited Researcher from Clarivate Analytics (2018), the KAIST Grand Prize for Academic Excellence (2015) and Presidential Young Scientist Award (2013). To date, He has published more than 277 SCI Journal papers and 105 patents relevant to the nanomaterial's science. Prof. Kim's H-index is 88 and the total citation number is more than 27000 (Google Scholar).

Novel 2D Nanomaterials for Energy Harvesting and Storage

Weiwei Lei*

Institute for Frontier Materials, Deakin University, Waurn Ponds Campus, Locked Bag 20000, Victoria 3220, Australia.

Abstract:

Advances in the design and fabrication of 2D nanomaterials and their membranes with improved flux, stability, scalable, and cost-effectiveness will have tremendous impact in several fields such as gas separation, organic solvent nanofiltration, water treatment and chemical sensors.1 Laminar membranes prepared by two dimensional (2D) based nanomaterials, including the graphene-family, BN, exfoliated dichalcogenides, layered metal oxides, zeolites, and metal–organic framework (MOF) nanosheets, MXene, offer an exciting opportunity for developing a new family of advanced nanomaterials and membranes featuring unique properties including super thermal stabilities, high resistance to oxidation, excellent chemical inertness, and electrical insulation.2-7 Such distinctive intrinsic characteristics endow these 2D nanomaterials and their membrane as promising multipurpose applications in water purification and energy generation and stoerage.

Here, we have reported a series of functionalized 2D nanomaterial membranes such as graphene, BN, MoS2, MXene, metal nitrides with unprecedented multipurpose molecular and ion sieving in water and in organic solutions with high permeation and selectivity, high rate of ionic transport for energy generation and storage, and broadband (UV-visible-Infrared) light absorption and excellent photothermal conversion efficiency for freshwater generation. Such multipurpose and super stable molecular-sieving membrane with high throughput manufacturing route facilitates the innovative application of 2D nanomaterial membrane to meet the rapid industrial development multi-demands.

Biography:

Weiwei Lei is an Associate Professor and ARC Future Fellow at the Institute for Frontier Materials, Deakin University. He received his PhD degree in Condensed Matter and Physics from the Jilin University in 2010. He then joined Max-Planck-Institute of Colloids and Interfaces, Germany, as Research Fellow. He was awarded an Alfred Deakin Postdoctoral Research Fellowship, Deakin University in mid of 2011. He was then granted a prestigious Australian Research Council Discovery Early Career Researcher Award (DECRA) in 2014. His research focuses on the development of new nanomaterials and nanotechnologies for sustainable water and renewable energy generation and storage including water cleaning, solar steam generation, photocatalysts for hydrogen generation, osmotic energy generation, and rechargeable batteries and supercapacitors. He has contributed 2 book chapters, 9 patents, >180 journal publications including Nature Communications, Joule, Advanced Materials, ACS Nano, Advanced Energy Materials, Journal of the American Chemical Society, etc, and over 20 keynote/invited presentations, which received >10,800 citations with an H-index of 55 (Google Scholar). As a Chief Investigator, Weiwei has attracted numerous competitive external grants over $20M, i.e., ARC DECRA 2014-2017, Discovery Project 2019-2022, ARC Future Fellowship 2022-2025, and Discovery Project 2022-2025, ARC industry Hub, Innovative Manufacturing Cooperative Research Centre (IMCRC) project, etc. He has won some prestigious awards including the 2014 Finalist of the Australian Innovation Challenge, 2015 TechConnect Innovation Award from the TechConnect Corporate & Investment Partner Committee, Washington DC, USA, 2016 Selected Global Young Scientists Summit, Awardee, Singapore., 2013 and 2019 Deakin's Vice-Chancellor's Early- and Mid-Career Researcher Awards for Research Excellence.

Quantum Nature and Confinement Control of Endohedral Lithium in [Li+@C60]PF6-

Hideo Ando[1]* and Yoshihide Nakao[2]

[1]Yamagata University, Japan; [2]Kyushu Sangyo University, Japan

Abstract:

A crystalline salt of lithium endohedral fullerene, Li+@C60, is an ideal system for studying the quantized translational motion of the Li+ nucleus under sub nanoscale confinement. The adsorbent potential within every C60 cage governs the quantized nuclear motion of Li+, which underlies terahertz (THz) spectra at low temperatures. To date, however, little is known about the microscopic factors determining the adsorbent potential and, thus, the Li+ motion. In [Li+@C60]PF6–, an archetypal Li+@C60 salt, the Li+ ion in each C60 cage is simultaneously localized at two disordered sites in $24\ K < T << 100\ K$, whereas it becomes mostly localized at one of the two sites below 24 K (i.e., two-site disorder–order transition). We theoretically study the origin of this temperature-dependent Li+ behavior (PCCP, 2021, 23, 9785; PCCP, 2023, accepted). We developed a model adsorbent potential that fits highly-accurate post-Hartree–Fock energies and obtained hundreds of nuclear wave functions of Li+ using the Fourier grid Hamiltonian method. Our results indicate that weak distortion of C60 above 24 K (ca. 10–2 Å) sterically and electrostatically deepens the potential wells at the two disordered sites, at which low-energy nuclear wave functions are localized. Upon cooling below 24 K, inversion-symmetry-breaking distortion of the C60 cage and the PF6– coordination sphere correlates closely with the two-site disorder–order transition. Its spectral fingerprints evidently appear in the THz frequency range, namely blueshifts of two absorption peaks. Our approach will help deepen the fundamental understanding of nanoporous host–guest science, particularly at low temperatures.

Biography:

Hideo Ando received his Ph.D. from Kyoto University in 2013 under the supervision of professor Hirofumi Sato and emeritus professor Shigeyoshi Sakaki. In 2013, he joined the group of distinguished professor Shaul Mukamel as a postdoctoral scholar at Department of Chemistry, University of California, Irvine. He started to work as an assistant professor at Department of Physics, Faculty of Science, Yamagata University in 2015 and was promoted to a lecturer in 2019. His interest is theoretical quantum molecular science, in particular, concerning coupled behavior of electronic and nuclear quantum states.

Synthesis of Novel Carbon Materials from Designed Organic Precursors using High Temperature High Pressure Processing

Toshihiro Shimada, Seiya Yokokura, Ichiro Yamane, Taijiro Tadokoro, Minako Aikawa, Teruki Ando

Division of Applied Chemistry, Faculty of Engineering, Hokkaido University, Japan

Abstract:

High pressure synthesis is a versatile tool for creating new materials. Under high pressure, interatomic distances are reduced and electronic structure is modified. Designing molecules and finding proper conditions for polymerization and hydrogen elimination will be an effective route towards the synthesis of novel carbon materials with designed nanostructures. There are some reports on the high-pressure processing of molecules to make carbon solids. Three-dimensional topotactic polymerization of C60 fullerene is an example. Very hard materials are obtained by polymerization of co-crystal between fullerene and other molecules. Photocatalytic graphitic-carbon nitride changed bandgap by compression due to the holes vanishing in the carbon-nitrogen networks. When aromatic molecular solids are placed under high pressure, it is expected that a Diels–Alder-like reaction occurs and the molecules polymerize or oligomerize. In this presentation, we report the polymerization of nitrogen-containing large aromatic molecules quinoxalino[2′,3′:9,10] phenanthro[4,5-abc] phenazine (TQPP) and dibenzo[a,c] dibenzo[5,6:7,8]quinoxalino[2,3-i] phenazine (DDQP)[1]. The products were examined using various spectroscopic methods, x-ray diffraction and MALDI-TOF-MS. Under 5 GPa compression at room temperature, DDQP showed origomerization (trimer formation) even after quenching to ambient pressure. TQPP showed dimerization. Examination of the effect of heat treatment under higher pressure using diamond anvil cell is underway.

Biography:

Toshihiro Shimada is professor of Applied Chemistry at Faculty of Engineering, Hokkaido University, Japan. He graduated from The University of Tokyo and obtained Dr. Sc. Degree from the research on the interfaces formed by van der Waals epitaxy. He studies crystal and thin film growth of various materials, physical properties of layered materials including some topological materials, surface spectroscopy, organic semiconductors as well as the present topic of novel carbon materials.

Na-catalyzed Rapid Synthesis of Graphite Intercalation Compounds

Akira Iyo*, Hiraku Ogino, Shigeyuki Ishida, Hiroshi Eisaki

National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Ibaraki, Japan

Abstract:

Graphite intercalation compounds (GICs) exhibit a wide range of functions due to their diverse material variations. As research on the applications of GICs progresses, it is crucial to develop efficient synthetic methods for GICs. For GICs intercalated with donor-type atoms, such as alkali metals (AM) and alkaline earth metals (AE), effective synthetic techniques, including vapor phase and molten salts methods, have been proposed. While these methods are capable of synthesizing high-quality GICs, they might not be well-suited for the rapid mass synthesis necessary for practical applications. We have made a significant discovery indicating that Na possesses a catalytic property, which greatly accelerates the formation of GICs [A. Iyo et al., Advanced Materials 35, 2023, 2209964]. In our study, we successfully synthesized LiC6n (n = 1, 2), KC8, KC12n (n = 2, 3, 4), and NaCx by simply mixing AM and graphite powder with Na at room temperature (~25 °C), and AEC6 (AE = Ca, Sr, Ba) are synthesized by heating Na-added reagents at 250 °C only for a few hours. The formation of NaCx, resulting from the mixing of C and Na, plays a crucial role as a reaction intermediate and acts as a catalyst, thereby significantly lowering the activation energy required for intercalation. This Na-catalyzed method allows for the rapid and mass synthesis of homogeneous GIC samples, surpassing conventional techniques in terms of simplicity and efficiency. We anticipate that this breakthrough will drive further research and development for GIC applications.

Biography:

Akira Iyo is a chief senior researcher at the National Institute of Advanced Industrial Science andTechnology (AIST) in Japan. Iyo is a materials scientist working on the development of novel superconductors (SCs), including copper oxides and iron-pnictides. Recently, Iyo has been utilizing a combinatorial chemistry method to efficiently search for novel SCs with the potential for room-temperature superconductivity. Serendipitously, during this search, the synthesis of Graphite Intercalation Compounds (GICs) using the Na-catalyzed method was discovered. Iyo is currently exploring the potential applications of Na-catalyzed GIC synthesis.

The Pressure and Time Effect in Hydrothermal Carbonization for Activated Carbon Production

Ratna Frida Susanti[1*], Leonardus Kenny[1], Kevin Cleary Wanta[1], Hans Kristianto[1] and Agung Nugroho[2]

[1] *Chemical Engineering Department, Industrial Technology Faculty, Parahyangan Catholic University, Ciumbuleuit 94, Bandung, West Java, Indonesia*

[2] *Chemical Engineering Department, Industrial Technology Faculty, Universitas Pertamina, Teuku Nyak Arief, Simprug, Jakarta*

Abstract:

Activated carbon is a material that is popular in many applications, including energy storage devices. Activated carbon is synthesized by carbonization and activation. In hydrothermal carbonization, variables such as temperature and time were often investigated; however, the pressure was different. The pressure effect was rarely to be investigated. In the batch reactor, if pressure is not maintained, the state of the liquid can go to vapor-liquid equilibrium, where the mixture of vapor and liquid occurs. On the other hand, pressure can be adjusted to maintain the water phase at its liquid state, called subcritical water. In this research, the effect of pressure was investigated on the properties of activated carbon produced.

The pressure of carbonization was varied at 100 bar and 250 bar while the time was varied at 1 hr and 5 hr. The temperature was kept constant at 200 °C. The activated carbon produced characterized the surface area, morphology, functional group, and crystallinity. The results show that, in terms of surface area, the pressure had a negligible effect on the activated carbon produced, except for the shortest time (1 hr). The sample processed at low pressure (100 bar) and short time (1hr) gave a different isotherm curve. The surface area grew with time. The O-H stretch was more pronounced at 250 bars. In addition, the XRD shows the different crystallinity between 100 bar and 250 bar samples.

Biography:

Ratna Frida Susanti is an associate professor in the chemical engineering department of Parahyangan Catholic University Indonesia. She currently serves as a vice dean for academic affairs in the Industrial Technology Faculty. Her research focuses on biomass carbonization, energy storage devices, supercritical fluid gasification, and supercritical fluid extraction. She has published her articles in the Journal of Industrial and Engineering Chemistry, International Journal of Hydrogen Energy, Material Letter, Energy, Journal of Membrane Science, Chemical Engineering Research and Design, Ionics, Journal of Applied Electrochemistry, etc.

Immobilization of Laccase on Magnetized Multiwall Carbon Nanotubes

Balakrishnan Kunasundari[1*], Hasnol Azahari Natasha Yasmin[1], Siew Hoong Shuit[2], Mohamad Fahrurrazi Tompang[1]

[1]Faculty of Chemical Engineering & Technology, Universiti Malaysia Perlis, 02600 Arau, Perlis, Malaysia

Abstract:

The interest in using magnetic nanoparticle (MNPs) as a carrier for immobilization is overwhelming due to high surface area and lightweight properties. However, the conventional synthesis of MNPs required use of high amount of chemicals and is a time consuming process. Thus, in the present research, magnetized multiwall carbon nanotubes (m-MWCNTs) was successfully synthesized via water-based system using simple steps. Laccases were immobilized on m-MWCNTs. The optimum laccase concentration required for immobilization was 7 mg/mL. Both free and immobilized laccases showed optimum activity at pH 5 whereas the optimum temperature was shifted from 40 °C to 50 °C in the latter. The immobilized laccase showed a wider range of stability at more extreme temperature compared to free laccase. The immobilized laccases retained more than 60% of relative activity at the fourth cycle of reusability study. Lignin degradation was observed based on the FTIR peak at 2921 cm-1 during paddy straw saccharification with immobilized laccase. Immobilized laccase on m-MWCNTs could be recovered at ease, which promote its application for biomass hydrolysis.

Biography:

Kunasundari Balakrishnan received her PhD degree from Universiti Sains Malaysia (USM), Malaysia in 2014. Her thesis is focused on the development of an animal model to recover poly(3- hydroxybutyrate) granules from dried cells of Cupriavidus necator H16. She was attached to Japan International Research Centre for Agricultural Sciences (JIRCAS), Tsukuba, Ibaraki, Japan as a research fellow for 9 months in Dec 2012. Currently, she is a senior lecturer at Universiti Malaysia Perlis (UniMAP), Malaysia. Her research interest included biopolymer production and use of magnetized carbon nanotubes immobilized enzyme system for utilization of lignocellulosic biomass.

Carbon Fibers Grown from a Copper Nanoparticle Encapsulated within Hollow Carbon Spheres

Manoko Maubane-Nkadimeng[1*], Pranav Gangatharan[1], Neil Coville[1,2]

[1]University of The Witwatersrand, South Africa.

[2]DSI-NRF Centre of Excellence in Strong Materials, South Africa

Abstract:

Research in the synthesis and applications of nanomaterials has grown exponentially in recent years. Control of nanostructures using, capping agents, templates etc. has led to an understanding of the methods used to grow these nanostructured materials. Studies on the synthesis of nanostructures in small nano-confined environments has been well documented. However, these nanostructures (eg. metals/oxides) are formed in open-ended structures, and the confinement is not in all dimensions1 . In order to synthesize nanomaterials that are fully confined and to develop simple procedures to make nanostructures with controlled dimensionality, we have used hollow carbon spheres (HCSs) as our model container. In particular, we have chosen to grow helical carbon fibres (CNFs) inside a HCS using a Cu catalyst. HCSs were synthesized using a template method and were infiltrated with Cu ions (1%) to produce CuO particles2 . Transmission electron microscopy of HCSs revealed a spherical morphology (od = ca. 310 nm) with encapsulated Cu particles (d = ca.20 nm). Acetylene was then used as a carbon source to grow helical CNFs within the HCS using a chemical vapor deposition technique. The diameter and helicity of the CNFs were influenced by the Cu content within a HCS, the limited Cu sintering as well as the dimensions of the sphere. The procedures employed suggest that the philosophy of building other structures/molecules with any elements within confined nanoreactors is possible. References: 1. Restrepo, C.V., et al. (2021) Environ. Nanotechnol. Monit. Manag. 15, 100428. 2. Li, S., et al. (2000) J. Mater. Chem. A, 4, 12686.

Biography:

Manoko Maubane-Nkadimeng (PhD) Manoko Maubane-Nkadimeng graduated her MSc in Chemistry Cum Laude in 2010, followed by a PhD in Chemistry (Materials) in 2013 at the University of The Witwatersrand (Wits). She is currently a Senior Instrument Scientist and Researcher at Wits. Her research interests are in structured nanocarbons, with emphasis on their properties and applications in water and energy. She is the vice chairperson of the Employment Equity committee at Wits, a member of the Centre of Excellence in Strong Materials and a Fulbright Scholar Alumnae. She also holds a Postgraduate Diploma in Higher Education qualification and in 2019 she was appointed by the University of Pretoria as the Advisory Board Member of the Faculty of Education.

Topological phonons and superconductivity based on T-carbon

Presenter*: Jing-Yang You

Department of Physics, Faculty of Science, National University of Singapore, Singapore

Abstract:

T-carbon as a new carbon allotrope was proposed theoretically in 2011 and then successfully synthesized in experiments recently. In this talk, I will first introduce exotic

topological phonon states in T-carbon, including nodal loops and type-I and type-II Weyl points. In terms of the lattice symmetries and k·p model analyses, these topological phonons are found to be protected by the corresponding symmetries and are material independent, which can thus be applicable to the materials with similar symmetries, such as diamond. In addition, because of the fluffy structure of T-carbon, several kinds of atoms can be intercalated into it, and we show that superconductivity can appear in Na-doped T-carbon with a superconducting transition temperature Tc of 11 K at ambient pressure, which can be enhanced to 19 K under a pressure of 14 GPa. The calculations on temperature dependence of specific heat and electrical and thermal conductivities show that the normal state of Na-doped T-carbon superconductor is a non-Fermi liquid at temperature below 50 K, where the Wiedemann-Franz law is remarkably violated. These studies would not only spur great interest both experimentally and theoretically to explore novel carbon-based topological states and superconductors, but also provide a platform to explore the emergent physics due to the interplay between topological phonons and electron-phonon coupling and thermal transport.

Biography:

Dr. Jing-Yang You received a doctorate in physics from the University of Chinese Academy of Sciences in 2020. Since then, he has served as a research fellow at the National University of Singapore. Dr. You's main research interest is to conduct theoretical research on the design and physical properties of new quantum functional materials, such as topological states of matter, magnetic semiconductors, superconductors, and carbon materials, using density functional theory combined with model analysis. He has published over 30 papers in SCI journals as the first author or corresponding author.

POSTER

CoMnxNy supported on carbon nanotube with atomically dispersed Co active sites for efficient hydrogen generation from hydrolysis of ammonia borane

Dawson Wai-Shun Suen, Lok-Yan Leung, Kelvin Sher-Kin Tang, Anthony See Yuen To, Chi-Wing Tsang*

Faculty of Science and Technology, Technological and Higher Education Institute of Hong Kong (THEi), Hong Kong, China

**Authors to whom correspondence should be addressed:*

Abstract:

As urban areas continue to grow and living conditions improve, finding an efficient, safe, and sustainable source of energy is crucial for ensuring the longevity of human civilization. This requires new approaches to deriving energy from renewable resources and storing and releasing it, particularly through chemical reactions and engineering techniques. In this paper, we investigate the potential of Co and MnxNy nanoparticles (NPs) and supported on carbon nanotube with atomically dispersed Co active sites (Co SACs) for the hydrolysis of ammonia borane, a hydrogen storage material, and evaluate their physicochemical properties and catalytic performance. The study involved preparing bimetallic NPs and CNT with SACs consisting of atomically dispersed Co atoms on N-doped CNTs. The results indicate that the calcination temperature, total mass composition of the two metals, and the Co:Mn ratio all play important roles in optimizing the catalytic efficiency of the hydrolysis reaction. The CoMnxNy catalyst showed superior performance compared to pure Co and Mn monoatomic catalysts, and remained durable even after 50 cycles. The study also provides a detailed characterization of the physical and morphological properties of the CoMnxNy/Co-N-CNT catalyst.

Keywords: Hydrogen storage materials, ammonia borane, hydrogen generation, heterogeneous catalysis

Biography:

Dr. TSANG is currently academic staff of Faculty of Science & Technology, Technological and Higher Education Institute of Hong Kong (THEi) and is a chartered chemical engineer and fellow member registered with the Institution of Chemical Engineers and Institute of Materials, Minerals & Mining, UK. His research interests lie primarily in the areas of i) catalytic hydrogen generation; ii) heterogeneous and homogeneous catalysts syntheses; iii) development of high phosphorus content polymer with unique catalytic properties; iv) decarbonization technology. Since joining THEi in August 2016, he has already obtained over HK$12 million research funding from external sources (including 3 Faculty Development Schemes as PI, 1 Collaborative Research Grant as Co-PI, 1 Innovation Technology Commission funded project as Co-I and 1 Environment and Conservation Fund as PI). (i.e. > 60 refereed journal articles and 8 patent applications). He has also been invited as associate editor of Frontiers in Chemical Engineering, and guest editors of Catalysts and Journal of Visualized Experiments.

ORAL

Role of Carbon traces and Interfaces in Metal Oxide Nanocomposite Catalysis for Pollutant Estimation and Degradation in Water

Chaitanya Lekshmi Indira

Plaksha University, Mohali, Punjab

Abstract:

Through my talk, I will discuss on carbaneous metal oxide nanocomposite systems and the role of interfacial interactions in enhancing electro and photocatalysis leading to efficient

pollutant detection and degradation in water. In our research, we have shown metal oxide nanocrystal (NC) modified carbon electrodes as excellent choice for amperometric electrode fabrication and miniaturization for sensing. NiO NC based graphite or polymer nanoelectrodes could also support hierarchical structures with enzymes that enhanced the sensitivity of detection in aqueous medium to nM regime. While NiO NCs in the composite framework enabled easy electron transfer with the analyte molecule at the electrode-electrolyte interface, carbon framework was found to provide excellent support for catechol sensing activity across a spectrum of templates. Metal oxide NCs embedded in largely exfoliated graphene oxide network or having carbon quantum dots dispersed in them also enable advanced oxidation of organic dye pollutants by enhancing the lifetime of charge carriers and with better matching of catalyst redox potentials with active intermediates. In my lecture, I will address some of the influencing factors in these nanocomposites for efficient pollutant detection and degradation in water.

C-based Materials for Solid State Hydrogen Storage: A New Perspective

Chiara Milanese[1*], T. Bellotti[1], A. Girella[1], M. Medina LLamas[1] M. Gaboardi[1], G. Magnani[2], A. Rinaldi[2], D. Pontiroli[2], M. Riccò[2]

[1]*Pavia H2 Lab, Chemistry Department & C.S.G.I., Viale Taramelli, University of Pavia, Italy*

[2]*Nanocarbon Laboratory, DSMFI, Parco Area delle Scienze, University of Parma, Italy*

Abstract:

In the last 10 years, our research groups started a deep investigation on the possibility to use C-based materials for solid state H2 storage. The research started with alkali cluster-intercalated fullerides: in particular, we prepared mixed Li-Na clusters intercalated fullerides belonging to the NaxLi6-xC60 ($0 \leq x \leq 6$) family able to covalently store up to 5.5 wt% H2 at 300 °C and 50 bar, thanks to the catalytic effect of the alkali clusters. The addition of Pt and Pd nanoparticles to Li fullerides increases up to 5.9 wt% H2 the absorption capacity and of about 35% the absorption rate.

Being the price of C60 quite high for large scale applications, our attention moved to biochar, the carbon side-product in the pyrolysis/gasification of residual waste biomasses. Biochar can be converted into activated carbon (specific surface area > 1000m2/g) through a chemical treatment with bases giving a new cost-effective C material. In this frame, we prepared super-activated C materials from biochar derived by the pyrolysis of several different agrifood wastes. The materials obtained from rice bran and melon peels (surface area up to 3000 m2/g) adsorbed up to 4.5 wt % of H2 in around 30 seconds at 77K. Some unconventional wastes likes bean pods and asparagus stems were also considered, obtaining an adsorption higher than 3 wt% H2. Work is in progress to optimize the pyrolysis and activation conditions and to improve the sorption performance by intercalating with metals (Na, Li) and doping with metals oxides.

Biography:

Chiara Milanese is associate Professor at the Physical Chemistry Section of the Chemistry Department – Pavia University, where she is the scientific coordinator of the Pavia Hydrogen Laboratory. Her main research activities regard the preparation and characterization of innovative materials for solid state hydrogen storage and energy storage and topic linked to circular economy. She is Italian expert of the task 40 "Energy storage and conversion based on hydrogen" activated by IEA and member of the International Hydrogen Carrier Alliance. She is author of 230 papers on materials science topics on high impact factor journals (h index 35).

Engineering Bismuth Electrodes for Green Formate Synthesis from Carbon Dioxide Electroreduction

Juqin Zeng[1,2,] Nicolò B. D. Monti[1,2], Marco Fontana[1,2], Mattia Bartoli[2], Micaela Castellino[1], Pravin Jagdale[2], Candido F. Pirri[1,2]

[1]Politecnico di Torino, Italy

[2]Istituto Italiano di Tecnologia, Italy

Abstract:

In the last decade, electrochemical conversion of CO2 into valuable chemicals and fuels has attracted worldwide attentions and been considered as a promising approach to achieve a carbon neutral circular economy. The present work aims at realizing efficient CO2 reduction to HCOO−/HCOOH with excellent selectivity and high current density. Such targets have been achieved by utilizing bismuth (Bi)-based gas diffusion electrodes simply prepared via two different methods: 1) inkjet printing of precursor solution followed by in-situ restructuring; 2) microwave-assisted synthesis of BiOx nanoparticles and then drop-casting of the catalyst onto the carbon substrate. These electrodes result in excellent HCOO−/HCOOH selectivity in a wide potential range in both KOH and KHCO3 electrolyte. In addition, the HCOOH selectivity also reaches good values at pH value as low as 2. Such outcomes imply that the herein proposed Bi-based electrodes have good potential to be implemented in industrially relevant processes for CO2 valorization. Particularly, the direct production of HCOOH in acid is of high interest, since it is also a promising liquid hydrogen energy carrier due to the high energy density of 1.77 kWh/L that is comparable to the commercial high pressure hydrogen tanks. Green HCOOH is identified to be the most cost-effective carrier when the entire supply-chain cost is considered, the only green carrier that is more affordable to produce than its fossil-based counterpart, and the safest of the studied carriers like ammonia and methanol. It can also be used as a fuel in direct formic acid fuel cells.

Biography:

Zeng is currently an assistant professor in Politecnico di Torino, and mainly works on applied electrochemistry in different research fields like fuel cells, Li-O2 batteries and CO2 electrolyzers. She has (co)authored 38 papers in international journals with high impacts and two patents. She was awarded Premio di Dottorato 2013 "Fondazione De Nora" by Società Chimica Italiana. She has great passion in training young researchers, and has been tutoring numerous master and Ph.D students in materials Science and Technology, Chemical Engineering, Nanotechnology and Physics.

Carbon Nanotube Aerogel: An Exciting Material for Flexible Supercapacitor

Divya Nechiyila*, Jyoti Prakasha [b], Rajath Alexandera and Kinshuk Dasguptaa[b]

[a]*Materials Group, Bhabha Atomic Research Centre, Mumbai, 400085, India*

[b]*Homi Bhabha National Institute, Anushakti Nagar, Mumbai, 400085, India*

Abstract:

Supercapacitors possess the potential to revolutionize current energy storage technologies, enabling the development of more efficient, reliable, and sustainable storage devices. They offer several advantages over batteries, including high power density, long cyclic stability, fast chargedischarge capability, high energy efficiency, and low maintenance requirements. The demand for flexible and lightweight supercapacitors is increasing due to their broad applications in wearable electronics, hybrid electric vehicles, robotics, and aerospace. In response to this demand, our research delves into the remarkable potential of carbon nanotube (CNT) aerogel as a highperformance material for supercapacitor applications. The CNT aerogel, comprising a lightweight and self-supporting CNT network, serves a dual role as both a supercapacitor material and a current collector due to its advantageous features of high surface area and exceptional electrical conductivity. The flexible and bendable CNT aerogel supercapacitor exhibits exceptional performance in terms of specific capacity, energy density, and power density. Additionally, these flexible supercapacitors demonstrate long cyclic stability. This study opens up pathways for the commercial production of flexible, portable, and cost-effective supercapacitors, leveraging the scalable and robust production capabilities of CNT aerogel.

Biography:

Divya Nechiyil is currently serving as a research associate at Bhabha Atomic Research Centre, Mumbai, India. Her primary area of research focuses on the development of CNT aerogel-based flexible supercapacitors, reflecting her profound interest in energy storage advancements. Throughout her professional journey, Dr. Divya has actively engaged in different research projects, demonstrating her passion for exploring innovative research problems. She has 12 papers in peer-reviewed journals. Her research endeavors have covered a broad spectrum of subjects, encompassing the utilization of carbon nanomaterials in solar cells, sensors, and supercapacitors, as well as the applications of 2D nanomaterials in optoelectronic devices.

GO scaffolds for tissue regeneration

Giorgio Speranza[1, 2, 3, *], Firas Awaja[4], Heike Kaltenegger[5], Débora Coraça-Huber[6], Birgit Lohberger[5]

[1]*CMM - FBK, v. Sommarive. Trento – Italy*

[2]*IFN - CNR, CSMFO Lab. & FBK CMM, via alla Cascata, Trento, Italy*

[3]*Department of Material Engineering, University of Trento, v. Mesiano, Trento, Italy*

[4]*Regenerative Medicine Institute (REMEDI)and CÚRAM Centre for Research in Medical Devices, National University of Ireland, Galway, Ireland*

[5]*Department of Orthopedic Surgery, Medical University Graz, Auenbruggerplatz, Graz, Austria*

[6]*Department of Orthopaedic Surgery, Experimental Orthopaedics, Medical University Innsbruck, Innrain, Innsbruck, Austria*

Abstract:

Osteo-integration and tissue regeneration are vital for the longevity, durability, and unremitting functionality of medical implants/scaffolds implanted in vivo. To induce the cellular secretion of growth factors needed to induce tissue generation, it is essential playing with biomaterials properties since the administration of artificial growth factors, in vivo, is largely prohibited.

Bioactive coatings made of GO and aC/DLC functionalized with O2 and N2 were successful used to induce favorable cellular secretion of growth factors important for osteo-integration of medical implants. More precisely, Graphene Oxide (GO) stabilized in a hybrid structure induced the expression of vascular endothelial growth factor (VEGF) and osteoprotegerin (OPG) growth factors in human fibroblasts (hGF) and, more remarkably, in human osteoblasts (hOB) cells. We also observed a negative trend between hGF fibroblasts, but not hOB osteoblasts, cellular viability and GO presence in the hybrid films that might indicate the phenomenon of oxidative stress. We traced that back to the presence of higher concentrations of carboxyl and the carbonyl groups on the surface of the GO rich coatings.

The above-described properties provided by GO coatings might be desirable for bio-selectivity applications and for the reduction of the undesired fibrosis process that is associated with medical implants in vivo environment.

Biomass-Derived Carbon Dots as Photocatalysts to Decompose Pollutants in Wastewater

Le Thi Thu Huong[1]*, Nguyen Thi Hong Hanh[1], Chu Thi Thanh[1], Ngo Thi Thuong[1]

[1]*Vietnam National University of Agriculture, Vietnam*

Abstract:

Biomass is considered as a low-cost and environmental-friendly source for synthesis of carbon nanodots. In this study, carbon nanodots were prepared from different biomass. The synthesized carbon nanodots were characterized by transmission electron microscopy (TEM), infrared spectroscopy (FTIR), fluorescence spectroscopy (PL) and UV-Vis spectroscopy before applied as a photocatalyst. The carbon dots were in the size range of 4 to 8 nm and capable of photocatalyzing to decompose up to 95% methylene blue (MB) in water at initial MB concentration of 10 ppm after 20 minutes. The results showed that the carbon nanodots are potential for environmental applications.

Biography:

Le Thi Thu Huong did her graduate work at the Graduate University of Science and Technology, Vietnam Academy of Science and Technology (Ph.D. degree in 2019). Thereafter, she did postdoctoral training in chemistry at Institute of Chemistry, Vietnam Academy of Science and Technology and Vietnam National University of Agriculture. She is currently the vice head of Department of Chemistry, Faculty of Natural Resources and Environment, Vietnam National University of Agriculture. She is the co-author of more than 20 publications on nanomaterials for environmental and biomedical applications.

Tailoring Single-molecule Conductance with Structured Graphene Electrodes

Cristina Díaz[1*], and Joel G. Fallaque[2,3],Sandra Rodríguez-González[4], Fernando Martin[2,3,5]

[1]*Dept de Química Física, Fac. de Ciencias Químicas, Univ. Complutense de Madrid, 28040, Madrid, Spain*

[2]*Dept. Química, Univ. Autónoma de Madrid, 28049, Madrid, Spain*

[3]*Instituto Madrileño de Estudios Avanzados en Nanociencia, 28049, Madrid Spain*

[4]*Dept. de Química Física aplicada, Univ. Autónoma de Madrid, 28049, Madrid, Spain*

[5]*Condensed Matter Physics Center (IFIMAC), Univ. Autónoma de Madrid, 28049, Madrid, Spain*

Abstract:

Modulation of electric currents through single-molecule junctions can be achieved by

synthesizing molecules with desired functionalities, together with appropriate molecule-electrode contacts through specific anchoring groups. However, an alternative to this standard approach, scarcely explored so far, is to use structured electrodes. Using this kind of electrodes, conductivity can be controlled by changing the specific anchoring site within the very same electrode. In this project, we have investigated, from a theoretical point of view, how to exploit the pronounced anisotropy of corrugated graphene deposited on Ru(0001) (Gr/Ru) to tailor single-molecule conductivity in two largely different organic molecules, aniline and 4-aminobenzonitrile. Our results show that the currents induced in different anchoring positions in the Gr/Ru moiré are rather different, irrespective of the investigated molecule. The magnitude of these currents can differ by as much as an order of magnitude at specific bias voltages. We also show that both molecules display rectifying properties, which can differ by up to a factor of five in different anchoring sites. Interestingly, the observed modulations strongly depend on the chemical binding nature between the molecule and the electrode, covalent bond for aniline and physisorption for 4-aminobenzonitrile. From our analysis, we conclude that Gr/Ru can be an ideal electrode to modulate single-molecule electric conductivity under experimental conditions available in many laboratories.

Biography:

Cristina Díaz received her PhD in 2004 from the Universities Autónoma of Madrid and Bordeaux I. She has worked at Leiden University, Univ. Autónoma de Madrid, and since December 2019 she is professor of Physical Chemistry at the Univ. Complutense of Madrid. Her research has been mainly focused on surface dynamics molecular phenomena on graphene-based materials. Her scientific work has yielded more than 80 publications in peer-review journals and her h-index is 27 (https://scholar.google.es/citations?user=nSV-rl4AAAAJ).

PLENARY PRESENTATIONS

Carbon-based Materials for Biomedical Applications

Luke P. Lee*

Harvard Medical School, Brigham Women's Hospital, USA

Abstract:

In this talk, I will present the biomedical applications of carbon-based materials and devices, and the biological effects of carbon nanomaterials. First, I will discuss significant examples of carbon-based nanomedicine: therapeutic drug delivery, biomedical imaging, biosensing, photothermal therapy, and tissue engineering. Second, I will also examine the toxicity of carbon nanomaterials. Even though carbon nanomaterials are applied well in

life sciences and healthcare, examining their toxic effects in biological systems is critical. Third, after highlighting a few excellent examples of in vivo and in vitro applications of carbon nanomaterials-based biosensors, I will explain how to gaze at the health status with a grain of sand with carbon nanomaterials and find solutions for preventive medicine against a global pandemic such as COVID-19. Due to the lack of on-site fast, reliable, sensitive, and low-cost polymerase chain reaction (PCR) testing, we were limited to executing early detection, timely isolation, and epidemic prevention and control. However, low-cost carbon nanomaterials-based PCR chips are now created for a rapid, mobile, efficient diagnostic of infectious diseases via on-chip PCR: MEDIC-PCR. It shows excellent diagnostic accuracy of 97%, sensitivity of 94%, and specificity of 98%. Carbon nanomaterials-based MEDIC-PCR can contribute to preventive global health in the face of a future pandemic. It will also impact quantitative life sciences, precision personalized medicine, and global health.

Biography:

Prof. Lee received his BA in Biophysics and Ph.D. in Applied Physics and Bioengineering from UC Berkeley. He became the Arnold and Barbara Silverman Distinguished Professor at Berkeley. He also served as the Chair Professor in Systems Nanobiology at ETH Zürich. He founded the Biomedical Institute for Global Health Research & Technology (BIGHEART). He served as Associate President (International Research and Innovation) and Tan Chin Tuan Centennial Professor at the National University of Singapore. Currently, he is a Professor of Medicine at Harvard Medical School. His focus is global healthcare, neurodegenerative diseases, and quantum life sciences.

Probing the Nanoscale with a Combination of Spatially Resolved Spectroscopy and Theory

Sokrates T. Pantelides

Vanderbilt University, Nashville, TN, USA

Abstract Not Available!!

Keynote Session-II

Moisture Kinetics and LongTerm Post Thermal Aging Response of Carbon/Epoxy Composites

Vistasp M. Karbhari

Department of Civil Engineering & Department of Mechanical and Aerospace Engineering; University of Texas Arlington; Arlington; Texas 76019; USA

Abstract:

Carbon/epoxy composites have broad applicability in marine, offshore, and naval applications. Cost and scale considerations often result in the use of ambient and moderate temperature cure nonautoclave processes. These structures are not only subject to seawater and moist environments over extended periods of time but also thermal spikes due to operating temperatures, fires, and other regimes of elevated temperature. The mechanisms related to this combined and sequential exposure are different from those seen from individual effects and provides a challenge for design andprediction of longterm durability. This presentation presents a fundamental understanding of the synergistic mechanisms of degradation. Characteristics of thermooxidative resistance and post thermal aging seawater exposure of wet layup carbon/epoxy composites used in civil, naval, and offshore sectors are investigated. The interaction and competition between mechanisms of are elucidated with specific focus on moisture kinetics and dynamic characteristics and glass transition temperature. The relative effects of period of exposure and temperature are investigated and results used to determine operational limits for these materials.

Biography:

Vistasp M. Karbhari is a Professor in the Departments of Civil Engineering, and Mechanical and Aerospace Engineering, at the University of Texas at Arlington. An internationally reputed researcher, Prof. Karbhari is an expert in the processing and mechanics of composites, durability of materials, infrastructure rehabilitation, and multithreat mitigation. He is a fellow of the American Association for the Advancement of Science (AAAS); the National Academy of Inventors (NAI); the American Society of Civil Engineers; ASM International; the International Institute for Fiber-reinforced Polymers in Construction; the International Society for Structural Health Monitoring of Intelligent Infrastructure. ASCE's Structural Engineering Institute, and is an elected member of the European Academy of Science and Arts.

Nanostructures of Carbon and Related Materials for Energy Conversion and Chemical Sensing

Oomman K Varghese[1,2*]

[1]Department of Physics, University of Houston, Houston, Texas 77204, USA.

[2]Texas Center for Superconductivity, University of Houston, Texas 77204, USA.

Abstract:

Growing concerns over adverse impacts of accumulation of fossil fuel derived carbon compounds in the planet, especially CO2 in the atmosphere, have brought recycling of carbon and carbon materials using sustainable options as a promising risk reduction strategy. Converting carbon dioxide to fuels, synthesizing carbon materials from natural organic resources and transforming carbon waste to products using renewable energy are some of the widely explored approaches. The application scope of carbon materials has increased dramatically since the advent of low dimensional carbon materials such as carbon nanotubes, graphene and carbon dots. These materials derived from sustainable sources have shown remarkable properties. In this presentation, the characteristics of these materials and compounds applied to environmental sensing for medical diagnosis, and solar fuel production processes such as solar photocatalytic/photoelectrochemical carbon dioxide conversion and water splitting are discussed.

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.

Carbon Molecular-Sieve Membranes Developed from a Tröger's Base Polymer for Enhanced Carbon-capture Technologies.

Richard J. Spontak[1*]**, Zhongde Dai**[2]**, Jing, Deng**[3]**, Liyuan Deng**[4]

[1]North Carolina State University, USA
[2]Sichuan University, China
[3]ALTR FLTR, USA
[4]Norwegian University of Science & Technology, Norway

Abstract:

Carbon molecular-sieve membranes possess tremendous practical advantages over unary polymer membranes by providing high gas-separation performance levels, coupled with excellent mechanical and chemical stability. Improving their overall effectiveness greatly expands the competitiveness of this class of membranes. In the present study, carbon membranes are fabricated from a Tröger's base polymer as the precursor. The chemical structure of the aromatic polymer precursor is given by the following:

By optimizing the carbonization conditions, the gas-separation performance of the resultant membranes are significantly enhanced. Under optimized conditions, a H2 permeability of up to 1135 Barrer is achieved, with a corresponding H2/CH4 selectivity of 1170 and a CO2/CH4 selectivity of 238. While increasing the operating temperature slightly reduces the selectivity, it still remains in the high-separation region. Overall, the measured separation performance levels for H2-related separations, i.e., H2/CH4, H2/N2 and H2/CO2, all substantially exceed the Robeson upper bound. Moreover, the CO2/CH4 separation efficacy also lies above the 2019 upper bound, indicating that the carbon membranes developed in the present work are versatile and promising for several different gas-separation applications.

Biography:

Richard Spontak, a Distinguished Professor at NC State University, received his Ph.D. from UC Berkeley and pursued post-doctoral research at Cambridge University before joining P&G in 1990 and NC State in 1992. He has published over 300 peer-reviewed journal papers and 40 book chapters and invited works. He has received numerous research awards including the NC State Holladay Medal for Excellence, the ACS-PMSE Tess Award, the SPSJ International Award, the IChemE Underwood Medal, the ACS-RUBB Chemistry of Thermoplastic Elastomers Award, and the IOM3 Colwyn Medal. An IOM3, ACS-PMSE, APS and RSC fellow, he is a member of the Norwegian Academy of Technological Sciences.

Developments in Directed Metal-Catalyzed C-H Bond Functionalization

Hamad H. Al Mamari*

Department of Chemistry, College of Science, Sultan Qaboos University, Al Khoudh 123, Muscat, Sultanate of Oman

Abstract:

C-H Bond functionalization has emerged as a powerful strategy for transforming inert nonreactive C-H bonds into reactive ones. Due to ubiquitous presence of C-H bonds in natural products and numerous organic molecules, functionalizing such inert bonds would be a vial approach towards accessing functional molecules and materials in an expeditious

manner. This strategy will then allow recycling of otherwise wasted hydrocarbons and their reuse in an efficient and environmentally benign manner. Therefore, functionalization of C-H bonds is considered a green approach. Recent research has aimed at developments of new strategies tailored at making C-H bond functionalization more efficient. One of the strategies utilized to solve the regio-selectivity issue to the use of directing groups. The use of mondentate and bidentate directing groups allows delivery of the transition metal catalyst to a proximal C-H bond and accordingly functionalization of such bond. Thus, chelationassistance allows cleavage of an ortho C-H bond with respect to the directing group. Directing groups have allowed a wide range of CH bond functionalization reactions catalyzed by various second and the more earth abundant, first row-transition metals. The presentation will report developments in metal-catalyzed C-H bond functionalization reactions assisted by directing groups. This includes research carried out in metal-catalyzed C-H bond functionalization of benzamides containing 8-aminoquinoline as a N,N-bidentate directing group and strategically designed bidentate directing groups, such as the novel triazole-based N,N-directing group the triazolyldimethylmethyl (TAM) group. In addition, the presentation will cover novel design-based removable N,O-bidentate directing group based on cheap and commercially available starting materials such as 4-aminoantipyrine (AAP).

Biography:

Hamad Al Mamari obtained his PhD degree (2006) at the University of Oxford under the supervision of Professor David Hodgson. Upon completion of his PhD, he returned to his home institution, Sultan Qaboos University, Oman. In 2012/2013 he spent one-year sabbatical at Georg-August University, Göttingen, Germany where he worked in the field of C-H bond functionalization (Host: Professor Lutz Ackermann). Later, he spent short-term visits at the Department of Chemistry, School of Science, University of Tokyo (Host: Professor Eiichi Nakamura) (2015 & 2017), the Julius-Maximilians-Universität,

Würzburg, Germany (Host: Professor Todd Marder) (2016), and University of Ljubljana, Slovenia (Host: Professor Dr. Bogdan Štefane). In the period of 2021/2022, Dr. Al Mamari spent a one-year research visit/visiting scholar at Julius-Maximilians-Universität, Würzburg, Germany (Host: Professor Todd Marder). Dr. Al Mamari currently hold the rank of an associate professor of chemistry at the Department of Chemistry, College of Science, Sultan Qaboos University, Sultanate of Oman. His research interests Are themed in organic synthesis with emphasis in developments of methods and reactions in the field of C-H bond functionalization and their applications in natural product synthesis.

The Role of Metal-Organic Frameworks for Energy Storage Materials

Ali A. Ensafi

Department of Chemistry, Isfahan University of Technology, Isfahan 84156-83111, Iran

Department of Chemistry & Biochemistry, University of Arkansas, Fayetteville, AR, USA

Abstract:

Presently, 80% of the world's energy is supplied by fossil fuels which thus leads to strong global warming effects. These crises urge scientists to take advantage of other energy sources with no environmentally destructive effects, including wind and hydropower, fuel cells, and solar energy. To benefit from these energy sources, significant efforts are required to develop and design high-performance devices for efficient energy conversion, storage, and green electricity production. Thus, there is an immediate requirement for energy storage and conversion systems. As for electrochemical and electrochemical energy storage devices, supercapacitors and fuel cells have gained tremendous attention from both industry and academia due to their unique characteristics such as ultra-long durability, environmentally friendly, and good reliability.

The assembly of metal ions with organic ligands through the formation of coordination bonds gives crystalline framework materials, known as metal-organic frameworks (MOFs), which recently emerged as a new class of porous materials. MOFs are a new class of porous coordination compounds with remarkable properties, such as large surface area, adjustable structure, and tunable pore sizes. MOFs have emerged as one kind of important porous solid and attracted intensive interest in different subject areas. MOF composites can be divided into four parts according to their dimensions, including MOF/zero dimension (0D), MOF/one-dimension (1D), MOF/two dimension (2D), and MOF/three-dimension (3D), each of their special properties. Subsequently, many types of MOFs were reported with designed structural, magnetic, electrical, optical, and catalytic properties by choosing appropriate metal ions and organic ligands.

Biography:

Prof. Ensafi graduated in Chemistry (Ph.D.) in 1991 (Shiraz University, Iran). He became a full professor in 2001 at Isfahan University of Technology. He joined as an Adjunct Professor in Department of Chemistry & Biochemistry, University of Arkansas (USA) in July 2021. He has H-index of 73 and published more than 550 papers. He has awarded three international awards. He is the editor and co-authors of 18 books, associate editor of Biosensors & Bioelectronics X, Journalof Iranian Chemical Society, and editorial board of 15 scientific journals. His research program is developing biosensors and nanomaterials for fuel cells and supercapacitors.

Understanding the Role of GO on the Synthesis of GO-Based Membranes for Membrane Distillation Desalination

Lucy Mar Camacho[1*], Olubayo O. Oginni[1], Saketh Merugu[2], Anju R. Gupta[2]

[1]*Texas A&M University-Kingsville, Unites States*

[2]*University of Toledo, United States*

Abstract:

Graphene oxide (GO) has been identified as a promising material for membrane synthesis. In addition to its remarkable mechanical and thermal properties, GO has the ability to modify the pore structure of the membrane, impart antifouling properties, and increase the hydrophilicity and surface charge of the membrane. More research needs to be conducted to explore the characteristics of GO-based membranes dedicated to the vapor-pressure-driven process of membrane distillation (MD), which is one of the main limitations that prevent MD from commercialization as a promising separation process for desalination. Membrane distillation, identified as a thermal-membrane process, requires membranes with unique characteristics. Contrary to existing polymer membranes, which are commonly hydrophilic and dense, membranes for MD need high hydrophobicity and porosity. We combined the properties of GO and polysulfone (PSF) to fabricate MD-dedicated membranes. This combination imparted not only antifouling and porous properties. It also provided hydrophobic properties and resilience to pH change and chemical attacks. We characterized the GO material and the morphological properties of the GO-PSF membrane with respect to the GO content. We tested the membrane to separate high concentrations of minerals from produced water by MD and compared the results with commercial membranes. GO provided the unique membrane conditions for high flux, salt rejection, and antifouling conditions for successful MD separation.

Biography:

Lucy Mar Camacho is an Associate Professor in the Department of Environmental Engineering at Texas A&M University-Kingsville. She received her Ph.D. degree in Chemical Engineering from New Mexico State University (NMSU) in 2000. She received an M.S. in Electrochemical Engineering Processes and a B.S. degree in Chemistry from the Technische Universität Dresden, Germany. She also conducted a postdoc at NMSU. Dr. Camacho has more than 15 years of laboratory research experience in the area of water desalination and innovative water treatment technologies. She is currently developing graphene oxide (GO) membranes for water treatment and other separation applications.

Paraffin-Olefin Separation by Ag(I) and Cu(I)-doped Nanoporous Carbons

Dipendu Saha

Associate Professor and Department Chair, Widener University, 1 University Place, Chester PA, USA

Abstract:

Among different types of adsorbents, nanoporous carbons are highly attractive because of their lowest cost, versatile synthesis protocol, wide range of precursors, easy functionalization protocol, and efficient separation. Light olefins, like ethylene and propylene, are the precursors of most modern-day plastics. An olefin is always mixed with the corresponding paraffin at the time of production, and therefore it needs to be separated from paraffin to produce polymer-grade olefin (99.95%). It is extremely difficult to separate olefins from paraffin owing to their similar physicochemical properties. The current state-of-the-art separation technique, cryogenic distillation, is highly expensive and hazardous. On the other hand, adsorption in a suitable material, like porous carbon can be a sustainable solution for the olefin separation and enrichment. In this presentation, the role of pi complexation with a few selected metals, like Ag(I) and Cu(I) on the surface of porous carbons towards the separation of ethylene and propylene will be discussed from both experimental and computational perspectives.

Biography:

Dipendu Saha is the associate professor and chair of chemical engineering department Widener University. He received his Ph.D. 2009 from the Chemical Engineering department of New Mexico State University. He completed his postdoctoral appointments from University of Quebec-Trois Rivieres (Canada) and Oak Ridge National Laboratory (USA). Dr. Saha has received the Outstanding Researcher Award in recognition of his exemplary achievements in research and scholarship from Widener University. His research area includes design and synthesis of nanoporous carbons for water purification, carbon capture, gas separation and critical elements recovery. His research has been supported by several organizations in the U.S.A

Carbon Nanofiber Z-threaded Carbon Fiber Reinforced Polymer Composites: the Interactive Role Between the Carbon Fiber and Carbon Nanofiber and the Future

Kuang-Ting Hsiao*

University of South Alabama, USA

Abstract:

Carbon nanotubes and nanofibers (CNFs) have been extensively investigated for improving carbon fiber reinforced polymer (CFRP) composites over the past decades. Literature reported significant effort in understanding and eventually recognizing the critical influence of dispersion and alignment of the nanoparticles in the polymer matrix. However, the interaction between the CNF (or CNT) vs. the carbon fibers was hardly mentioned nor addressed systematically. The inconsistence and complexity among different material systems and the great uncertainty of data made such effort extremely challenging and remaining largely unanswered.

The carbon nanofiber z-threaded carbon fiber reinforced polymer (ZT-CFRP), as unique class of nano-enhanced CFRP, has long carbon nanofibers to zig-zag thread between continuous carbon fibers perpendicularly to form the mechanically interlocked nanofiber-

microfiber reinforcement network, and have achieved robust and repeatable improvements in the mechanical properties, thermal conductivities, electrical conductivities, and some other novel phenomena due to the unique 3D-multiscale reinforced micro-structure. The zig-zag mechanically-interlocked structure of the ZT-CFRP and its repeatable experimental data could be useful to understand the potential roles of interaction between CNF (or CNT) and the carbon fiber, and how the interaction could affect the composite's properties. This presentation will discuss the role of interaction between the CNF (or CNT) and the carbon fibers and the future development including application of nano-enhanced CFRP composites in 3D printing.

Biography:

Professor Kuang-Ting Hsiao is a tenured full professor of mechanical engineering at the University of South Alabama. His current research interests are in the manufacturing, characterization, and micro-mechanics modelling of nano-enhanced multifunctional carbon fiber composites, and the integration of new composite materials with new additive manufacturing techniques. Prof. Hsiao has published 1 book, 6 book chapters, 32 journal papers, 70 conference papers, and holds 15 patents and 6 pending patent applications. Prof. Hsiao's research has been funded by NSF, NASA, DOD, DOE, Alabama Commission on Higher Education, Alabama Department of Commerce, and Industries.

Fischer-Tropsch Synthesis in 3D-Printed Stainless Steel Microreactors

Debasish. Kuila*, Meric Arslan, Saif Hassan, Juvairia Shajahan, Sujoy Bepari, Nafeez Mohammad, and Richard Abrokwah

Department of Chemistry and Applied Sciences and Technology, Joint School of Nanoscience and Nanoengineering, North Carolina A&T State University, Greensboro, NC

Abstract:

One of the main objectives of our NSF-CREST bioenergy Center is to develop robust catalysts for Fischer-Tropsch (F-T) synthesis using syngas (CO:H2) containing CO2 obtained from biomass gasification. Our previous F-T studies at 1 atm involved the use of silicon(Si) and 3-D printed stainless steel (SS) microreactor to explore the effect of metal-support interaction on formation of hydrocarbons.1-4 These studies have been extended to 20 bar and scaled-up to obtain liquid fuels using Co-Ru-KIT-6, a mesoporous silica supported bimetallic catalyst, in a SS microreactor. 5 This catalyst was used for CO2-enriched syngas conversion to higher hydrocarbons at 20 bar. 6 Currently, the effect of iron and cobalt-based bimetallic core-shell catalysts using mesoporous silica and SiO2-Al2O37 , and the use of graphene oxide as support and metal promoters on Fe-catalysts 8 for F-T synthesis at 20 bar are being investigated. An overview of these on-going studies including metal-support interactions will be presented.

Biography:

Debasish Kuila, previous Chair and Professor of chemistry, is the Research Director of NSF-CREST Bioenergy Center and the PI of the DOE-BES and DOE-EERE projects at North Carolina A&T. He is an affiliate of JSNN and an adjunct professor of Wake Forest School of Medicine. He spent over 14 years at Hoechst Celanese and Great Lakes Chemical Corporations, Purdue, and Louisiana Tech University. His research interest spans from materials/biomaterials, CO2 capture/conversion, cell biology, to catalysis. He was the 2020 Senior Researcher of the CoST, and received 2019 Chemcon Distinguished Speaker Award at the International Conference on Energy & Environment, Jaipur, India.

From Waste Graphite Fines to Revalorized Anode Material for Li-ion Batteries

Juan Carlos Abrego-Martinez[1*], Youling Wang[1], V. Vanpeene[2], Lionel Roué[1]

[1]Institut National de la Recherche Scientifique (INRS) - Centre Énergie, Matériaux, Télécommunications (EMT), Varennes, Canada.

[2]X-Ray Nanoanalysis beamline ID16B, European Synchrotron Radiation Facility (ESRF), Grenoble, France

Abstract:

More than 50% of natural graphite material is wasted during the spheroidization process in the production of battery grade graphite for lithium-ion batteries. The waste product consists of graphite fines that are not suitable for use in lithium-ion batteries due to their small particle size (<10 µm), therefore, graphite fines are discarded or sold at a loss. In this work, we report a method for graphite fines re-agglomeration and subsequent coal tar pitch coating that allows for revalorization and recycling of waste graphite from the spheroidization process. Resulting agglomerate particles showed a particle size distribution comparable to a commercial battery grade natural graphite reference and proved structurally sound to withstand the electrode calendering process. Pitch-coated agglomerate particles exhibited lower surface area and improved cycling stability with respect to non-coated agglomerate particles. Overall, the material obtained through this method shows great potential for re-introduction in the production chain of battery grade natural graphite for lithium-ion batteries.

Biography:

Juan Carlos Abrego Martinez holds a PhD in energy and materials science from the Institut national de la recherche scientifique. His research focuses on energy conversion and storage systems such as lithium-ion batteries, microfluidic fuel cells and supercapacitors.

Microstructure and Oxidation Analysis of Cemented C/C/C Fabricated by Laser

Jorge A. Ramos-Grez*[1], David Bourell[2] and Madhavrao Govindaraju[3]

[1]*Pontificia Universidad Católica de Chile, Macul, Santiago, Chile;*

[2]*University of Texas at Austin, Austin, TX, USA;*

[3]*University of Texas at San Antonio, San Antonio, TX, USA*

Abstract:

C/C composites of cylindrical shape have been cemented using a raster-scanned CO2 laser beam in a four-step sequence. Complete and homogenous surface cementation as well as thermal stability of the composites was achieved. The heat line created from the laser beam impinged parallel to the axis of rotation of the pre-coated cylinder, while suspended from one end. Different slurry compositions were prepared, all containing chloride salts from refractory elements, some including silicon. The latter was pre-deposited by air spraying it over each specimen and then the laser heat treatment was applied. Heat applied sublimed the chlorine ions resulting in silicide compounds that reacted with the carbon substrate forming a bond layer. Comprehensive microstructure characterization was done immediately after the cementation was consolidated and after heat treatment under argon, using scanning electron microscopy, energy-dispersive spectroscopy, and x-ray diffraction. Oxidation weight loss tests after 9 h of exposure were performed up to 1423 K under argon and air, showing a decrease of 9.8 and 30.6% in weight, respectively. A 28% weight loss was obtained with a glass overcoat layer applied over the cemented specimens, performed at 1273 K for 20 h in air.

Biography:

Jorge A. Ramos-Grez is a Professor at the Department of Mechanical and Metallurgical Engineering, Pontificia Universidad Católica de Chile. His research interests include materials engineering, modern manufacturing methods, and laser applications in manufacturing: cutting, welding, heat treatments, coatings, ab initio and semi-classical modeling, and synthesis of shape memory alloys.

Transmission Electron Microscopy (TEM) Analysis of MWNT/PMMA composite samples made by three different methods

Morgan R. Watt,[1] Rosario A. Gerhardt*,[1], Chanchal Gosh[2], Manish K. Singh[2], Stephen Jett [3], John Watt [4] and C. Barry Carter[2]

[1]*Georgia Institute of Technology*

[2]*University of Connecticut*

[3]*Sandia National Laboratories,*

[4]*Los Alamos National Laboratory, United States (USA)*

Abstract:

The effect of processing on the arrangement of multiwalled carbon nanotubes (MWCNT) embedded in a thermoplastic poly-methyl methacrylate (PMMA) polymer was investigated. MWCNT/PMMA composites were fabricated using three different mixing methods (mechanical, solution, and melt mixing) followed by compression molding. Each mixing method used resulted in vastly different electrical properties. Percolated composite specimens made by the three different mixing methods, which displayed the same electrical resistivity, were chosen for detailed TEM analysis. Samples were prepared by microtoming and the lamellas were collected on 3 mm C-coated Cu grids. All samples were coated with a fine layer of C (~ 5 nm). The TEM studies were carried out using a Tecnai F30 TEM operated at 300 kV and a FEI Talos operated at 120 kV. Image processing and analysis were carried out using the 'Digital Micrograph' and 'Image J' image analysis software. In all the specimens, the CNTs were found to be 12-15 nm in diameter while the lengths of the nanotubes vary. Selected-area diffraction patterns indicate that the nanotubes in all three specimens are identical in phase and structure. The contrast in the amorphous matrix is due to rumpling. Images reveal that the MWNT arrange themselves along the polymer boundaries in the mechanical-mixed sample while they are evenly distributed throughout in the melt-mixed sample with the formation of some micron-sized agglomerates. The solution-mixed samples did not show any distributed MWNT and instead all nanotubes form mostly agglomerates with different surface characteristics from those observed in the melt mixed samples.

Biography:

Rosario A. Gerhardt is a full professor at the Georgia Institute of Technology in Atlanta, GA, USA where she focuses on research that links the underlying structure of materials to their electrical, optical and magnetic properties. She has conducted research on carbon black, graphite nanoplatelets and carbon nanotubes for 20 years. Morgan Watt graduated with her PhD from Georgia Tech in 2020. This work was done in collaboration with the Center for Integrated Nanotechnologies (CINT) located at Sandia and Los Alamos National Labs with the help of Prof. C.B. Carter and his students.

Copper-based Approaches in the War Against Cancer: Taking Advantage of Inorganic Physiopathology

Valentina Oliveri*

Department of Chemical Sciences, University of Catania, Italy

Abstract:

Among various medical challenges, cancer remains the leading cause of death worldwide. The development of new effective therapies should aim to reduce side effects, increasing

the selectivity of the administrated drugs. In addition, these agents should overcome cancer cell resistance and target cancer stem cells. Since the key role exerted by Cu in the etiology, severity, and progression of cancer diseases, it could be a vulnerable point to target for arresting cancer development (1). Some copper-involving agents (i.e. Cu ionophores, Cu complexes, Cu chelators and Cu nanosystems) have revealed anti-cancer activity, boding well for the development of new agents that can overcome cancer drug resistance (2). Here we report some systems based on the quinoline scaffold that, when co-administered with copper ions, can trigger cancer cell death, probably through a Cu-dependent mechanism, recently reported as cuproptosis (3). On the other hand, cuproplasia is copper-dependent cell growth and proliferation and some strong copper chelators based on quinoline scaffold can arrest cancer growth, suggesting that copper depletion and copper supplementation may be viable approaches for developing novel anticancer therapies. We also evaluated a series of strategies to increase the selectivity of our copper-binding compounds, for example, designing and evaluating stimulus-responsive systems of 8-substituted quinolines.

Biography:

Valentina OLIVERI received her Ph.D. in Chemical Sciences cum laude in 2014 from the University of Catania (Italy). She was a visiting PhD student at the University of Sussex in 2012 where she gained skills to design and synthesize metal-binding ligands. Currently, she is an Assistant Professor (RTD-b, tenure-track position) at the University of Catania. As a bio-inorganic and supramolecular chemist, she has explored the chemistry and exploited the properties of different metal centers also in supramolecular networks using different techniques. Her research has been recognized with several distinctions and awards including funding from PRIN 2022 and Italfarmaco award.

Novel Topotactic Route of Fabricating Multiwalled Cerium Oxide Nanotubes from Multiwalled Carbon Nanotubes

Jorge R. Vargas-García[1*], Sarahi Pacheco-Espinoza[1], Alejandro I. Cuesta-Balderas[1], Jorge Vázquez-Lujano[1], Abril Rosiles-Aguilera[1], María A. Hernández-Pérez1, Felipe Cervantes-Sodi[2], Fei Chen[3], Qiang Shen[3], Ron Tu3, Lian-Meng Zhang[3]

[1]*Instituto Politécnico Nacional, Mexico*

[2]*Univ. Iberoamericana, Mexico*

[3]*Wuhan University of Technology, China*

Abstract:

The development of new strategies for synthesizing 1D cerium oxide (CeO2) hollow nanostructures has attracted much attention in recent years due to the importance of the superior surface-to-volume ratio and highly anisotropic geometry. Herein, we present the

topotactic transformation as an effective route for synthesizing novel multiwalled CeO2-d nanotubes from functionalized-MWCNTs. The entire volume of f-MWCNTs is converted into multiwalled CeO2-dnanotubes through oxidation/dehydration topotactic reactions. The stable CeO2 (111) planes grow topotactically parallel to the curved C (002) planes. In their initial condition, novel nanotubes consist mainly of CeO2-x(OH)x with residual fractions of carbon. As heating in air up to 500 °C, CeO2-x(OH)x transforms gradually by topotactic dehydration into CeO2-d, while the residual carbon is oxidized. The multiwalled CeO2-d nanotubes prepared in this study exhibit an outstanding presence of surface oxygen vacancies and maintain their structural integrity up to about 600 °C. In fuel cell applications, novel CeO2-d nanotubes show attractive electrochemical performance as catalytic supports for methanol oxidation.

Biography:

Jorge Roberto Vargas Garcia received the B.S. and M.S. degrees in Metallurgical and Materials Engineering from Instituto Politécnico Nacional and the degree of Doctor of Engineering in the subject of Materials Science from Tohoku University. Currently he is a Professor at Instituto Politécnico Nacional, where he leads the Functional Nanomaterials Laboratory. He was director of the Centre for Nanoscience and Nanotechnology at Instituto Politécnico Nacional. He has authored or co-authored over 100 research papers and he serves on Editorial Boards of international journals. His current research interests are in thin film deposition, materials characterization, and nanomaterials synthesis.

Friction and Degradation of Graphite: A Nanotribological Approach

Arnaud Caron* and Jaemoo Kim

KOREATECH – Korea University of Technology and Education, School of New Materials and Chemical Engineering, Republic of Korea

Abstract:

We investigated the friction and wear of graphite by atomic force microscopy in sliding contact with SiOx, Pt, and diamond tips with contact forces up to several micronewtons. Graphite's tribology strongly depends on the chemistry of the counter body. With a SiOx tip, friction is governed by puckering. Wear initiates at surface steps by mechanical destabilization of folds. With a Pt tip, the adhesive effects lead to the exfoliation of graphite. At higher loads, friction crosses over from exfoliation to puckering. For SiOx and Pt, the wear rate is low in ambient conditions. In the case of diamond tips, we measured a friction coefficient and a wear rate of an order of magnitude larger than with SiOx or Pt tips.

Biography:

Arnaud Caron is a materials scientist with expertise in the mechanical behavior of materials, surfaces, and components. Arnaud Caron is a faculty member at KoreaTech, Rep. Korea. Arnaud Caron obtained his engineering degree in Materials Science in 2004, and he earned his doctoral degree in materials science in 2009 from the University of Saarland, Germany. Arnaud Caron worked at the IMNM at the University of Ulm, Germany, the WPI-AIMR at the Tohoku University, Japan, and the Leibniz – INM, Germany.

Design Thick Electrodes to Improve the Comprehensive Lithium Storage Performance

Hongtao Sun

The Pennsylvania State University, University Park USA

Abstract:

Developing electrochemical energy storage that enables simultaneously delivering high areal, volumetric, and gravimetric performance is a grand fundamental and technological challenge. It is straightforward but problematic to make electrodes thicker and denser for high areal and volumetric performance while sustaining a high level of gravimetric performance. The insufficient charge transports in these electrodes with high mass loading and electrode density could severely degrade the energy storage performance. Herein, we developed an energy-efficient fast sintering method (e.g., Spark Plasma Sintering) to fabricate a structural cathode with a high electrode density (2.0–2.3 g cm^{-3}) and high mass loading (70–100 mg cm^{-2}). The vertically aligned carbon networks and anisotropic pore channels in the ultrathick electrodes (300–500 µm) are designed and tailored for efficient charge transports throughout the whole thickness. As a result, the sintered structural electrodes perform high areal (8.6 mAh cm^{-2}), volumetric capacity (246 mAh cm^{-3}), uncompromised gravimetric performance (164 mAh g^{-1}) at normal current and stable cycling with a capacity retention of 84% after 200 cycles under a current density of 4.5 mA cm^{-2} .

Biography:

Hongtao Sun is an assistant professor in the Department of Industrial and Manufacturing Engineering at the Pennsylvania State University. Prior to Penn State, he was a postdoctoral fellow at UCLA from 2015 to 2018. He received his Ph.D. degree in Mechanical Engineering from Rensselaer Polytechnic Institute (RPI) in 2014. His research lies at the intersection of energy science, functional materials, and advanced manufacturing. Dr. Sun has published 50 peer-reviewed papers in leading journals such as Science, Nature Reviews Materials, Nature Communications, and Nature Catalysis with a total citation number of over 8000 and an h-index of 43.

Enhancing Antimicrobial Properties of Graphene derivatives on Metallic Substrates for Biomedical and Environmental Applications

Sasmita Nayak[1,2]

[1]*School of Biotechnology, Kalinga Institute of Industrial Technology Deemed to be University (KIIT-DU), India*

[2]*Kalinga Institute of Medical Sciences, Kalinga Institute of Industrial Technology Deemed to be University (KIIT-DU), India*

Abstract :

The global emergence of multidrug-resistant pathogens poses a threat to public health, necessitating the development of innovative antimicrobial materials. Our work focuses on harnessing the antimicrobial potential of graphene oxide and derivatives, when applied to bare metallic substrates, offering solutions towards biomedical and environmental applications. Initially, we introduced an eco-friendly approach involving natural shellac-derived GO coatings on metallic films, underscoring their environmental significance. Our findings illustrated the remarkable antibacterial potential of GO coatings on a variety of metallic substrates, including Zn, Ni, Sn, and steel against a Gram-negative bacterium. The connection between electrical conductivity and antibacterial activity within GO-metal systems remained a focus of this study. Additionally, we provided detailed mechanistic insights, elucidating how GO-metal interactions function as highly efficient electron sink for bacterial respiratory chain, leading to the generation of reactive oxygen species (ROS) and potent bactericidal effects. As an extension of this work, we further explored the antimicrobial potential of rGO on bulk aluminum substrates. Our findings revealed substantial inhibition of Gram-positive and Gram-negative bacteria as well as fungi when compared to control (Glass, Bare Al) surfaces showcasing the superior broad-spectrum antimicrobial activity of rGO-Al substrates. SEM analysis confirmed structural damage to microbial cell membrane. A mechanism was proposed involving surface hydrophobicity directed sustained microbial interaction followed by conductivity driven electron transfer leading to ROS mediated membrane damage. The current research will have an essential impact on designing and understanding of the biocidal roles of graphene-based materials with promising uses in industrial and biomedical sectors.

Biography:

Sasmita Nayak is an experimental biologist with a passion of improving health and wellbeing. She began her journey with a Bachelor of Medicine and Surgery from S.C.B. Medical College Hospital, India. After E.C.F.M.G. certification, she worked as a visiting physician at various hospitals in USA. Her research career took off as a research assistant at the Centre for Immunology and Microbial Diseases, Albany Medical Centre, USA. In 2012, she earned her Ph.D. from RPI, USA. Her current research focus includes exploring the inhibition strategies against ubiquitous microbial components within our surroundings. She currently holds an Associate Professor position in KIIT School of Biotechnology and as Adjunct Associate Professor at the Microbiology Department of Kalinga Institute of Medical Sciences.

Chemistry of Spirobifluorene-Based Macrocycles

Toru Amaya*

Graduate School of Science, Nagoya City University, Japan

Abstract:

Shape-persistent macrocyclic compounds containing carbon-rich π-electron systems have been researched because of their unique molecular geometry and associated characteristic properties. Here, I would like to report our recent results on such carbon-rich π-electron systems based on spirobifluorenes as a building block. More specifically, the synthesis and characterization of a linear [3]spirobifluorenylene, 1 consisting of the double strand of S-shaped p-sexiphenyl, will be presented. The characteristic spiro-conjugation,2 host-guest chemistry,3 and intramolecular electron transfer in radical cation species4 of the cyclic [n]spirobifluorenylenes will also be reported in this presentation.

References:

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Biography:

Toru Amaya received his Ph.D. Degree from Tokyo Institute of Technology in 2003. He was as a postdoctoral fellow with Professor Julius Rebek, Jr. at Scripps Research Institute (2003-2004). In 2004, he was appointed as an Assistant Professor at Graduate School of Engineering, Osaka University. He was promoted to Lecturer in 2018, and Associate Professor in 2019. In 2021, he established his independent group at Nagoya City University, as a Professor. His research interests include functional organic chemistry and synthetic organic chemistry.

Ultra-fine Nano-$CaCO_3$ Based-epoxy Composites: A High-strength Nano-filler Engineered *via* Planetary Ball Milling for Advanced Structural Applications

Neha Uppal [a,b*], Asokan Pappu [a,b], Vijaya Kumar Sorna Gowri [a,b]

[a] *Academy of Scientific and Innovative Research (AcSIR), Ghaziabad-201002, India*

[b] *CSIR-Advanced Materials and Processes Research Institute, Bhopal, Madhya Pradesh-462026, India*

Abstract:

CaCO3 fillers offer high stiffness and impact resistance, but their rigid, brittle behavior makes it challenging to attain good tensile properties in epoxy matrices. Herein, we report a high tensile strength and stiff nano-CaCO3 /epoxy composites engineered via planetary ball milling for the first time. Remarkable improvement in strength of ~ 51% (51.90 MPa) and modulus of ~ 28% (522.62 MPa) at 1 wt% was observed with respect to micron-sized counterparts. A fascinating observation of ~ 40% enhancement in ductility was also seen. The results imply that nano-CaCO3 particles (38-52 nm) showed promising results to be used as sustainable concrete nanofiller in the greener construction industry and other commercial building applications.

Keywords: Sustainable nano-CaCO3, Planetary ball milling, Nanocomposites, Elastic properties

Biography:

Dr Uppal received her doctoral degree from AcSIR, CSIR-Advanced Materials and Processes Research Institute, Bhopal, India in 2023. Her research interests include the applications of industrial wastes in conjunction with nanocellulose/biofibers based polymeric composites, materials characterization, structure-property relationship of composites for advanced structural applications.

Engineering Active Sites of 2D Materials for Active Hydrogen Evolution Reaction

Jeong Hyo Kim[1], Da Yeon Lee[1], Ning Ling[2], Yongjoon Lee[3], Heejun Yang[3], Suyeon Cho[1*]

[1] *Division of Chemical Engineering and Materials Science, Graduate Program in System Health Science and Engineering, Ewha Womans University, Seoul, 03760, Republic of Korea*

[2] *Department of Energy Science, Sungkyunkwan University, Suwon, 16419, Republic of Korea*

[3] *Department of Physics, Korea Advanced Institute of Science and Technology (KAIST), Daejeon 34141, Republic of Korea*

Abstract:

Hydrogen evolution reaction (HER) is a promising solution for sustainable and clean energy source with zero carbon emission. Numerous studies have been conducted with versatile low dimensional materials, and the development of highly active electrochemical catalysts for HER has been one of the most important applications of the materials in the studies. Despite such extensive research, the physical origin of active catalytic performances from low dimensional materials remains unclear, which is distinguished from classical transition metal-based catalysts. Here, we review recent studies on intrinsic catalytic activity of two-dimensional (2D) semimetals, particularly among transition metal dichalcogenides (TMDs), highlighting promising strategies for the design of materials to further enhance their catalytic performances. An attractive approach for active HER is fabricating single-atom catalysts in the framework of TMDs. While electrochemical reaction at a catalytic atom for hydrogen evolution has been discussed by the Sabatier principle, we describe the phenomenon by Gibbs free energy for hydrogen adsorption via down-sizing, alloying, hybridizing, hetero-structuring, and phase boundary engineering mostly with TMDs. Thus, unique advantage of TMDs and their derivatives for HER are summarized, proposing research directions for promising design of low dimensional electrochemical catalysts for efficient HER and their energy applications.

Biography:

Suyeon Cho is currently an Associate Professor in the division of Chemical Engineering and Materials Science, Ewha Womans University, Korea. She received her Ph.D. degree at the department of Physics and Astronomy, Seoul National University in 2012, and then she worked as a Post-Doctoral Research Fellow at the ANTARES beamline in the synchrotron SOLEIL, France in 2013–2014 and at the Center for Integrated Nanostructure Physics (CINAP) in Sungkyunkwan University, Korea in 2014–2017. Her research interests include the synthesis and characterization of energy conversion/storage materials.

Near-Infrared responsive Carbon Nanostructures based on CholineCalix[4]arene-Gold for Photothermal Cancer Treatment

Salvatore Petralia[1], *Ludovica Maugeri[1], Valeria Consoli[1], Valeria Sorrenti[1], Gianpiero Buscarino[2], Simonpietro Agnello[2], Luca Vanella[1], Giuseppe Forte[1] Grazia Maria Letizia Consoli[3]

[1]Department of Drug Science and health, University of Catania, 95125 Catania, Italy

[2]Dipartimento di Fisica e Chimica, University of Palermo, Palermo 90133, Italy

[3]CNR-Institute of Biomolecular Chemistry, 95126 Catania, Italy

Abstract:

The development of novel chemical approaches for the fabrication of gold nanostructures with localized surface plasmon resonance (LSPR) falling in the near-infrared (NIR) region is one challenging topic in nanomaterials science. Due to their optical and photothermal properties triggered by light excitation in the therapeutic window (650−1300 nm), gold-based nanostructures are appealing candidates in anticancer nanomedicine. Here, we report a novel method to prepare water dispersible hybrid carbon-gold nanostructures with NIR-LSPR (λ 600−1000 nm) properties. The gold nanostructures were achieved in a single step by an unconventional method using NADH as a reducing agent and an amphiphilic choline-calix[4]arene derivative (Chol- Calix) forming micelles as a template. The CholCalix-Au nanostructures were characterized by UV−visible spectrophotometry, Raman spectroscopy, and atomic force microscopy. Agglomeration of the nanostructures due to multiple crosslinking interactions was observed and supported by modeling simulation. Effective anticancer photothermal-induced effect of the CholCalix-AuNPs was demonstrated on human breast cancer cells irradiated with biofriendly light at 808 nm.

Biography:

Salvatore Petralia, received the PhD in Chemistry from University of Catania (Italy), in 2003. In 2020 he joined University of Catania as Researcher of Chemistry. From 2004-2020 he was Technology Development sect. Manager at STMicroelectronics, covering several R&D positions and leading multidisciplinary teams focused on the development of nanostructured materials and chemical processes for biosensing application. The research activity over the years has covered multidisciplinary aspects of chemistry, photochemistry, nanostructured materials, biosensing and bioMEMS silicon technology. In this field he is co-author of 128 peer reviewed scientific publications, 1 chapter of book and co-inventor of 12 patent applications

Carbon Nanodots and Their Nanocomposites: A Photophysical Study

Alice Sciortino

Physics and Chemistry Department – Emilio Segrè, University of Palermo, Palermo, Italy

Abstract:

Carbon Nanodots (CDs) are an emerging family of carbon-based nanoparticles characterized by intense and tunable light absorption-emission in the visible range. Besides, their optical response is very sensitive to external agents (solvent molecules, ions in solution, nanoparticles…), a property which may be very useful for several applications, if deeply understood. For example, CD emission decreases in presence of metal ions in solution because of a high electron donor capability of CDs. In contrast, CD emission can be strongly enhanced, under certain conditions, through the interaction with plasmonic metal nanoparticles. The versatility of their possible behaviours promisingly projects the use of CDs as suitable substitutes of quantum dots in many optoelectronic or photo/electro-catalysis applications. Here, we will present a summary of our scientific work on

the photophysics of CDs. In particular, we will focus on the fundamental photophysics of two different classes of composite nanomaterials, obtained by coupling CDs to Carbon Nanotubes or Gold nanoparticles respectively, in order to show the variety of CD optical responses and the wide range of possible applications.

Biography:

Alice Sciortino took her PhD in 2019 in “Material science and nanotechnology”. Her PhD research has been carried out under a joint supervision between the University of Palermo (Italy) and the University of Bern (Switzerland). Dr. Alice Sciortino is a researcher working at University of Palermo (Physics and Chemistry department). The focus of her studies is the characterization of luminescent nanomaterials by optical investigation method including ultrafast spectroscopic techniques. Among fluorescent nanomaterials, a great part of her research is focused on the study of the photophysics of carbon-based nanomaterials as carbon nanodots and their nanocomposites.

Magnetic Activated Carbon as a Sustainable Sorbent for Removal of Antibiotic From Water

Hasan Sayğılı[1*] **and Gülbahar Akkaya Sayğılı**[2]

[1]*Vocational School of Technical Sciences, Department of Chemistry and Chemical Process Technology, Batman University, Batman, Turkey*

[2]*Department of Science, Faculty of Education, Dicle University, Diyarbakır, Turkey*

Abstract:

Tetracycline (TC) is one of the most widely used antibiotics that causes contamination of aqueous environments and has raised serious concern during the past few years. In this work, an alternative utilization of agro-industrial lentil factory waste (LFW) as raw material for the synthesis of magnetic adsorbent aiming the TC removal is proposed. The synthetized adsorbent, denominated magnetic activated carbon (MAC), was prepared by co-precipitation of copper ferrite (CuFe2O4) onto activated carbon surface. Characterization of MAC was carried out by nitrogen adsorption-desorption isotherms, X-ray diffraction, and vibrating sample magnetometer. The batch technique was used in order to demonstrate the influence of temperature and adsorption isotherm. The consequences reveal that the Freundlich model and Langmuir model are able to adequately describe the adsorption isotherm parameter. Adsorption isotherm studies on MAC revealed multilayer adsorption with Freundlich isotherm. The Langmuir isotherm model demonstrated that TC adsorption capacity on MAC was 384.62 mg g−1 at its maximum. The findings demonstrate the practical views of a facile preparation of MAC in simplifying the separation in a fast and cost-effective manner for wastewater treatment.

Biography:

Hasan SAYĞILI is currently working as an Assoc.Prof. in the Chemistry and Chemical Process Technology Department, Vocational School of Technical Sciences, Batman University, Turkey. He has an experience in the field of carbon-based materials for environmental applications. He holds a PhD in activated carbon production from biowastes from Dicle University, Turkey. His primary research interests include carbon nanomaterials, waste minimization, environmental pollution, hydrothermal carbonization, cleaner production technology and wastewater treatment. He has published 27 SCI papers.

Graphene for Interconnect Applications: Requirements and Challenges

Inge Asselberghs, Zsolt Tokei

IMEC, Leuven, Belgium

Abstract:

Different types of carbon allotropes have been proven to have unique properties. After almost two decades of intensive research on graphene, the material is named for its potential in different applications fields, ranging from composite materials, batteries, spintronic, electronic, photonics and sensor application. Depending on the application, significant different requirements are expected in terms of material properties and fabrication capabilities at an industrial scale.

In the upcoming technology nodes, Cu is challenged as the interconnect material. Many alternative metals are considered, while only a few are making it on top of the list. In this context, graphene is mentioned either a conductor, Cu-barrier, or capping layer. Once more, the requirements on the material properties, deposition and post processing conditions, and integration flows will go together to define the likeliness of industry uptake.

In this work, an overview of the status of the field will be discussed, while also providing considerations regarding the requirements and challenges for fabrication in a CMOS compatible fab.

Biography:

Inge Asselberghs is Program Manager Process and Module Innovation at imec. She received the M.Sc. and Ph.D. degrees in chemistry from the University of Leuven, Leuven, Belgium. After a Post-Doctoral Fellowship in nonlinear optics, she joined imec in 2011. Her research interest covers new materials, process set-up, and integration pathfinding from the laboratory scale to fab infrastructure. She holds the position of division leader of the 2D-experimental pilot line, an EU funded initiative working on the enablement of 2D-materials-based device fabrication in an industry-relevant environment.

Ca-Doped MgMn2O4Based Cathode Materials for Magnesium Ion Cells

Z. Osman*[1,2], N. Harudin[1,2], M.Z. Kufian[1,2] and R. Rosli[1,2]

[1] *Centre for Ionics Universiti Malaya, Universiti Malaya 50603 Kuala Lumpur, Malaysia*

[2] *Physics Department, Universiti Malaya, 50603 Kuala Lumpur, Malaysia*

Abstract:

Electrospinning is a versatile and efficient fabrication method for one-dimensional (1D) nanostructured fibers of hydrocarbons, metals, composites and metal oxides. The features of electrospun nanofibers depend crucially on technological parameters as aspect of volume ratio, viscosity, type of polymer and applied voltage. There are several combination methods of electrospinning for synthesizing electrode materials being applied such as combustion, solidstate reaction and spray drying. In the present work, Ca-doped based cathode materials were synthesized by using a combination of self-propagating combustion and electrospinning method with annealing temperature of 900°C. The electrospun nanofibers have been characterized morphologically through FESEM and XRD, and the electrochemical performance has been evaluated through galvanostatic charge discharge. The electrospinning process was carried out by using solutions of polyacrylonitrile (PAN) diluted in N,N dimethylformamide (DMF) and a cathode material with a ratio of 1:1, a uniformly nanoparticles fiber was obtained. FESEM micrographs shown that the smaller particle size of Ca-doped sample was observed when electrospinning method is applied. A smaller particle size gives a larger surface area where it is expected to facilitate in ion intercalation and de-intercalation during the charge–discharge processes, hence giving a better cycling performance of the magnesium ion cells. Therefore, electrospun Ca-doped based cathode material is a promising approach to obtain novel cathode materials product for magnesium ion cells. Biography: {Max words limit 100} Professor Dr Zurina Osman is a professor from the Department of Physics, Universiti Malaya, Kuala Lumpur, Malaysia. Her research interests focusing on energy materials, particularly polymer electrolytes and electrode materials which are used in electrochemical devices such as batteries, solar cells and supercapacitors. She has published her research works in many reputable journals. She has also involved in various administrative positions at Faculty level and University level. She has been appointed as the Head of Department, the Department of Physics, Universiti Malaya from 2019 to 2021. Since 2018, she has appointed as the Head of Research Centre (Centre for Ionics Universiti Malaya).

Graphene-doped PEDOT:PSS Acting as Hole Transport Material in Photovoltaic Device.

Teresa S. Ripolles[1,2]* Carlos Redondo-Obispo,[2,3] Sandra Cortijo-Campos3, Angel Luis Álvarez[2], Esteban Climent-Pascual[4] Alicia de Andrés[3], Carmen Coya2

[1]Institute of Materials Science (ICMUV), University of Valencia, C/ del Catedrátic José Beltrán Martinez, 2, 46980 Valencia Spain

[2]Escuela Técnica Superior de Ingeniería de Telecomunicación, University Rey Juan Carlos, C/ Tulipán s/n, 28933 Madrid, Spain

[3]Instituto de Ciencia de Materiales de Madrid, Consejo Superior de Investigaciones Científicas, C/ Sor Juana Inés de la Cruz 3, 28049 Madrid, Spain

[4]Escuela Técnica Superior de Ingeniería Industrial, Universidad Politécnica de Madrid, C/ José Gutiérrez Abascal 2, 28006 Madrid, Spain.

Abstract:

The undesirable reactions from poly(3,4-ethylenedioxythiophene):poly (styrene sulfonate) (PEDOT:PSS), which presents hygroscopic and acid character of PSS- group, reduces drastically the stability and efficiency of inverted perovskite solar cells. We developed a facile synthesis method of graphene platelets into PEDOT:PSS solution in order to block these unstable reactions. The homogenous graphene-doped PEDOT:PSS layer show up to 10 times improvements on its conductivity, maintaining high optical transmittance. Additionally, the standard CH3NH3PbI3 film grown on graphene-doped PEDOT:PSS layer exhibits large perovskite crystallite size and a reduction of PbI2 content, leading high stability over time. The hydrophobic character of graphene probably blocks undesirable reactions hampering degradation. The inverted perovskite solar cells based on graphene-doped PEDOT:PSS as hole transport layer show better photovoltaic parameters by increasing charge extraction analyzed by impedance spectroscopy. This simple and low-cost preparation method leads to a successful candidate to synthetize effective hole transport layer to be considered in optoelectronic devices.

Biography:

As a researcher, I published a total of 40 peer-reviewed papers, and the h-index is 24. I received my Bachelor Degree in Chemistry at University Jaume I (Spain). At the same university, I studied master and PhD in Nanoscience and Nanotechnology; then I moved to Kyushu Institute of Technology (Japan) as an Assistant Professor to develop all-inorganic perovskite solar cells. Then, I worked at University Rey Juan Carlos as a Jr. Research Fellow, where I studied the perovskite material properties. Currently, I am a Principal Investigator at University of Valencia. My area of expertise is lead-free tin perovskite solar cells.

Computational Modelling of Carbon Nano Tube (CNT) Based Nanocomposites

Khalid I. Alzebdeh[1*], Musa S.M. Al-Kharusi[1], and Tasneem Pervez[1]

[1]Department of Mechanical and Industrial Engineering, College of Engineering, Sultan Qaboos University, P.O. Box 33, Al-khod 123, Sultanate of Oman

Abstract:

The effective mechanical properties of Single Wall Carbon Nano Tubes (SWCNTs) are predicted using an atomistic-based continuum approach. This is achieved by equating the stored energy in a representative unit cell for SWCNT at atomistic scale to the strain energy of an equivalent continuum medium under prescribed boundary conditions. At macroscale, the SWCNT is taken as cylindrical continuum solid with transversely isotropic mechanical properties. A comparison of elastic constants obtained from current modelling concur with results reported in literature. With the multifunctional properties of these nanomaterials, determination of their elastic moduli will facilitate a better design of nanocomposite materials. Furthermore, a new finite element model nanocomposites is developed taking into account of all possible interactions between individual atoms within SWCNT and the surrounding polymer. The interatomic potential functions are used to derive the constitutive behavior of the finite elements thereby reducing the computational complexity of the problem while maintaining the accuracy of the model. This nano-model is capable to create a link between nanoscale reinforcement material and surrounding polymer matrix material. Results revealed that the effective properties of the underlying nanocomposite are strongly dependent on size and chirality of embedded SWCNT, the thicknesses of the interfacial and polymer layer, and the stiffness ratio.

Biography:

Khalid Alzebdeh has completed his PhD from Michigan State University, USA and postdoctoral studies from Michigan State University and Georgia Institute of Technology, USA. He is currently an Associate Professor at the Department of Mechanical and Industrial Engineering, Sultan Qaboos University, Sultanate of Oman. He has published more than 40 papers in reputed journals and has been serving as an editorial board member of several journals. Dr. Alzebdeh is a registered Professional Engineer in the state of Minnesota, USA. His current research interests include technology innovation, processing of advanced materials, which include, bio-composites, nano-structured and cellular materials.

Unearthing the Hidden Territory of π-conjugated Thiocarbonyl Chemistry

Yi-Lin Wu

School of Chemistry, Cardiff University, UK

Abstract:

Promising applications of thiocarbonyl derivatives (R2C=S) in biomedicine, optoelectronics, and photocatalysis were not revealed until recently. Although these compounds can be easily derived from their carbonyl analogues (R2C=O), which are widely recognized as organic electron-accepting materials, a comprehensive understanding of the structural,

electronic, and (photo-) reactivity aspects of thiocarbonyl remains relatively limited. With the evidence from experimental, computational, and statistical analysis, compelling evidence has emerged regarding the significance and intricate roles of the orbital orientation, energy, and size of the sulfur atom in thiocarbonyl. I will discuss how the non-covalent interactions, electronic properties, luminescent behavior, and reactivities of π-conjugated materials can be controlled or enhanced when introducing thiocarbonyl functionalities alongside other structural modifications.

Biography:

Yi-Lin Wu is a Lecturer in Materials Chemistry at Cardiff University. He obtained his doctorate from ETH Zürich in 2012 under the guidance of François Diederich. Following his time in Zürich, he received the Swiss National Science Foundation Fellowship to pursue postdoctoral research with Michael Wasielewski at Northwestern University, where he was subsequently appointed as Research Associate Professor (2017). He takes the combined synthetic and spectroscopic approaches to interrogate the interplay between the self-assembly nanostructures and excited-state electron/energy dynamics in materials relevant to biology and photovoltaics.

Polymer-Metal & Polymer-Ceramic hybrids materials in 3D-FDM printing: structuro-functional versatility

Séverine A.E. Boyer[1*], Alain Burr[1]

[1]*MINES Paris PSL, CEMEF CNRS 7635, Sophia Antipolis, France*

Abstract:

Inspiring polymer-based research approaches give rise to novel processing of metals and ceramics in Fused Deposition Modelling (FDM) [DOI: 10.1108/RPJ-05-2019-0133]. In our study, polylactic acid (PLA) loaded with metallic and with ceramic particles were printed with a ToolChanger & Motion System (E3D, UK). The experience around several fundamental stages in shaping by 3D printing is detailed and presented, i.e. the definition of a 'scaffold structures' ceramic, "thermo-chemical debinding sequences" and "high temperature curing and sintering". The use of a refractory powder bed during thermal debinding sequences gives sintered structures capable of supporting their own weight seen as a compressive force. Discussion highlights also the effect of gas confinement during the thermal scheme. In addition to the stability of the scaffold structures, the shrinkage can be anisotropic, depending of the orientation of the printing pattern, abstraction done of the orientations of the metallic or ceramic fillers that could induce a potential cause of the anisotropy. The application of ceramic and metal FDM permits to extend the versatility to complex scaffolds. Different targeted applications will be presented through some achievements. Acknowledgments: IMT with ALaRM ("Automatization of Laboratory Equipment through Rapid Manufacturing of Biopolymeric Multi-Material Parts") and

Roaming (“A Roadmap for Industrializing Additive Manufacturing”) projects.

Biography:

Séverine A.E. Boyer activities conduct fundamental and finalized studies on the mechanisms of the polymorphogenesis/deformation of structural synthetic and natural organic systems to develop or to recycle functional and hybrid materials. Are developed chains of original experimental and numerical models linking the multi-scale structure, from chemical-molecular size to macroscopic size, in complex and extreme environments. International recognitions: Thesis - ‘William F. Giauque Student Award, CALCON 2003 (USA)‘; Young Researcher - “ICTAC Young Scientific Award, ICTAC 2012 (Japan)” (1st time awarded to a French researcher); ‘First Place Best Poster, PPS 2019 (South Africa)‘; and Awards deserved to her collaborative colleagues.

Graphene Filler Influence on Thermal, EMI Shielding, and Electrical Properties of Polymer-based Nanocomposites

Anna Łapińska[1*], Natalia Grochowska[1,3], Klaudia Żerańska[1], Anna Dużyńska[1], Kamil Dydek[2]

[1]Warsaw University of Technology, Faculty of Physics, Koszykowa 75, 00-662 Warsaw

[2]Warsaw University of Technology, Faculty of Material Science and Engineering, Wołoska 141, 02-507 Warsaw

[3]Warsaw University of Technology, Faculty of Chemistry, S. Noakowskiego 3, 00-664 Warsaw

Abstract:

In an era of advanced electronics, issues like adequate electromagnetic interference protection and effective heat dissipation are crucial due to the malfunctioning that they may cause. The high density of electronic elements forced by the miniaturization trend intensifies problems, and a solution is urgently needed.

Polymer nanocomposites are materials able to combine multiple features in one and may be treated as alternatives to currently existing solutions in providing electromagnetic compatibility (EMC) or effective heat dissipation. Therefore, comprehensive studies of electrical, thermal and electromagnetic shielding properties induced by graphene nanoplatelets are shown here.

Different preparation method had been employed like powder mixing, and hot pressing; extrusion, or 3D printing (FDM).

The following example results have been achieved: thermal conductivity, κ = 5.34 W/mK, obtained for PVDF/GNP samples, which gives 2800% enhancement compared with

pure PVDF matrix, EMI shielding effectiveness, SETOT = 17 dB at 5 GHz, with absorption as the primary shielding mechanism for THV/GNP/MWCNT composite, and electrical conductivity σ = 40 S/cm for PVDF/GNP composites.

The finding presented here is the first step in developing multifunctional material with outstanding EMC protection features and thermal properties that may be applied in airborne and space.

Biography:

ANNA LAPINSKA – a young, female physicist with certified knowledge in Agile Project and Program Management, Change Management, Management of Risk, IPR protection. The beneficiary of national programs aimed at young scientists. Currently, the PI of such a program concerning with multifunctional polymer nanocomposite production for airborne and space. Founder and CEO in start-up to be (opening date: 2023)) with the main activity of manufacturing thermally conductive composite materials for effective cooling.

Utilization of carbon derived materials for Microextraction of environmental pollutants from food and water samples prior to instrumental analysis

Mohamed A. Habila[1*], Adibah M. Almutairi [1], Zeid A. AlOthman[1], and A.Y. Badjah Hadj Ahmed[1]

[1]*Department of Chemistry, College of Science, King Saud University, P.O. Box 2455, Riyadh 11451, KSA.*

Abstract:

International organizations such as the Food and Agriculture Organization (FAO) and the World Health Organization (WHO) have established a food national controlling system which gives a guideline for the developing countries to improve food quality and provide a healthy meal, especially after the appearance of foodborne diseases and their hazards. To ensure the quality of available food and agreement of the contaminant concentrations with the allowed limits stated by FAO and WHO, it is important to develop a suitable and reliable analytical system for screening of the most toxic substances in food. The proposed analytical method should be accurate and sensitive even when applied for samples from different matrices. This research work aims to utilize the carbon materials for development of microextraction procedures for precontraction of environmental pollutants. This serve for sample purification as well as enrich the concentration of the trace contaminates from food or water samples. Carbon materials possess a stable structure with porous nature which facilitate the adsorption of pollutants from food extract and isolate the targeted analytes. The second step is to elute the loaded analyte and introduce to the instrumental analysis such as chromatographic or spectroscopic derived techniques. The

tested pollutants include organic contaminates such as carbaryl, malathions, metals and dioxins derivatives.

Biography:

Mohamed A. Habila works as associate professor of chemistry, King Saud University. He is a board member of Saudi Chemical Society. He is interested in nanotechnology for development of clean methods for separation of environmental pollutants, improvement of solid phase extraction and dispersive microextraction, water and wastewater treatments, and synthesis and characterization of nano-porous multifunctional core-shell structures for various applications. Dr Habila supervised more than 7 MSc and PhD. Students. Dr Habila has published more than 110 scientific articles, and has delivered more than 25 public lectures in chemistry in local and international conferences and scientific events. He received IAAM Young Scientist Medal, 2022, from International Association of Advanced Materials. Acknowledgements The authors extend their appreciation to the Deputyship for Research & Innovation, Ministry of Education in Saudi Arabia for funding this research work through Institutional Funding Program For Research and Innovation (project no IFKSUDR_F122)

3D Printed Electrodes for High Performance Li-Ion Batteries

Vinay Gupta[1*] and Shanmugam Kumar[2]

[1]Department of Physics; [2]Dapartment of Mechanical Engineering, Khalifa University of Science and Technology, Abu Dhabi, United Arab Emirates

Abstract:

3D-printed porous PLA/LiF/CNT-based nanocomposite electrodes for high performance Li-Ion batteries were realized. The LFP/PLA/CNT cathodes with different CNT loadings (3, 5, 7, and 10 wt%), interconnected porosities (10%, 30%, 50%, and70%), and thicknesses (100, 200, and 300 μm) were 3D printed by utilizing in-house nanoengineered filaments. The nanocomposite cathodes exhibit a specific capacity of 155 and 127 mAh g−1 and an areal capacity of 1.7 and 4.4 mAhcm−2 for 100 and 300 μm thick electrodes, respectively, at 0.40 mA cm−2. Moreover, we observe that the specific capacity of the thicker electrode (300 μm) enhances from 125 to 151 mAh g−1 without any loss in areal capacity with an increase in porosity. The results demonstrate that the effect of thickness on the specific capacity can be negated by engineering desired porosity, and thereby specific and areal capacities can simultaneously be enhanced. The convergence of emerging nanoscale additive manufacturing and the ability to design ever-more tightly controlled nano-and micro-architected hierarchical structures will enable the creation of high-performance LIBs.

Biography:

VINAY GUPTA is working as an Assistant Professor in the Department of Physics at Khalifa University, Abu Dhabi, UAE. He has research interests in Solid state physics, organic and perovskite solar cells, supercapacitors, lithium-ion batteries, and water filtration. He is a recipient of several international and national awards, including the prestigious Shanti Swarup Bhatnagar (SSB) award (2017), and the Thomson Reuters India citation award (2015)

Graphene Functionalization of Polyrotaxane Encapsulated PEG-based PCMs: Fabrication and Applications

Guang-Zhong Yin[1, 2, *] Xiao-Mei Yang [2], Alba Marta López[2] Javier García Molleja[2], Mei-Ting Wang[3] De-Yi Wang [1, 2]

[1]Escuela Politécnica Superior, Universidad Francisco de Vitoria, Ctra. Pozuelo-Majadahonda Km 1.800, 28223 Pozuelo de Alarcón, Madrid, Spain

[2]IMDEA Materials Institute, C/Eric Kandel, 2, 28906 Getafe, Madrid, Spain

[3]Shenyang University of Chemical Technology, Shenyang 110142, China

Abstract:

In recent decades, phase change materials (PCMs) have received much attention in thermal regulation of electronic devices. But the main limitation for the use of organic PCMs are the low thermal conductivity and leakage during the phase change process. This work will try to improve these limitations, to increase thermal conductivity of the leakage proof PCM formed by a polyrotaxane that serves as a support material to encapsulate Polyethylene glycol (PEG) as work substance. For this purpose, different contents of graphene nanoplatelets (GNP) would be blended. To facilitate its post-industrial production and to meet ecological standards, the synthesis of this PCM is simple and only use water as a solvent. The PCMs can be thermal processed conveniently by hot press. Furthermore, the PCMs created in this work achieves a high thermal performance with high enthalpy values (132.9 -142.9 J/g), due to the action of GNPs as thermal conductive fillers, also experiencing an increase of 60%-257% in thermal conductivity values the higher the GNP content, and also shows a great shape stability and no leakage during its phase change. These improvements solve the main problems of organic PCMs thus making PLR-PEG-GNP based materials a good candidate to be used as thermal energy storage material in industrial applications as thermoregulator of solid-state disks or realizing the “shaving peaks and filling valleys” effect for thermoelectric generator.

Biography:

Guang-Zhong Yin received his PhD degree in Materials Science and Engineering at Beijing

University of Chemical Technology in 2016. Currently, he is a researcher at Francisco de Vitoria University (Spain) and an adjunct researcher at IMDEA Materials Institute (Spain). His research interests include polymeric functional materials, phase change materials and bio-based fire-safe nanocomposites. He published 56 peer-review articles or chapters (40+ of them are in JCR Q1 journal). He was selected as Youth Editorial Board Member for the international journals, such as, Nano Research Energy and Nano Materials Science. He was selected as MSCA fellow with full marks (100/100).

Study of Thermal Decomposition of Cycloalkanes Using Flash Pyrolysis Vacuum Ultraviolet Photoionization Mass Spectrometry

Kuanliang Shao and Jingsong Zhang*

University of California, Riverside, USA

Abstract:

Cycloalkanes are important components in hydrocarbon fuel usage and transformation. In this work, thermal decomposition of several cycloalkanes, cyclopentane, cyclohexane, and cycloheptane, at temperatures ranging from 295 K to 1310 K were studied using flash pyrolysis coupled with vacuum ultraviolet (118.2 nm) photoionization time-of-flight mass spectrometry. The experimental results revealed that the major initiation reactions of the cycloalkane decomposition were C-C bond fission leading to the formation of diradicals. The diradicals could isomerize to 1-alkenes and decompose into several fragments. The diradicals could also undergo direct dissociation; the unique fragments via the diradical intermediates were observed, serving as evidence of the diradical mechanism. Quantum chemistry calculations at UCCSD(T)/cc-pVDZ level of theory on the initial reaction pathways of the cycloalkanes were performed and found to be consistent with the experimental conclusions. These studies help provide more insight into the pyrolysis mechanisms of cycloalkanes.

Biography:

Jingsong Zhang is a Professor of Chemistry at University of California, Riverside. His research focuses on chemical reaction kinetics and mechanisms important in combustion and atmospheric chemistry. He received B.S. degree in Chemical Physics from University of Science and Technology of China (1987) and Ph.D. degree in Physical Chemistry from University of California, Berkeley (1993). In 1993-1996, Dr. Zhang was a postdoctoral fellow at University of Southern California. In 1996, Dr. Zhang started as an assistant professor in the Department of Chemistry and an assistant research chemist at the Air Pollution Research Center (APRC) at University of California, Riverside.

Comparison of GaAsSb Nanowires-based Near-Infrared Photodetectors in the Axial and Core-Shell Configurations

Shanthi Iyer

North Carolina A&T State University, Department of Nanoengineering, 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. Relaxation of lattice mismatch constraints in this configuration permits the implementation of various architectures, many exclusive to this geometry. These, combined with their remarkable quantum, surface, and outstanding optical absorption properties, allow innovative bandgap engineering of the NW-based heterostructures to achieve high-performance III-V-based optoelectronic devices integrated on mainstream Si platforms.

This talk will be focused on the Ga-assisted molecular beam epitaxial growth of GaAsSb nanowires on (111) Si substrate in axial and core-shell architectures. A comparison of the performance of NW-based photodetector devices, namely n-i-p junction and avalanche photodetectors in axial and core-shell configurations, will be presented. These devices in the near-infrared regime cover high-impact applications across wide-ranging fields, from remote sensing to imaging to communication.

Biography:

Shanthi Iyer, Professor in the Nanoengineering Department at the Joint School of Nanoscience and Nanoengineering, has initiated and developed NCA&TSU's state-of-the-art 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.

Cyclodextrin-Based Liquid Crystals and Their Applications

Chang-Chun Ling* and Austin Che, Jayar Espejo

Department of Chemistry, University of Calgary

Abstract:

Cyclodextrins (CDs) constitute a special class of glucose-based macrocyclic hosts with a truncated cone-shaped geometry, they are water-soluble and biodegradable and have foundwidespread utilities in pharmacy, agriculture, and many other indistries. During

recent years, we have developed several families of amphiphilic CD derivatives capable of forming thermotropic liquid crystals; these systems have polar oligoethylene groups placed at either the primary or secondary face of β-CD, and apolar aliphatic chains on the opposite face. The role that β-CD macrocycle serves is to pre-organize the hydrophobic from hydrophilic regions and separate them to facilitate a nanophase segregation. These systems have found to be capable of self-assembling into different mesophases at wide temperature ranges, such as smectic and hexagonal columnar. The synthesis and thermotropic properties of this class of novel materials will be presented.

Biography:

Chang-Chun Ling graduated with a BSc degree in Chemistry from the University of Lanzhou (1986) and PhD from the Université de Paris Sud (1991). After spending several years as a post-doctoral fellow or research associate at the University College Dublin, Université Pierre et Marie Curie, University of Alberta, Alberta Research Council, he was appointed as an Assistant Professor at the Department of Chemistry, University of Calgary in 2006, he become a full professor since 2021. His current research is focused on the development of carbohydrate-based therapeutics to treat infectious disease and autoimmune conditions and carbohydrate-based nanomaterials for different applications.

An Inverse Electron Demand Diels-Alder Reaction for Fullerene and Metallofullerene Functionalization

Jianyuan Zhang* and Yue Sun

Rutgers, The State University of New Jersey, USA

Abstract:

Chemical functionalization of fullerenes is a powerful approach to introduce desirable properties. Among the methods to functionalize fullerenes, fullerenes typically play an electron-accepting role, which leads to somewhat consistent reactivity and regioselectivity. To functionalize inert fullerene and metallofullerene species, and to access new regioselectivity, we developed an inverse electron demand Diels-Alder (IEDDA) reaction where fullerene/metallofullerenes are electron donors. In this presentation I will discuss our effort in the new IEDDA reaction on C60, C70 and metallofullerene Lu3N@C80.

Biography:

Jianyuan Zhang received his undergraduate degree from Beijing Normal University. After completing his PhD program studying fullerenes and metallofullerenes at Virginia Tech, and two postdoctoral studies at University of Washington and Massachusetts Institute of Technology, he started his independent research at Rutgers University – New Brunswick. The research of the Zhang group includes the chemistry, physical properties, and biomedical application of fullerenes and metallofullerenes.

Reactive Adsorption of Small Sulfur Compounds on Ruthenium Supported Graphene – an Ultra-high Vacuum Surface Science Study

T. Stach, U. Burghaus*

Department of Chemistry and Biochemistry, North Dakota State University, Fargo, North Dakota, USA

Abstract:

The molecular and reactive adsorption of small sulfur compounds on graphene grown on ruthenium(0001) (hereafter denoted as Gr/Ru) was characterized at ultra-high vacuum (UHV) conditions using Auger electron spectroscopy (AES) and multi-mass reactive thermal desorption spectroscopy (RTDS). Detection of the parent masses in RTDS indicates the presence of a molecular adsorption pathway for all compounds studied. Interestingly, in addition extra masses were detected by RTDS which are absent in the gas-phase fragmentation pattern of the probe molecules, i.e., RTDS indicates the formation of decomposition products. Furthermore, AES detected sulfur adsorbed on Gr/Ru after the RTDS experiments. Thus, both techniques RTDS and AES show consistently that the compounds dissociate on Gr/Ru. Importantly, according to AES, Gr/Ru remains intact. In other words, the carbon signal in AES spectra does not change due to the adsorption of the sulfur compounds. Two different synthesis procedures were used to nanofabricate Gr/Ru which leads to the formation of grain boundaries (without vacancy defects) in Gr in one case and generates defect free Gr/Ru in the other case. The reaction rates were unaffected by the defect density which rules out defects as the active sites for the decomposition of the sulfur compounds. Part of the results were published in J. Vac. Sci. Technol. A, 39 (2021) 042201. The application of graphene as a carbon catalyst was demonstrated which may lead the way to the design of metal free catalysts (see e.g., Current Physical Chemistry, 2022, 12, 2-10).

Biography:

Uwe Burghaus' research is focusing on experimental surface chemistry. His studies include projects on nanocatalysis, heterogeneous catalysis, molecular beam scattering, adsorption dynamics, kinetics, and spectroscopy (AES, XPS) for studying materials including metal oxides, supported nano metal/oxide clusters, nanoparticles, nanotubes, bimetallic systems, nanocarbon (CNTs, graphene), and inorganic nanostructures (nanotubes, inorganic fullerenes). He was originally educated as a physicist, but he moved into the physical chemistry field. He is faculty at NDSU (Fargo, ND, USA) since 2003, and graduated in 1995 from the Fritz-Haber Institute of the Max Plank Society in Berlin, Germany

A Molecular Rationale for the Exotic Photophysical Properties of Curved Nanographenes

Inés Corral[1*], Fernando Romeo-Gella[1], Lara Martínez-Fernández[1] Sergio Ramírez-Barroso[2,3], Jesús Manuel Fernández-García[2], Siyang Feng[3], David García-Fresnadillo[2], Nazario Martín[2,3], Reinhold Wannemacher[3]

[1]Universidad Autónoma de Madrid, Spain; 2Universidad Complutense de Madrid, Spain; IMDEA Nanoscience, Spain

Abstract:

The optical properties of p-conjugated organic systems have attracted the attention of the material science community in the last decades for their potential use as advanced optoelectronic devices.[1] Among organic nanostructures, nanographenes hold particular interest due to their electronic bandgap and visible photoluminescence, which can be adjusted by modifying the size, shape, terminal groups, or chemical composition of their sp2 carbon network.[2] A further twist in the design of novel nanographenes with unique electronic and optical properties relies in the change of their curvature by incorporating five, seven or eight membered rings into the hexagonal lattice of these systems.[3]

The aim of this contribution is to provide an overview of the main photophysical properties of selected members of the family of nanographenes consisting of corannulene and hexabenzocoronene fragments, with different degrees of constraint of the helicene. These systems were found to present multiple emission and remarkable singlet oxygen yields.[4] In addition, thermally activated delayed fluorescence (TADF) in a limited temperature range has been also reported for these systems, suggesting to a quite complex potential energy landscape, with an intricate interplay between singlet and triplet excited sates. Resorting to Density Functional Theory calculations, we have mapped the topography of the excited and ground potential energy surfaces and modelled the absorption and emission spectra of these systems, establishing a mechanistic frame for the experimental observations.

Biography:

[1] See for instance: F. Yuan, Y.-K.Wang, G. Sharma et al. Nat. Photonics 2020, 14, 171; X. Wang, X. Zhang, X. Gu et al. Adv. Opt. Mater. 2020,8, 2000239.

[2] L. Li, G. Wu, G. Yang, J. Peng, J. Zhao, J.-J. Zhu, Nanoscale 2013, 5, 4015.

[3] J. M. Fernández-García, P. J. Evans, S. Medina Rivero, et al. J. Am. Chem. Soc. 2018, 17188.

[4] Sergio Ramírez-Barroso, Fernando Romeo-Gella, Jesús Manuel Fernández-García, Siyang Feng, Lara Martínez-Fernández, David García-Fresnadillo, Inés Corral, Nazario Martín, Adv. Mat. 2023, https://doi.org/10.1002/adma.202212064.

From 2D graphene to Functional Materials Via Computational Design

Zhao Qin*[1,2] and Kamalendu Paul[1,3]

[1]Laboratory for Multiscale Material Modelling, Syracuse University, 151L Link Hall, Syracuse University, Syracuse, NY 13244, USA

[2]Department of Civil and Environmental Engineering, Syracuse University, 151L Link Hall, Syracuse University, Syracuse, NY 13244, USA

[3]Department of Physics, Syracuse University, 151L Link Hall, Syracuse University, Syracuse, NY 13244, USA

Abstract:

Ultrathin 2D nano materials like graphene, MoS2 and MXene are highly versatile due to their high strength, thermal and electrical conductivity. Understanding the structure-mechanics relationships in architected materials composed of these building blocks is essential for using the same material to achieve better functionality. Here, we use multiscale modeling and computation to investigate the mechanics of a series of hierarchical carbon nanoarchitectures with structural features quantitatively characterized. Inspired by natural and architected 3D composites of high mechanical toughness, we introduce architected defects to the 2D materials and study their fracture in molecular dynamics simulations. We find that the length of the defects in the shape of parallel bridges is crucial to fracture toughness, as long bridges can significantly increase the toughness of graphene and MoS2 but decrease the toughness for MXene, while the short bridges show opposite effects. This strategy can increase the toughness of 2D materials without introducing foreign materials or altering the material chemistry, providing a general method to enhance their mechanical performance.

Biography:

Dr. Zhao Qin is working as an Assistant Professor at Department of Civil and Environmental Engineering at Syracuse University, USA. His study focuses on structure-function relationship of nano and biological materials of hierarchical structures. His lab is currently working toward combining experiments and multiscale computational tools for functional biocomposite designs through natural processes. He has published over 100 papers and received a 2022 CAREER Award from the National Science Foundation.

Evaluating Electrolyte Decomposition at Graphite and Graphite-Blended Electrodes Using Symmetric-Cell Techniques for Long Cycle-Life Li-ion Batteries

Zilai Yan[1,3]* and Mark N. Obrovac[1,2]

[1]Department of Chemistry, Dalhousie University, Halifax, N. S, B3H 4R2, Canada

[2]Department of Physics and Atmospheric Science, Dalhousie University, Halifax, N. S, B3H

4R2, Canada

[3]Current address: Solid Energy Systems, LLC, Woburn, Massachusetts, United States 01801

Abstract:

Graphite-based electrodes have been dominantly used in Li-ion battery systems as the negative electrode, due to their high specific/volumetric capacity, low average potential, and high reversibility. [1] The demand for a better battery, particularly towards higher energy density, has significantly driven the development of new negative electrode materials, such as Si-alloys, and new electrolyte systems. These promising electrode materials are preferably blended with graphite in more commercially relevant electrodes. It is a common routine to test the cycling performance of new electrode/electrolyte systems, to estimate their cycle life in practical batteries. Typically, the electrode of interest is paired with a Li metal electrode (assembled as half cells) or a positive electrode (assembled as full cells). Unless expensive high-precision chargers are used, the irreversible signal needs to accumulate over months or years to measure. This sluggish feedback greatly hinders the progress towards longer cycle-life batteries.

Symmetric cells are a cell format including two identical working electrodes. This special format holds superior advantages in efficiently measuring the irreversible capacity without the use of high-precision chargers and avoiding interference from a different electrode. This talk will introduce the use of symmetric-cell techniques to probe the electrolyte degradation at graphite and graphite-blended electrodes of Li batteries and discuss the progress in cell assembly and data analysis to achieve reliable results. [2, 3, 4] The general considerations and conclusions of this talk are widely applicable to other battery systems, such as Na, K, Mg, and Ca batteries.

References:

[1] Mark N. Obrovac and Vincent L. Chevrier. Chemical reviews 114.23 (2014): 11444-11502.

[2] Zilai Yan. Journal of The Electrochemical Society 170 (2), 020521

[3] Zilai Yan, Y Liu, TD Hatchard, B Scott, Y Cao, S Cao, Mark N. Obrovac. Journal of Power Sources 530, 231281

[4] Zilai Yan, C Wei, MN Obrovac. Journal of Power Sources 438, 226955

Biography:

Zilai Yan obtained his Ph. D. from Dalhousie University (Canada) (2021) and worked as a postdoc at Princeton University (2022-2023) before joining SolidEnergy Systems, LLC as a senior scientist. He is the author of 10 refereed journal papers. His research interest includes battery techniques and electrochemistry in general and methodologies that can provide accurate and unbiased results.

Advanced Two-dimensional Materials for Electrochemical Energy Storage and Conversion

Fei Yao[1*], Sichen Wei[1], Maomao Liu[2], Yu Fu1, and Huamin Li[2]

[1]*Department of Material Design and Innovation, University at Buffalo, USA,*

[2]*Department of Electrical Engineering, University at Buffalo, USA*

Abstract:

The development of clean energy technology is indispensable in mitigating climate change and meeting future energy demand. Electrochemical energy strategies including energy storage and electrocatalysis have drawn tremendous attention lately. Two-dimensional (2D) post-graphene materials (PGMs) including transition metal dichalcogenides (TMDs) and transition metal carbides/nitrides (i.e., MXenes) have demonstrated enormous potential as electrode materials due to their large surface area, superior chemical stability, and versatile material engineering possibilities. Nevertheless, their practical application is hindered by the intrinsically low electrical conductivity arising from the semiconducting nature of 2H phase TMDs and the undesired oxidation of MXene. In this talk, I will introduce effective strategies for PGMs structure-property engineering with the aim of optimizing the electrochemical performance for the development of the next-generation Pt-group-metal-free electrocatalysts and lithium-ion battery anodes.

Biography:

Fei Yao received her dual Ph.D. degree in Energy Science from Sungkyunkwan University (SKKU), Korea, and in Physics from Ecole Polytechnique, France, in 2013. Currently, she is an assistant professor in the Department of Materials Design and Innovation at the University at Buffalo. Her research interests include low-dimensional materials synthesis, property engineering, and their applications in electrochemical energy storage and conversion, electrochromic devices, and electronic devices.

Soft Matter Systems Investigated by Small-Angle X-Ray Scattering

Cristiano Luis Pinto de Oliveira[1*]

[1]*Physics Institute, University of São Paulo, São Paulo, SP, Brazil*

Abstract:

Soft matter is a fascinating research field. In this topic one finds an enormous number of systems and products we consume and use in our everyday life. Food, washing products, plastics, liquid crystals are just few examples of such systems. One striking property of soft-matter is its ability of self-assembly in highly hierarchic structure. Surfactant systems, for example, in aqueous media can form different types of micelles or supramolecular

arrangements, depending on the system characteristics (concentration, temperature, etc). The structural investigation of this type of system has to be performed in such a way that does not disturb its thermodynamic equilibrium. Scattering methods, in particular small-angle X-ray scattering (SAXS), are very suitable for these studies since it has a minimum interaction with the system, preserving the equilibrium. Even though the experimental data provides information in the so-called reciprocal space, requiring the use of specialized modeling and analysis methods, the information reflects a reasonable ensemble average, since the data results from the contribution of a very large number of scatterers. In this talk several examples of the use of the SAXS methods for investigating soft matter systems, with the development of advanced modeling methods, will be shown. Advanced studies of lipid membranes, protein systems, nanoparticles, liquid crystals, human hair and several other examples are presented and discussed [1]

Biography:

Undergratuation in Applyed Physics (1998), teaching habilitation (2004), MsC in Physics (2001) and PhD in Physics (2005) all from State University of Campinas (UNICAMP). Postdoc at Brazilian Synchrotron Light Laboratory (2005-2006) and at Chemistry Department of Aarhus University/Denmark (2006-2009). Assistant professor at Aarhus University with a Lundbeck Fellowship (2009). Professor at the institute of Physics, University of São Paulo since 2010. His expertise are soft matter, condensed matter, biophysics and material sciences with large experience on scattering methods, experimental and theoretical developments. Lecturer of dozens of invited talks wordwide, author of more than 140 articles, with Hfactor 34.

Photochemistry by Molecular Dynamics

Dmitri S. Kilin*

Department of Chemistry & Biochemistry, North Dakota State University, Fargo, ND, USA

Abstract:

Several aspects of electromagnetic field to matter interaction are addressed by computational modeling of transitions between ground and excited state potential energy surfaces, driving molecular system away from the equilibrium. Photoinduced bond breaking events are enhanced for molecular systems placed in the center of resonant microcavity via formation of a bound matter-to-field polaritonic state. A description of matter-to-electromagnetic radiation interaction is is integrated with on-the-fly ab initio molecular dynamics and electronic structure methods. Validity and predictive power of several algorithms applicable for the IR and UV-vis range excitations are discussed. A vibrational polariton algorithm is tested by exploring an ensemble of hydrogen fluoride molecules in the IR cavity. A time-dependent excited state dynamics (TDESMD) algorithm is applied to a several UV-photoactivated reactions ranging from formation of

luminescent defects at surface of carbon nanotubes [1] to photodegradation of polymers and plastics [2] to photopolymerization of molecular precursors for fabrication of silicon nanostructures. [3] Introduced TDESMD algorithm seems most useful in the limit of multiple reaction pathways and multiple products. Validation of TDESMD predictions is based on comparison of computed and measured distribution of products and mass spectra. Optical properties, such as lifetimes, and photoluminescence quantum yield of the molecular structures are computationally evaluated through implementation of nonequilibrium dynamics of excited electronic states.[4] Support of NSF-1944921 is acknowledged.

[1] Nature Comm. 2022, 13 (1), 4439.

[2] J. Phys. Chem. Lett. 2022, 13 (19), 4374-4380.

[3] J. Phys. Chem. Lett. 2018, 9 (15), 4349-4354.

[4] J. Phys. Chem. Lett. 2022, 13 (39), 9210-9220.

Biography:

D. Kilin completed his B.S. and M.S. degrees in physics at Belarus State University, (Minsk, Belarus) and received his doctoral degree from Chemnitz University of Technology, (Chemnitz, Germany) in Michael Schreiber's group in 2000. After subsequent postdoctoral internships with Jeff Cina at the University of Oregon, Oleg Prezhdo at the University of Washington, and David Micha at the University of Florida, he joined the University of South Dakota as a research faculty. In 2015 he became an assistant professor, and in 2021 an associate professor in the Department of Chemistry and Biochemistry at North Dakota State University.

Layered Rotated Graphene Promises Breakthrough in the Efficiency of Li-ion Batteries

Tereza M. Paronyan

HeXalayer, LLC, Louisville, KY, USA

Abstract:

Li-ion batteries (LIB) dominate the rechargeable battery market due to their ability to restore the charge and provide consistency in the power. Carbon-based materials remain the most reliable anode in such a battery for long-term cycling and safety. Layered graphene consisting of many rotated layers has been demonstrated as a most reliable high-capacity anode for Li-ion batteries [1-3]. HeXalayer develops a new innovative technology of scaling up a new class of rotated multilayer graphene with a unique structural property that is beneficial anode for high-energy density Li-ion batteries. We study the correlation of

these graphene structural and binding features with Liintercalation process. The analysis of Raman spectra, X-ray diffraction, and HRTEM/SAED results revealed a novel hidden structural feature inside of graphene layers showing unusual stacking order that results high rate of Lithium intercalation therefore high-capacity Li-ion batteries. This rotated graphene-based anode exhibits extremely high (up to 2,000 mAh/g) reversible capacity in LIB throughout 300 cycles with over 98% Coulombic efficiency. It promises to bring into the market a new class of LIBs that would deliver over 600Wh/kg specific energy with reduced battery weight. References [1] T.M. Paronyan et al., Incommensurate graphene foam as a high-capacity Lithium intercalation anode. NATURE, Sci. Rep. 7, 39944; doi: 10.1038/srep39944 (2017). [2] T. M. Paronyan et al. Exceptional Lithium Intercalation Capacity of Incommensurate Graphene Foam in Rechargeable Batteries- ECST V77.p 311-320 (2017) [3] T.M. Paronyan Weakened interlayer interaction of incommensurate graphene as a key factor for superior lithium intercalation. JMR 36, 2872–2880 (2021).

Nanomechanical Characterization of Carbon Fiber and Composites

Dayakar Penumadu[1*] and Dr. Vivek Chawla[2]

[1]Fred N. Peebles Professor, [2] Post-Doctoral Scholar, University of Tennessee, Knoxville, TN USA

Abstract:

Carbon fiber reinforced polymer and ceramic composites are exceptional materials with low weight and large stiffness and strength. Nano-mechanical testing provides unique opportunity to evaluate tensile behavior of single carbon fibers, interface/interphase shear strength with matrix, and much insight into fracture toughness directly. Such measurements are essential to provide detailed material parameters for use in predictive approaches of macroscopic behavior of fiber reinforced composites. Since interface is essential for optimizing mechanical and thermal transport for effective composite performance, nanoindentation techniques provide valuable insight. This presentation will summarize the latest progress in relating manufacturing science, structure, process, property relationships of carbon fibers and its composites and will demonstrate a case study involving the role of environmental degradation studies using such novel techniques for composites exposed to harsh sea environment.

Biography:

Penumadu has been a faculty member in the Department of Civil & Environmental Engineering at the University of Tennessee, Knoxville (UT) since fall 2001. He currently holds Fred N. Peebles professorship and the Institute for Advanced Materials and Manufacturing (IAMM) Chair of Excellence position. He served as the Head of the Department of Civil and Environmental Engineering from 2007 to 2014. Prior to joining UT, he was a faculty member at Clarkson University for 8 years. His research interests include: carbon fiber reinforced polymeric composites and sandwich structures, environmental degradation, and multi-scale mechanics.

Multi-Element Scanning Thermal Analysis of Solid Carbonaceous Samples

Yuch-Ping Hsieh

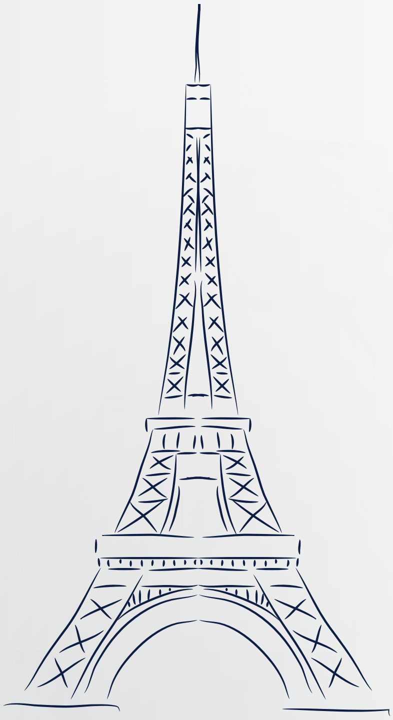
Florida A&M University, USA

Abstract:

Analytical technologies for solid samples are much more limited in comparison to those for liquid or gaseous samples. We have developed a Multi-Element Scanning Thermal Analysis (MESTA) technology that can sensitively and conveniently analyze solid carbonaceous samples. MESTA technology characterizes the thermochemical property of a solid sample by its C, N, S, and H thermograms in a given temperature range, and thermal scanning rate under a given composition of the carrying gas. MESTA technology is particularly suitable for the analysis of carbonaceous solid samples. In this report, I will present the principle of MESTA and examples of its application on the thermochemical properties of biochar, aerosols, C60, and C60 derivatives.

Biography:

Yuch-Ping Hsieh is a professor of wetland ecology at Florida A&M University, USA. He has 35+ research experience in soil and environmental chemistry. He has been responsible for the development of many original methods that are used by the researchers of the fields, including 14C and 13C isotopic tracer methods for the dynamics of soil organic carbon, diffusion methods for reduced inorganic sulfur species, a rapid method for soil microbial biomass carbon and multi-elemental scanning thermal analysis (MESTA) technology.



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Tel: +1-469-854-2280/81; **Fax:** +1-469-854-2278; **Email:** secretary@carbon-conferences.com
Web: https://carbon.unitedscientificgroup.org/