

ABSTRACT BOOK

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ABSTRACTS

PLENARY

Title: Multifunctional Synergy Strategies for Materials Design, Processing and Applications

Shi Xue Dou

Institute for Superconducting & Electronic Materials, Australian Institute for Innovative Materials, University of Wollongong, Australia

Abstract

Significant advances in development of strategies and approaches on novel materials design and processing have been made. Here we particularly highlight the advantages of combination of multi-functionalities to achieve synergetic effect on energy materials performance towards applications. These include combination of carbon coating with band engineering for alteration of electronic properties; universal general approach for morphology control; combination of physical confinement with catalytic effect to control polysulphide loss in metal sulphur battery; Multiple strain engineering for increase of reactive sites in catalysts; Additive & subtractive engineering for controlled growth of nanomaterials with designed size, shape and composition. Multiple dimension manipulation to achieve optimised electronic and ionic properties; Hybridisation at materials, structure & device level to achieve high reactivity in energy storage materials. Among these the interface/surface science and engineering is the most critical element for energy materials design and processing at both fundamental and applied level. Most of the research is limited within the block of research inputs to research outputs while there is a huge gap between research outputs and commercial benefits which need to be addressed. Scaling-up remains as a great challenge to facilitate industry transformation processes from laboratory to real world applications. The design and construction of battery pack driven minning veicles through development of advanced battery management system by UOW team sets unique example for transferring lab success to industry applications.

Biography

Shi Xue Dou is a Distinguished Professor at University of Wollongong, the founding director of ISEM and UOW Research Ambassador for Asia. He received his PhD at Dalhousie University, Canada in 1984 and DSc at the University of New South Wales in 1998 and was elected as a Fellow of the Australian Academy of Technological Science and Engineering in 1994. He was awarded the Australian Government's Centenary Medal in 2003 and Australian Order of Member in 2019 for his contribution to materials science and engineering, multiple Australian Professorial Fellowships from 1993 to 2011, the Vice-Chancellors Senior Excellence Award in 2008, Outstanding Partnership Award in 2012 and the Life Achievement Award from ASTS in 2018. He is named as a highly cited researcher in materials science by Thomson Reuters with citations of 60,000 and h-index of 115(Scopus).

His research focusses on energy and electronic materials. He has supervised and co-supervised more than 100 PhD students, more than 60 postdoctoral and visiting fellows. He is program leader for Auto CRC 2020 on electrification program and the on-going ARENA 2016-2020 on smart sodium storage system program.

SPECIAL TALK

Graphene Functionalization and Functional Free-standing Graphene Membranes

Martin Kalbac1*

J. Heyrovsky Institute of Physical Chemistry of the Czech Academy of Sciences, Dolejškova Prague, Czech Republic

Abstract

Functionalization of 2D materials represents a logical strategy to boost potential for application of these materials. However, in contrast to surfaces the functionalization of 2D materials also may lead to changes in their electronic structure. Therefore, a careful control of this process is very desirable. We proposed several ways to control the functionalization reaction. It will be also shown how tailored functionalization can be applied to optimize function of supercapacitor in graphene /PANI composite. Furthermore, preparation of active graphene membrane by deposition of cerium oxide nanoparticles using pulsed laser deposition in ultra-high vacuum conditions and a systematic study of the influence of preparation conditions on ceria nanoparticles and their interaction with CVD graphene will be discussed. Finally, the influence of graphene membrane on cerium oxide catalytic properties towards methanol will be presented.

Biography

Martin Kalbac graduated in inorganic chemistry from Charles University, Prague, Czech Republic, (1998), where he also received his Ph.D. degree in 2002. Since 2001 he has worked at the J. Heyrovsky Institute of Physical Chemistry of the Academy of Sciences of the Czech Republic. Currently, he is a vice-director of the institute and the head of the Department of Low dimensional Systems. His research interests include carbon nanotubes, graphene, Raman spectroscopy and Spectro electrochemistry, isotope engineering of carbon nanostructures and sensorics.

KEYNOTES

Graphene Oxide Liquid Crystal for Real-World Applications

Sang Ouk Kim*

National Creative Research Initiative (CRI) Center for Multi-dimensional Directed Nanoscale Assembly, Department of Materials Science & Engineering, KAIST, Daejeon, Republic of Korea

Abstract

Graphene Oxide Liquid Crystal (GOLC) is an emerging 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 in 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, prototype liquid crystal display 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 research particularly focusing on the nanoscale assembly of functional nanostructures, including highly oriented 1D fibers, 2D films and 3D nanoporous structures. Besides, relevant research

works associated to the nanoscale assembly and chemical modification of various low dimensional materials, including 1D carbon nanotubes, 2D TMDs and MXene, will be presented particularly aiming at energy and environmental applications.

Biography

Kim attained his Ph.D. in 2000 from the Department of Chemical Engineering at KAIST and joined the Department of Materials Science & Engineering of KAIST as a professor in 2004. He has developed the molecular level self-assembly principle for the general material fabrication methodologies based on various nanomaterials, including polymers and low-dimensional carbon materials. One of the prof. Kim's well-known research achievements is the world-first discovery of graphene oxide liquid crystal. Significantly, graphene oxide liquid crystal offers a valuable precursor state for the mass-production of sub-5-layer level high quality graphene powders. His academic contribution has been widely appreciated by prestigious honours, including the youngest fellow of the Korea Academy of Science and Technology (2020), Highly Cited Researcher from Clarivate Analytics (2018), the KAIST Grand Prize for Academic Excellence (2015) and Presidential Young Scientist Award (2013).

Advanced Nanocarbon Materials for Energy and the Environment

Aristeidis Bakandritsos^{1,2}, * Giorgio Zoppellaro,¹ Veronika Sedajova¹, Iosif Tantis¹, Jan Kolarik¹, Ievgen Obraztsov¹, David Panacek¹, Michal Otyepka¹, Radek Zboril^{1,2}

¹Regional Centre of Advanced Technologies and Materials, CATRIN, Palacký University, Olomouc, Czech Republic.

²Nanotechnology Centre, Centre of Energy and Environmental Technologies, VŠB–Technical University of Ostrava, Czech Republic

Abstract

Functionalization of graphene can mitigate its tendency for restacking and boost interactions with target chemical species. Functionalization must be selective and dense if high performance is required, combined with stability in challenging environments. Such properties are pre-requisites for sustainable sorbents and electrode materials for energy storage and catalysis.

By leveraging the susceptibility of fluorographene to nucleophiles, advanced and tailored graphene derivatives can be obtained for targeted applications. Graphene acid (GA), cyanographene (G-CN), superdoped graphene are indicative examples. GA bears carboxyls which are strong metal-coordination sites. Therefore, GA exhibits high proclivity for sorption and sensing of Cd²⁺ and Pb²⁺, as well as for the valorization of waste Pt for developing electrocatalysts for the oxygen reduction reaction. The all-covalent and spacer-free C-COOH bonds render GA bullet-proof in highly acidic media, enabling metal recovery and full sorbent regeneration.[4] As Li-ion battery anode, GA reveals i) high redox capacity stemming from its carboxyl groups, ii) high conductivity, boosting the rate capability, and iii) extra charge storage due to the co-presence of high content in sp² moieties serving as Li intercalation sites. The nitrile groups of G-CN display the required coordination strength and electronic communication with the aromatic skeleton of graphene for preparing undercoordinated and mixed valence catalysts, enabling the effective production of pharmaceutical synthons via cooperative mixed valence single atom catalysts.

Such graphene derivatives lay the ground for the development of the next generation materials for energy storage, catalysis, sorption and environmental monitoring.

Biography

Aristeidis Bakandritsos is a senior researcher and head of the Magnetic Nanostructures group at CATRIN-RCPTM, Palacky University of Olomouc in Czech Republic. He received his BSc in 2001 and PhD in 2006 in chemistry from the A.U. of Thessaloniki and from NKUA&N.C.S.R. "Demokritos" in Athens, respectively. In 2012 he appointed at the Dept. of Materials Science, University of Patras as a lecturer and later as an assistant professor until 2015-2016, when he joined RCPTM. His research interests involve the functionalization of nanomaterials and their application key technological areas. Research results have been published in more than 100 articles (h-index 30) in international refereed journals (google scholar).

Insight into a Silent Role of Nanopores in Carbon Catalysts Promoting Oxygen Reduction Reaction

Teresa J. Bandosz*

The City College of New York, New York, NY

Abstract

In search for efficient non-metal-based oxygen reduction catalysts carbon-based materials are considered as promising candidates. The most often explored research path to increase their catalytic activity is an incorporation of heteroatoms to a carbon matrix with a main focus on nitrogen. Recently, a high catalytic activity of heteroatom-free carbons has been reported and their performance was linked to the presence of defects. We have found that besides defects, porosity might also play an important role in enhancing the oxygen reduction process. It is owing to a strong adsorption potential and the ability of hydrophobic pores to withdraw oxygen from an electrolyte, followed by bond splitting, reduction and hydrogenation. On highly porous carbons the number of electron transfer reaches 4, and they exhibit a high catalytic stability and tolerance to methanol. The results indicate the existence of two parallel mechanisms: 1) on catalytic centers and 2) pore/adsorption forces mediated. Based on extensive studies of ORR on porous carbons, the objective of this communication, is to demonstrate that pores contribute to ORR, however, the process is complex, as complex is the surface of nanoporous carbons.

Biography

Bandosz is a professor at the City College of New York (Ph.D.; D.Sci.). Her work during last 30 years has resulted in 8 US patents and over 420. Her recent research interests include synthesis of new materials for separation and energy harvesting applications, photoactivity of carbonaceous materials, energy storage, ORR/CO₂ERR catalysts and CO₂ sequestration and reduction. She is coeditor of Journal of Colloid and Interface Science and serves on the Editorial Boards of various Journals. She is a Fulbright Senior Scholar, Fellow of the American Carbon Society and Fellow of the Japan Society for the Promotion of Science.

Emerging Carbon Architectures for Rechargeable Batteries

Vilas G. Pol*

Davidson School of Chemical Engineering, Purdue University, West Lafayette, IN

Abstract

ViPER (Vilas Pol's Energy Research) experimental laboratory at Purdue University, IN, USA focuses its research activities on developing unique electrode, electrolyte and separator materials for longer life, safer rechargeable batteries. Considering the advantages and limitations of known synthesis techniques, a solventless, single step ViP processing technology has been developed to fabricate a variety of unique anode and cathode materials for lithium-ion, Na-ion, K-ion and Li-S batteries. The technique has particular merit for producing carbon cavities and metal-carbon composites from inexpensive starch-based precursors. This presentation will reveal selective results on the novel synthesis of 3-dimensional carbon hotels that accommodates electrochemically active, high capacity Sn, Co or Si based nanoguests, mitigating pulverization. These carbon hotel rooms are also used to accommodate in-situ formed nanosulfur guest as a cathode of Li-S batteries in presence of fluorinated ether-based electrolytes. ViPER's recent efforts on structural, morphological and electrochemical properties of various electro-chemistries will be demonstrated.

Biography

Vilas G. Pol is a Chemical Engineering Professor at Purdue University, USA. He authored/ co-authored >215 research publications (h index 47) and an inventor on 12 issued US patents and 20 applications. Pol delivered hundreds of invited, keynotes, plenary talks including 'TEDx'. He is honored with British Carbon Society's Brian Kelly, ACS's 'Grand Prize' & 'Salutes to Excellence', MRS's Science as Art first prize, AIChE's 'Sustainable Engineering Forum Research' and 'Professional Achievement', ACerS's 'Richard M. Fulrath' awards, The MMMS's Best Energy Paper Award, Guinness World Record and Purdue's Bravo, Outstanding Engineering Teacher, Seed for Success and Faculty Scholar awards.

Synthesis and Processability of Ortho-Diynyl Arene Resins toward Polynaphthalene Networks and High Yield Carbon-Carbon Composites

Ernesto I. Borrego, Behzad Farajidizaji, Gustavo Munoz, Charles U. Pittman, Jr., and Dennis W. Smith, Jr.*

Mississippi State University, Mississippi State, MS

Abstract

High temperature polynaphthalene networks via step-growth thermal cyclopolymerization of bis-ortho-diynylarene (BODA) monomers results in unusually high yielding glassy carbon upon pyrolysis (75+%). To enhance BODA processability for carbon-carbon composite applications, we have introduced mono-ortho-diynylarene (MODA) co-monomers to control reactivity, branching, viscosity, and ultimate crosslink density for specific pre- and post-carbonization applications. Specialty MODA monomers were prepared in a single step from the Sonogashira coupling of substituted alkynes with diiodobenzene to yield aryl diynes of varying terminal substitution. Thermal co-polymerization of MODA with BODA affords reactive resins with enhanced processability via controlled molecular weight, polydispersity, viscosity, and latent enediyne content.

Biography

Dennis Smith is Professor of Chemistry and Department Head at Mississippi State University. He received a B.S. in chemistry and mathematics from Missouri State University (1988), and a Ph.D. in chemistry from the University of Florida (1992). His interests include science & technology leadership, technology transfer, entrepreneurship, and chemistry/materials research. He was a Dow Chemical post-doctoral Fellow in Germany (1993), Dow Project Leader (1993-1998); Chair, Local ACS Section (1996); Professor of Chemistry and Material Science & Engineering (MSE); co-founder and Center Director at Clemson University (1998-2010), Co-Founder of Tetramer Technologies, LLC (2001), Visiting Professor - University of Heidelberg (2001), Robert A. Welch Distinguished Professor of Chemistry & MSE at the University of Texas at Dallas (2010-2014); Director of NSF-I/UCRCs; Chair, ACS Division of Polymer Chemistry (2009), Officer of IUPAC, founder of FLUOROPOLYMER (2000-2018), Editor of Polymer Bulletin, Journal of Nanoscience & Technology, and several other journal Boards. He is Fellow of the American Chemical Society (2010), IUPAC Fellow (2016), Cottrell Scholar of Research Corporation (2001), and ACS Charles Stone Award recipient (2008). Dr. Smith has published 146 refereed journal articles (H=45), 28 US patents issued or pending, 300+ conference papers, 5 book editorships, and 200+ invited lectures. He has graduated 22 Ph.D., 7 M.S. students, and mentored 20+ post-doctoral, and 80+ undergraduate, foreign exchange, and high school students and science teachers. Dr. Smith is a board director, consultant for organic & materials science, entrepreneurship, and expert opinion.

Towards Carbon Neutral World: Materials World Transformation: Sustainable Renewables

Mohini Sain*

University of Toronto, Canada

Abstract

Depleting non-renewables resources prompted a global urge to transform conventional materials to more sustainable and carbon neutral materials discovery. To this end bio-oil derived from forest floor residues considered as a by-product in most kinds of industrial productions from the industrial combustion and the extraction of the plants. This presentation will highlight an overview of this low carbon science and engineering for a carbon neutral materials world and will focus on forest biomass/industrial waste and reuse them into the creation of a product through facile and low-cost fabrication. A number of case studies will be presented ranging from energy devices to medical equipment using carbonized cellulose, lignin used bio-oil as an precursor to meet a number of applications in flexible device products by tuning their functional properties by graphene nanoplatelets. Taking a stringent approach to device efficiency, this study proposes disposable and energy-efficient flexible devices that can be used to produce biodegradable medical diagnostics, energy devices, sensors, electro-chemical and electro-thermal ion carriers and many more. It is a viable alternative to non-reusable devices because it breaks down quickly and contributes significantly toward a material circularity platform.

Biography

Currently a Professor of Mechanical and Industrial Engineering Department and, the Director of the Centre for Bio composites and Biomaterials Processing he was former Dean of the Faculty of Forestry at the The University of Toronto. Dr. Sain, a fellow of Royal Society of Chemistry UK and Canadian Academy of Engineers, specializes in advanced bio nanotechnology, functional bio composites and nature-inspired advanced devices at the University of Toronto. Globally known for his pioneering work on Biocar and is a globally acclaimed consultant in Low Carbon Materials.

DAY-1

Development of Diamond MOSFET Logic Circuits

Jiangwei Liu*

National Institute for Materials Science, Namiki, Tsukuba, Ibaraki, Japan

Abstract

It is well-known that wide bandgap semiconductors such as GaN, SiC, and diamond are suitable to replace silicon partly for fabrication of high-temperature, high-power, and high-frequency electronic devices. According to figure of merit, diamond-based electronic devices have the largest power-frequency product, the highest thermal limitation, and the lowest power-loss at high-frequency. Thus, diamond is considered to be a 21st-century material. Because the activation energies of diamond dopants (370 meV for boron and 570 meV for phosphorus) are much higher than the room temperature thermal energy, many diamond metal-oxide-semiconductor field-effect transistors (MOSFETs) have been fabricated on hydrogenated diamond (H-diamond) channel layers, which can accumulate holes on surface with sheet hole density of 10^{12} - 10^{14} cm^{-2} .

In our previous reports, the H-diamond MOSFETs with a bilayer gate insulators deposited by radio-frequency sputtering deposition (SD) and atomic layer deposition (ALD) techniques were fabricated. It was demonstrated that the SD-oxide/ALD-oxide/H-diamond MOSFETs showed enhancement-mode (E-mode) characteristics. Recently, controlling conditions for depletion-mode (D-mode) and E-mode MOSFETs have been clarified. There are two necessary conditions for the fabrication of E-mode MOSFETs, which are SD-oxide/ALD-oxide bilayer gate structure and an annealing process. Otherwise, if there is only single gate insulator on the H-diamond channel layer, the MOSFETs operate with D-mode characteristics. After fabricating D/E-mode H-diamond MOSFETs controllably, next challenge is to combine these devices to be logic circuits. In this presentation, H-diamond enhancement-mode MOSFETs and MOSFET NOT and NOR logic circuits composed of D- and E-modes MOSFETs will be demonstrated.

Biography

Jiangwei Liu is currently an Independent Scientist at Research Center for Functional Materials of National Institute for Materials Science (NIMS), Japan. He received his Ph. D degree from the University of Tokyo in 2012. From Oct. 2016, he became a tenured Independent Scientist at NIMS. He is an elected person of MEXT-LEADER Program in 2016, NIMS-ICYS Program in 2014, and JSPS-GCOE Program in 2009. He is presently interested in single crystalline diamond growth and diamond electronic devices. He has authored and co-authored over 60 Journal publications and three Japanese Patent.

Efficient Functionalization of Single-walled Carbon Nanotubes for Dispersant-free Colloidal Dispersion and its Electrical Applications

Joong Tark Han^{*,1,2}

¹Nano Hybrid Technology Research Center, Electrical Materials Research Division, Korea Electrotechnology Research Institute, South Korea

²University of Science and Technology, South Korea

Abstract

Surface functionalization of carbon materials such as carbon nanotubes (CNTs) and graphene nanosheets facilitates their dispersion in solution, without using a dispersant, by overcoming the van der Waals interactions between the nanoscale carbon materials¹⁻³. Unfortunately, permanent functionalization can compromise some of the electrical properties which make these carbon materials so valuable. In particular, single-walled CNTs (SWCNTs) tend to be shortened and damaged under harsh oxidation conditions because their curved surfaces have higher reactivity than the graphene basal plane. In this talk, we present the rational oxidation method of SWCNTs via acid treatment by minimizing defect formation on the surface. Importantly, the structure of the oxidized SWCNTs (Ox-SWCNTs) could be recovered by chemical, thermal, photothermal, or solvothermal reduction, enhancing the electrical conductivity of the Ox-SWCNT films from ~ 100 to ~ 1000 S cm^{-1} . The electrical conductivity, Raman analysis, and XPS data all demonstrate the structural recovery of highly oxidized SWCNTs without compromising their electrical or electrochemical performances. Our results demonstrate that remarkable electrical or electrochemical performances were obtained after deposition of SWCNT inks or pastes that were dispersed in water and various organic solvents (without additional dispersant). Supercapacitors and LIB cathode electrodes using Ox-SWCNTs and reduced Ox-SWCNTs showed high electrochemical performances compared to those employing pristine SWCNTs. The high solution dispersibility and structural recovery of oxidized carbon materials are expected to facilitate their application as electrical or electrochemical components in next-generation devices.

Biography

Joong Tark Han received his Ph.D. in Chemical Engineering from Pohang University of Science and Technology (POSTECH) in 2005. He is currently a principal researcher in the Nano-Hybrid Technology Research center at Korea Electrotechnology Research Institute (KERI). His research interests are in exploring nanostructures and electronic structures of electrical nanomaterials such as nanocarbon materials (carbon nanotube, graphene, etc.), nano-metal, metal oxide nanoparticles, for future smart electric devices.

Fundamental Properties of Li-intercalated Layered Graphene's and Graphene Nanoribbons

Ngoc Thanh Thuy Tran^{*}

Hierarchical Green-Energy Materials (Hi-GEM) Research Center, National Cheng Kung University, Taiwan

Abstract

The essential properties of Li-intercalated layered graphene and graphene nanoribbon (GNR) systems are investigated with the use of the first-principles method. The detailed calculations cover the bond length, structure stability, atom-dominated band structure, adatom-induced free carrier density as well as

energy gap, spin-density distributions, spatial charge distribution, and atom-, orbital- and spin-projected density-of-states (DOS). The magnetic configurations are clearly identified from the total magnetic moments, spin-split energy bands, spin-density distributions and spin-decomposed DOS. Moreover, the single- or multi-orbital hybridizations in Li-Carbon, Li-Li, and Carbon-Carbon bonds can be accurately deduced from the careful analyses of the above-mentioned physical quantities. They are responsible for the optimal geometric structure, the unusual electronic properties, as well as the diverse magnetic properties. These theoretical predictions are compared with available experimental data, and potential applications are also discussed.

Biography

Ngoc Thanh Thuy Tran obtained her Ph.D. in physics in 2017 from the National Cheng Kung University (NCKU), Taiwan. Afterward, she began to work as a postdoctoral researcher and then an assistant researcher at Hierarchical Green-Energy Materials (Hi-GEM) Research Center, NCKU. Her scientific interest is focused on the fundamental properties of 2D materials and rechargeable battery materials by means of the first-principle calculations.

Tough, Transparent, Semi-conductive Polymer Nano-composite Substrates for Bendable Electronic Devices

Anasuya Bandyopadhyay,* Uday Shankar

IIT Roorkee, Saharanpur Campus, India

Abstract

The interest in optoelectronic devices with flexible substrates has been overgrowing day by day due to their lightweight and possibilities in bending, folding, and mounting to surface, which can be extensively used in daily lives such as state-of-art electronic gadgets. This growth has also been boosted by the exciting advancement in organic thin films for displays and low-cost optoelectronic devices. In addition, an increasing number of products employing organic electronic devices have become commercialized, which has stimulated the age of organic optoelectronics. Therefore, flexible organic optoelectronic devices such as touch screens, organic light-emitting diodes, organic solar cells, and many others require highly transparent and flexible alternative substrates. A series of copolymers were synthesized with methyl methacrylate (MMA) with Acrylonitrile and MMA with Styrene in different weight-percent ratios via solution polymerization process. All the copolymers were characterized using various techniques to understand the effect of introducing different proportions of comonomers on PMMA backbone. The optimum composition was chosen based on copolymer's mechanical properties, optical transparency, and ultraviolet shielding properties. Then, a series of nanocomposites of MWCNT with optimized matrices were fabricated through the solution blending method to achieve suitable dispersions. Different advanced characterization techniques used for a detailed study about the dispersion of MWCNTs in the matrix. The thin film's optical transmittance and electrical conductivity were characterized thoroughly. An optimized formulation of nanocomposite with 0.25% MWCNT has shown enhanced conductivity of 10⁻² S/cm with ~94% optical transparency at 550 nm for P(MMA70-co-AN30) and 10⁻⁵ S/cm with ~88% optical transparency at 550 nm for P(MMA70-co-Sty30).

Biography

I did my undergraduate and post-graduate studies from the University of Calcutta, WB, India. Then, I have completed my doctoral research in the Indian Association for the Cultivation of the Science in the year

2007, and degree was conferred by Jadavpur University. I have joined as MANA post-doctoral researcher in the National Institute for Materials Science, Tsukuba, Japan, under Dr. Masayoshi Higuchi in the year 2008, and came back to India in the Year 2012 after completion of the 3.5 years successful post-doc period. I have published several research papers in reputed international journals and one book chapter.

Fabrication of 3D Printed Flexible Electrodes of Carbon Nanomaterials

Satendra Kumar^{1,2*}, Prachi Soni³, Surender Kumar^{1,2}, N. Sathish^{1,2}, A. K. Srivastava^{1,2}

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²CSIR - Advanced Materials and Processes Research Institute (AMPRI), Bhopal, India.

³School of Nanotechnology, Rajiv Gandhi Proudyogiki Vishwavidyalay, Bhopal, India.

Abstract

As one of the most broadly developed three-dimensional (3D) printing technologies, fused deposition modeling (FDM) is utilized to fabricate electrodes for energy storage, energy conversion, and many more. One notable challenge resides in preparing printable suspensions with superior dispersing ability and stability. Here, we fabricated 3D printed space-filling and flexible electrodes with carbon nanomaterials. The space-filling curves provide more active sites within the geometrical area and flexible electrode open the path for numerous applications.

Figure: 3D printed space-filling (A, B, C) and interdigitated (D) flexible electrodes. (E) FESEM image of interdigitated finger.

Biography

Satendra Kumar has obtained his Bachelor of Technology degree from KIET, Ghaziabad, India in 2014 and currently pursuing Ph.D. from AcSIR center at Bhopal, India. His research interest is 'Studies of Structures, Growth Mechanism, and Physical Properties of Carbon-based Electronic Materials for Energy Storage Applications.

Graphene Quantum Dot Sensitizes GaN Nanotower/ZnO Nanorods Heterostructure Based Optoelectronic Devices

Govind Gupta^{1,2}

¹Sensor Devices & Metrology Group, CSIR - National Physical Laboratory (CSIR-NPL), Dr K. S. Krishnan Road, New Delhi, India

²Academy of Scientific & Innovative Research, (AcSIR), CSIR-HRDC Campus, Ghaziabad, Uttar Pradesh, India

Abstract

Heterostructure based devices has shown great potential in optoelectronic field. Heterostructure optoelectronic devices have been fabricated with unique taper ended nanotowers GaN (GaN-NT) and ZnO nanorods (ZnO-NRs) which exhibit higher photocurrent generation and significantly enhanced responsiveness towards UV illumination. The fabricated device displays substantial low dark current and

fast time-correlated transient response and very high photo responsivity in self-powered mode of operation. Further, chemically synthesized novel Graphene quantum dots (GQDs) has been utilized as sensitizer and GQDs sensitized ZnO-NRs/GaN-NTs heterostructure-based UV-PDs is also realized. The fabricated devices display remarkable enhancement in the performance parameters. The fabricated device demonstrates an excellent responsivity of 3200 A/W along with a very high external quantum efficiency of $1.2 \times 10^6\%$, superior switching speed, and signal detection capability as low as ~ 50 fW. The study also provides a new perspective toward energy-efficient opto-electrical device fabrication.

Biography

Govind Gupta is Senior Principal Scientist & Head, Sensor Devices & Metrology Group, CSIR-NPL, New Delhi, India and Professor, Academy for Scientific & Industrial Research (AcSIR). His core area of expertise is the of growth of III-Nitrides, metal oxide and layered 2-dimensional materials, fabrication of smart optical & gas sensors, surface & interface Physics, etc.. He has published ~ 250 research articles in SCI journals and supervised many Ph.D. theses. He is an Associate Academician of Asia Pacific Academy of Materials and received numerous awards & fellowships including MRSI medal, Young Scientist Medal-National Academy of Sciences, India, BOYSCAST fellowship, etc.

Preparation and Characterizations on Short Carbon Fiber Reinforced Acrylonitrile Butadiene Styrene Hybrid Nanocomposites Involving Carbon Nanotubes

Alinda Oyku Akar^{1*}, Umit Hakan Yildiz², Seha Tirkes³, Umit Tayfun⁴, and Ferda Hacivelioglu⁵

¹Gebze Technical University, Turkey.

²Gebze Technical University, Turkey

³Atilim University, Ankara, Turkey.

⁴Inovasens Ltd., Technopark Izmir, Izmir, Turkey.

⁵Gebze Technical University, Turkey

Abstract

Acrylonitrile butadiene styrene (ABS) terpolymer containing carbon fiber (CF) is one of the potential materials to become an industrial solution to achieve demanded limits, such as electrical conductance, ohmic heating, electromagnetic (EMI) shielding and electrostatic discharge (ESD). However, higher loadings of CF to increase the conductivity of polymer composites has a detrimental effect on the mechanical and tribological performance. Improving the electrical conductivity with incorporation of carbon nanotubes (CNT), while attaining higher mechanical characteristics was the prime objective of this study.

The preparation steps of composites were carried out using lab-scale twin screw co-rotating micro-extruder (15 mL micro-compounder[®], DSM Xplore) and injection-molding process. ABS copolymer was compounded with the loading ratios of 20 wt.% CF and 0.1, 0.5 and 1.0 wt.% of CNT. Mechanical, electrical, damping, thermal, melt-flow and structural investigations of ABS-based composites were conducted by performing tensile, impact, hardness, conductive atomic force microscopy (AFM), dynamic mechanical analysis (DMA), thermal gravimetric analysis (TGA), melt flow rate test (MFR), scanning electron microscopy (SEM) characterization techniques, respectively.

According to mechanical test data of resultant composites including tensile and impact test findings,

CNT additions led to remarkable increase in tensile strength and impact resistance for CF reinforced ABS composites. Formation of synergy between CNT nanoparticles and CF was confirmed by electrical conduction results. The conductive path in ABS/CF composite system was achieved by the incorporation of CNT with different loading levels. SEM micrographs of composites proved that CNT nanoparticles exhibited homogeneous dispersion into ABS matrix for lower loadings.

Biography

Alinda Oyku Akar received her bachelor's degree from Chemical Engineering Department of Middle East Technical University (METU), at year 2013. That same year, she began the graduate program of Polymer Science and Technology at METU. She graduated from M.Sc. degree with thesis work named "Characteristics of Poly(lactide) Composites Involving Montmorillonite and Boron Compounds". Currently, she is pursuing her Ph.D. studies at Gebze Technical University in Micro & Nanotechnology priority area under her thesis about the improvement of electrical, thermal, and mechanical properties of acrylonitrile butadiene styrene (ABS)/carbon fiber composites by addition of carbonaceous nano additives.

Characterization of Graphene using Contactless Terahertz Spectroscopy Methods

Justinas Jorudas^{1*}, Daniil Pashnev¹, Natalia Alexeeva¹, Ilja Ignatjev¹, Andrzej Urbanowicz¹, Roman Balagula¹, and Irmantas Kašalynas¹

¹Center for Physical Sciences and Technology (FTMC), Lithuania

Abstract

Sensitivity of the chemical vapor deposition (CVD) graphene films to the technological transfer and device fabrication steps requires the development of non-destructive contactless characterization methods. Here we developed the terahertz (THz) time-domain spectroscopy and Fourier-transform infrared spectroscopy methods for the investigation of graphene electrical conductivity described in terms of high-frequency Drude model. A commercial CVD graphene samples were wet-transferred to different substrates in order to demonstrate the advantages of remote characterization method over contact-based approaches, conventionally used to measure the carrier density and mobility values in two-dimensional materials. Namely spectroscopically obtained electrical properties were compared to the results of Hall experiment in Van der Pauw geometry. Contactless THz spectroscopy and Raman experiments revealed that our graphene films have a Dirac point relatively close to zero point.

Biography

Justinas Jorudas received the B.Sc. degree in applied physics from Kaunas University of Technology, Kaunas, Lithuania in 2017 and M.Sc. (magna cum laude) degree in optoelectronic materials and technologies from Vilnius University, Vilnius, Lithuania in 2019. He is currently working toward the Ph.D. degree at Terahertz Photonics laboratory, Center for Physical Sciences and Technology (FTMC), where he works on terahertz detectors and electrical characterization of graphene enhanced AlGaIn/GaN high-electron mobility devices.

Coherent White Emission of Graphene – towards Graphene-based White-light Laser

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²Optidea.pl, Wrocław, Poland

Abstract

Our recent experiments have shown the possibility of broadband, anti-Stokes, laser-induced white light emission generation (LIWE) from graphene-based composited like graphene ceramics [1] and foam [2]. Possible application of this remarkable phenomenon include whitelighting [3] or telecommunication. Characteristic features of observed LIWE include: (i) point emission only from the excitation spot, (ii) threshold dependence on excitation power density, (iii) saturation of emission intensity at high excitation power, (iv) relatively low temperature in emitting spot and (v) efficient photocurrent and electron emission. Recently the coherence properties of broadband white light emitted by graphene foam were investigated [4]. The interference fringes assigned to spatial and temporal coherence were observed for graphene white-light emission excited by two different excitation wavelengths of 975 nm and 808 nm of laser diodes. It was found that the coherence degree of white lighting depends on the excitation wavelength but not the excitation power. Origin of this phenomenon was discussed within the multiphoton ionization and stimulated emission due to the inversion population. It might result in the future construction of graphene-based white laser.

[1] Strek et al. Light Sci Appl 4, e237 (2015). [2] Strek et al. Sci Rep 7, 41281 (2017). [3] Strek et al. US Patent S 10,808,915 B2. [4] Strek et al. Appl. Phys. Lett. 116, 171105 (2020).

Biography

Wiesław Stręk works at Institute of Low Temperatures and Structure Research, Polish Academy of Sciences in Wrocław, Poland. His research activity covers laser spectroscopy, luminescence properties of rare earth and transition metal ions in crystal, glasses and nanostructures, theory of electronic relaxation in metal complexes, nonlinear optics, sol-gel materials, nanotechnology, size-effects in nanomaterials, nanophosphors, nanoceramics, optical sensors. He is recently interested in white light emission from carbon materials. He is coauthor of more than 500 papers with more than 10000 citations and co-creator of more than 30 patents and patent applications.

Carbon Nanotube Growth Controlled by Laser-Treatment of Substrates

N. Hampp*, M. Dasbach, S. Durbach

University of Marburg, Department of Chemistry, Marburg, Germany

Abstract

Laser treatment of stainless steel enables precisely controlled generation of arrays of iron oxide nanoparticles (NP) which in turn may be used to catalyze carbon nanotube (CNT) growth by chemical vapor deposition (CVD). In addition to the surface-bound formation of iron oxide NPs, the substrate itself may be structured, too. In combination with substrate topography and areal density of catalytic NPs, a wide range of CNT growth patterns may be realized ranging from low-density CNT flock-like coating to dense arrays of vertically aligned CNT, up to high-density cauliflower-like coatings. The latter ones may be grown on the

centimeter scale. Due to the considerable amounts of metallic NPs, these sponge-like structures are even magnetic. In addition, the various surface morphologies can be prepared on the same substrate side-by-side. The local morphology is controlled by the initial laser treatment. Finally, these structures may be soaked with e.g. silicon polymer precursor and after polymerization released from the substrate and transferred to any other surface fully preserving the internal structure.

Biography

Norbert Hampp, born in 1957, studied pharmacy and physics at the University of Munich, where he completed his first Ph.D. in plant tissue cultivation and genetics in 1986. In the same year, he received a post-doctoral grant for biosensor research at an Institute for Semiconductor Technology. From 1987 to 1993 he has been with the University of Munich and the Max-Planck Institute for Biochemistry, Martinsried. In 1992 he received his second Ph.D. in physical chemistry. From a position at Wacker-Chemicals, he moved in 1995 to a chair for physical chemistry at the University of Marburg. His research activities focus on technical applications of biological materials, implantable polymers, and laser material processing. He authored more than 250 scientific papers and 20 patents.

Atomistic Insights in Bonding, Nucleation, and Growth of Metals Confined in the Narrow Space of Single-walled Carbon Nanotubes and Graphene Pockets

Ute A. Kaiser

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Abstract

It is a growing demand in materials sciences of low dimensional matter to understand fundamental processes on the level of single atoms. atomic defects induced properties. For this purpose, a new type of transmission electron microscopes, the so called SALVE instrument has been developed operating at electron accelerating voltages between 80kV and 20kV, undercutting most of the material's knock-on thresholds. Using this instrument and employing single walled carbon nanotubes as test tubes, we identify the structure of electron-beam-stimulated modifications of molecules confined in the narrow dimension of a SWNT and unravel fundamental chemical properties and processes. We measure the bond length between two metal atoms and associate them with the bonding nature. Moreover, we demonstrate that the rotational motions within the SWNT are associated with mass transfer and show the interaction between the moving matter and the carbon nanotube and its function for carrying metal atoms to a nucleation seed. We further image in situ the initial steps of nucleation at the atomic scale. With three different metals we observed three main processes prior to heterogeneous nucleation, show the roles of the amorphous precursors and the existence of an energy barrier before nuclei formation. In all three cases, we find that crystal nucleus formation occurs through a two-step nucleation mechanism. Finally, we intercalate bilayer graphene in-situ by lithium, study in-situ the lithiation and delithiation processes, as well as the formation process of the new high-density crystalline Li- phase.

Biography

Ute Kaiser is Professor for Experimental Physics at Ulm University and Head of the Central Facility of Material Science Electron Microscopy since 2004. She studied physics/crystallography at Humboldt University Berlin and received her PhD in 1993. In 2002, she finished her habilitation with the work on

TEM on semiconductor quantum materials. From 2009-20018 she was the director of the Sub-Angstrom Low Voltage Electron Microscopy project, where she and her team focus on developments of low-voltage electron microscopy, instrumentation, methods, and applications for beam-sensitive low-dimensional materials. She authors more than 300 publications and was “highly cited researchers” in 2018.

Hierarchical Mesoporous Silica Nanoparticles as the matrix for b-glucosidase immobilization

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²Department of Agricultural Sciences Università degli Studi di Napoli Federico II, Via Università, Portici (Na), Italy

³Istituto di Scienze e Tecnologie per l'Energia e la Mobilità Sostibil -CNR, Napoli, Italy

Abstract

Fossil fuels depletion and environmental pollution have led to the search for alternative, environmentally sustainable and renewable energy sources, including biofuels.

lignocellulosic biomass is considered a strategic source of biofuels. The main component of lignocellulosic biomass is cellulose, a polymer composed of glucose units that can be hydrolyzed to glucose. Glucose is easily fermented into biofuels such as ethanol and butanol.

The enzymatic hydrolysis of cellulose is carried out by a complex of enzymes collectively called cellulases. Of these, b-glucosidase acts in the last stage of hydrolysis and constitutes the bottleneck of the whole process, as it performs the hydrolysis of the cellobiose, an inhibitor of the other enzymes of the enzymatic complex.

The drawbacks in the use of the enzymes is due to the high cost and high sensitivity to pH and temperature. To address these problems and make the enzymatic catalysis competitive at an industrial level, they can be immobilized on an insoluble support. Among a variety of organic and inorganic materials available, mesoporous silicates are excellent candidates for enzymes immobilization, since they offer high porosity and large surface area for high enzyme loading, large pore size for easy enzyme access, easy functionalization and thermal, chemical and biological stability. In this work, we have immobilized b-glucosidase on wrinkled mesoporous silica nanoparticles (WSN) by physical adsorption and covalent linking and evaluated the catalytic performance in the cellobiose hydrolysis by kinetic studies.

Biography

Aniello Costantini is Professor of Chemistry since December 2004 in the Department of Chemical Engineering, Materials and Industrial Production at the University of Naples Federico II. He received his Master Science in Engineering and his PhD in Materials Engineering from the same University. He is author in more than 100 publications in international high quality peer reviewed journals. His research work is focused on the synthesis of glasses, ceramics, glass-ceramics and nanostructured hybrids. He is highly skilled in synthesis of nanostructures through sol-gel. Accurate design of process parameters has been exploited to produce hybrid nanostructures, tuning size, shape and surface chemistry to obtain bioactive and nanocomposites, smart drug delivery carriers, mesoporous silica materials as supports for enzyme immobilization

Topography-driven Phenomena in Graphene – chemistry meets Physics

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¹Charles University, Czech Republic.

²J. Heyrovsky Institute of Physical Chemistry, Czech Republic.

Abstract

Graphene is a prototypic two-dimensional material featuring many unique properties due to its intrinsic flatness. Nevertheless, by introducing the topographic corrugations in a controlled manner, manifold modifications can be achieved. For example, both the curvature of the graphene and the position of the Fermi level are the key factors influencing its local reactivity. A comprehensive overview of the topography-driven phenomena in graphene will be discussed. We employed strategies including graphene transfer on substrates decorated with nanoparticles [1], fullerenes [2], and nanopillars [3]. Consequently, we achieved spatial modulation of the strain and doping with nanometre resolution. In this vein, we demonstrated spatially-resolved hydrogenation and fluorination applied to single-layer graphene with carefully controlled topography [4]. We also find out that the wrinkles may act as an ultra-small prison for the confinement of various molecules, like water. At the same time, the wrinkled graphene served as an extremely sensitive probe for monitoring the phase transitions of the supercooled nanowater [5].

Biography

Jana Vejpravova is a full professor in condensed matter physics at the Charles University, Prague (tsunamigroup.eu). After receiving her Ph.D. (2007), she took stays at the Hasselt University, NIMS – Tsukuba, MIT - Cambridge, and worked as a senior scientist & head of the department in the Institute of Physics, Czech Academy of Sciences (2011 – 2017). Her current research interests cover nanocarbons, nanomagnets, and two-dimensional materials. She published about 160 papers, managed ~ 15 national and EU projects as PI, and received multiple recognitions (e.g., ERC Starting grant - 2017, Scopus/Elsevier Award - 2010, F. Behounek Award - 2019).

One-step Microwave Synthesis of Nitrogen-doped Carbon Dots from Different Precursors

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¹University of The Witwatersrand, South Africa,

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

Abstract

Due to their excellent optical properties, carbon dots (Cdots) have attracted a great deal of interest from the research community. Among the carbon precursors used for the synthesis of Cdots, citric acid (CA) has been well-studied, and when combined with ethylenediamine (EDA), it is reported to produce nitrogen doped Cdots (N-Cdots) with high quantum yield (QY), which makes them suitable candidates for device applications. In particular, the highest QY was obtained when Cdots were prepared from CA and EDA (CAEDA) via the hydrothermal method as compared to other methods. However, the hydrothermal treatment method involve long reaction times, high temperatures and pressures, low production yields and expensive Teflon-lined stainless steel which are used as reactors. As such, there is a need for the synthesis

of Cdots with high QY using a more cost-effective method. Microwave-irradiation is the most promising method because it is cost-effective, involves shorter reaction times and have higher production yields.

Herein, we report the use of CAEDA, and for the first time the microwave irradiation of fumaronitrile (FN) as precursors, for the one-step synthesis of nitrogen doped Cdots (N-Cdots). Transmission electron microscopy analysis showed that both NCdots-CAEDA and NCdots-FN were quasi-spherical carbon nanoparticles with diameters less than 10 nm. The particle sizes of NCdots-FN were larger than those of NCdots-CAEDA. The X-ray photoelectron spectroscopy data confirmed the successful nitrogen incorporation in both samples. Both N-Cdots demonstrated excitation-dependent fluorescence behaviors, and that the optical properties of the synthesized N-Cdots were less dependent on the precursor used.

Biography

Manoko Maubane-Nkadimeng is a Senior Instrument Scientist and Researcher in the Microscopy and Microanalysis Unit at The University of The Witwatersrand, Johannesburg. She graduated her MSc with distinction (2010), followed by a PhD in Materials Chemistry (2013). Her research interests are in the synthesis and applications of nano-carbons. She is a member of executive committee of the South African Chemical Institute (Central) and has many accolades. She also holds a Postgraduate Diploma in Higher Education qualification (PGDipHE) and she is the Advisory Board Member of the Faculty of Education, University of Pretoria.

A Brief Review on the Structural Modification of Graphene's for Persulfate Activation

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¹Huazhong University of Science and Technology, Wuhan, PR China.

²Covenant University, Ota, Nigeria.

Abstract

This survey discusses the structural modification of graphene's along with its efficiency as a persulfate activator in the removal of organic contaminants. Based on the existing literature, the structural modification techniques were classified into thermal and chemical modification processes. The thermal modification process primarily involves the application of heat to alter the structural properties of graphene whereas, the chemical modification process essentially introduces heteroatoms (such as N and B) and/or metal ions into the graphene structure. Remarkably, modified graphenes have a higher persulfate activation performance than unmodified graphene and pure Co₃O₄. However, several limitations on the structural modification processes have been identified and further studies are required.

Biography

Daniel T. Oyekunle obtained his M.Eng. in 2019 from Covenant University, Nigeria. He was also a faculty member of the institution. He is currently pursuing his Ph.D. at Huazhong University of Science and Technology. He currently has more than 20 research publications with notable publications in Chemical Engineering Journal, Journal of Material Chemistry A, Chemosphere, Science of The Total Environment and Materials Today communications.

“Super” Accumulation of Hydrogen in the Know-How of Activated Carbon Nanofibers

Yury S. Nechaev

Kurdjumov Centre of Metals Science and Physics, Bardin Central Research Institute for Ferrous Metallurgy, Moscow, RUSSIA

Abstract

An effective methodology [1] was applied to analyze the well-known (but not reproduced by anyone) data [2,3] on the “super” sorption of hydrogen in the know-how activated graphite nanofibers (GNF). Such processing of the thermal desorption and thermogravimetric data [2,3] made it possible for the first time to determine (by two independent methods) the characteristics of the main hydrogen desorption peak, namely: the temperature of the highest desorption rate is 914 K, the activation energy of desorption is 39 ± 3 kJ/mol(H_2), the frequency factor of the rate constant of the desorption process is 0.15 s⁻¹, the amount of released hydrogen is 7 wt%. These results are in satisfactory agreement with the results of our analysis of data [4]. The know-how technology of GNV activation in works [2-4] can be disclosed by analyzing the corresponding data.

Biography

Yury S. Nechaev is a chief researcher-analyst (from 1998) in Kurdjumov Centre of Metals Science and Physics, within Bardin Central Research Institute for Ferrous Metallurgy, Moscow, Russia. He is Professor of materials science and metals physics (Dpt.), Doctor of physical-mathematical sciences. He has published more than 150 research articles in scientific journals.

Harnessing the Carbon Content of Coal for Graphene and Synthetic Graphite

Alexander Azenkeng*, Nicholas E. Stanislawski, Jason D. Laumb

University of North Dakota Energy & Environmental Research Center, Grand Forks, North Dakota

Abstract

The production of coal-derived graphene and synthetic graphite by harnessing the carbon content of abundant coal natural resources has been investigated on four U.S. coal ranks: lignite, subbituminous, bituminous, and anthracite. Physical and chemical methods for removing coalborne impurities and heteroatom content are being developed to transform the coal carbon content into a higher-quality precursor for high-value carbon materials. Preliminary results show a residual ash content of <1 wt% for lignite, <3 wt% for subbituminous and bituminous, and <7 wt% for anthracite coals and oxygen content reductions ranging from 8% to 24%. Production of synthetic graphite from the upgraded coal samples is in progress, while additional method refinements are planned to produce ultraclean coals with residual ash content of <0.5 wt% for production of high-grade carbon materials. Graphene quantum dots (GQDs) produced from raw and clean coal samples exhibit differences in their optical properties. Higher ultraviolet-visible (UV-vis) spectroscopy absorbances and redshifted photoluminescence maxima were observed from GQDs obtained from clean coal samples compared to those obtained from raw coal samples. In all cases, the emission maxima show an increasing redshift from lowest to highest coal rank. Excitation of anthracite-derived GQDs in the UV region produced little to no fluorescence signal, but a maximum emission signal was observed when excited in the visible region. These studies are relevant in tailoring specific optical applications of GQDs derived from different coal ranks and for producing high-value carbon materials from abundant coal natural resources.

Biography

Alexander Azenkeng serves as Associate Director for Critical Materials research at the University of North Dakota (UND) Energy & Environmental Research Center (EERC). He obtained B.Sc. and M.Sc. degrees in Chemistry from the University of Buea, Cameroon, in 1996 and 1998, respectively. In 2007, he obtained a Ph.D. in Physical Chemistry from UND. His research at the EERC includes coal upgrading; coal combustion and gasification; carbon capture and sequestration; unconventional reservoir characterization for CO₂ enhanced oil recovery; and coal-derived critical materials research on rare-earth elements, platinum group metals, and high-value carbon materials.

Functionalized Graphene and Carbon Nanotube for the Performance Enhancement of Epoxy Composites

Melissa Wunch¹, Samsuddin Mahmood¹, Sangmin Lee¹ and Duck Joo Yang^{1,2*}

¹The University of Texas at Dallas, Texas.

²GrapheneTX Inc., Texas.

Abstract

Graphene and carbon nanotubes (CNTs) are carbon-based materials with unique multi-functional properties. These properties can include, i.e., conductivity, hydrophobicity, tensile strength, barrier, etc. Graphene and CNTs have shown to be promising materials in a variety of fields, including coatings, composites or engineering plastics. Introduction of surface functional groups can help to enhance the properties of graphene or CNTs. Amination of graphene and CNTs was performed without the use of pre-treatment with strong oxidizers. Amination of graphene (AG) and CNTs (ACNTs) was performed using an eco-friendly aminating agent. Surface functionalization was determined through analytical techniques, including FTIR, XPS, and TGA. Both AG and ACNT materials were composited in an epoxy resin to observe their effect on mechanical properties. After functionalization the tensile strength of both composites increased versus pristine material. Both AG and ACNTs showed a 3-fold increase in mechanical properties of the epoxy composite over G and CNT based epoxy composite. Additionally, dispersion studies were performed with both functionalized graphene materials to observe their effect on dispersion stability. AG and ACNTs have shown stability in dispersions with organic solvents and water, with and without surfactant. These studies show that through functionalization the properties of graphene and CNTs can be enhanced. Additionally, the mechanical properties of epoxy composites were enhanced, versus pristine graphene or CNTs, by the inclusion of AG or ACNTs.

Biography

Duck J Yang, PhD in Chemistry from UC Berkeley, and E-MBA from Wharton Business School. Associate Dean of Research at UTD, and Co-founder & CTO of Graphene TX Inc. Industrial experiences at DuPont and Samsung with 50+ publications and 20+ patents.

DAY-2

KEYNOTES

Identification and Detailed Characterization of Metal Oxides and Carbon Nitrides by Electron Trap-Distribution Analysis

Bunsho Ohtani* and Mai Takashima

Institute for Catalysis, Hokkaido University, Sapporo

Abstract

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

Biography

The research work on photocatalysis started in 1981 when he was a graduate student in Kyoto University. Since then, he has been studying photocatalysis for 40 years and published more than 300 original papers (h-index: 71) and two single-author books. After gaining his Ph. D. degree from Kyoto University in 1985, he became an assistant professor in the university. In 1996, he was promoted to an associate professor in Hokkaido University and was then awarded a full professor in Institute for Catalysis in 1998. He was awarded several times from the societies related to chemistry, photochemistry, electrochemistry, and catalysis chemistry.

CARBON APPLICATIONS

ORAL PRESENTATIONS

Hydrogenated Carbon Electrodes by Silane Reduction as Antifouling Sensors for Dopamine

Danny K.Y.Wong* Rita Roshni, Simona Baluchova, Jan Klouda, Karolina Schwarzova, Jiri Berek

Department of Molecular Sciences, Macquarie University, Sydney, Australia

Department of Analytical Chemistry, UNESCO Laboratory of Environmental Electrochemistry, Charles University, Prague, Czech Republic

Abstract

A long-term goal of our work is to apply antifouling carbon electrodes to acquire meaningful results during in vivo detection of the neurotransmitter dopamine. Extracellular concentration of dopamine is often used as a diagnostic marker for several neurodegenerative diseases (e.g. Parkinson's, Alzheimer's, schizophrenia, depression). Very often, a major challenge during in vivo dopamine detection is electrode fouling, which arises from hindered electron transfer of dopamine on an electrode by an impermeable layer formed by non-specifically adsorbed amphiphilic proteins, peptides and lipids present in extracellular fluid. Diminishing transient dopamine signals in such work have yielded compromising results in time-dependent in vivo dopamine detection experiments. To minimise non-specific adsorption, we have developed a hydrophobic carbon electrode surface by hydrogenating the electrode using silane reduction. In such a hydrogenation process, (i) polycarboxylic acids, ketones, aldehydes and alcohols on a carbon surface are reduced to alkanes, (ii) all phenolic functionalities are converted to extended siloxane dendrimers, (iii) no effect on double bonds and ether. In this study, we have hydrogenated the surface of conical-tip carbon electrodes (~2 μm tip diameters and ~4 μm axial length) using triethylsilane, phenylsilane and diphenylsilane to obtain a hydrophobic surface. The antifouling properties of these hydrogenated carbon electrodes will be compared by evaluating the analytical detection of dopamine at these electrodes that were deliberately treated in a laboratory synthetic fouling solution containing bovine serum albumin, cytochrome c, caproic acid and human fibrinopeptide. The electrodes are further evaluated in real-life biological samples including dopamine cells and brain slices.

Biography

Danny Wong is a Senior Lecturer at the Department of Molecular Sciences, Macquarie University, in Sydney, Australia. His main research interests cover electroanalytical chemistry and electrochemical sensors for environmentally and biologically significant species. In particular, his research group is interested in developing antifouling, physically small carbon electrodes for in vivo detection of neurotransmitters. Since 2018, Danny has been the President of the NSW Branch of the Royal Australian Chemical Institute, actively involved in organising conferences, symposia and social functions. Danny is a Fellow of both the Royal Australian Chemical Institute and the Royal Society of New South Wales.

Graphene-based Heat Conductive Smart Windows: Towards Energy Efficient Green Buildings

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³Institute of Chemistry, the Hebrew University of Jerusalem, Jerusalem, Israel

Abstract

In a typical residential and commercial buildings in urbanized city, about 30% of total electrical energy consumption is consumed by indoor lighting and air conditioning. The sustainable energy consumption, an important feature of green building, may be catalyzed by the use of smart windows technology. Smart window technology allows windows to modulate (transmit or block) infrared radiation or to conduct heat laterally (hence to modulate heat transfer through the window) while maintaining high optical transparency through the window. Graphene-based materials (graphene, graphene oxide (GO), reduced graphene oxide (rGO) and graphene quantum dots (GQD)), have been used extensively for diverse applications owing to its excellent electrical and thermal conductivity. These materials are promising candidate materials for heat management in smart window application due to its visible light transparency, ability to reduce cross-sectional NIR (near-infrared) radiation transmission, and its superior optical properties. This presentation focuses on various types of graphene-based heat conductive smart windows which possess tunable heat modulation capability that can be used in energy efficient green building.

Biography

Alfred Tok (PK; Ph.D, NTU; C.Eng, MIMMM; MBA, NTU) has been a faculty in the School of Materials Science and Engineering since 2003. He studied Mechanical Engineering at the Queensland University of Technology, Australia, and graduated with a first-class honor in 1995. He was also conferred the Dean's Award for Excellence for being top graduate on the course. After graduation, he had worked as a mechanical engineer at ST Aerospace Engineering. In 1997, he was awarded 2 scholarships at Nanyang Technological University (NTU) to pursue his PhD in Mechanical Engineering. After graduation, he joined the Materials Engineering school as a Research Fellow in 2000 and took up the position of Assistant Professor in 2003. In 2009, he was bestowed the National Day Commendation Medal (PK) from the Singapore Prime Minister's Office. In the same year, he obtained his Nanyang MBA in the Dean's Honors List. He was then appointed Division Head of Materials Technology in MSE in 2009 and presently, he is the Deputy Director of the Institute for Sports Research. He also consults extensively for companies from various industries. Prof Tok leads the Nanomaterials Group that focuses on the synthesis, processing, consolidation and applications of nanomaterials (rare earth, carbon-based, functional ceramic nanoparticles). His current research is broadly based on 3 areas: carbon-based sensors, synthesis of nanostructured materials and hard & tough materials.

Spacer-Assisted Amine-Coiled Carbon Nanotubes for CO₂ Capture

Hyung Gyu Park^{1*}

¹Nanoscience for Energy Technology and Sustainability, Department of Mechanical Engineering, Pohang University of Science and Technology (POSTECH), Korea

Abstract

Architecture of a DNA-wrapped carbon nanotube (CNT) inspires rational design of a polymer-wrapped CNT effective for CO₂ capture. Polyethyleneimine (PEI) selected as a spiral wrapper of CNT is modified by insertion of spacer molecules loaded with amino groups such as siloxanes and purine to enhance the CO₂ capture performance. A porous adsorbent made by packing these functional nanowires (e.g., PEI-purine-CNT) reveals CO₂ uptake as large as 3.875 mmol/g. Adsorbent materials from this biomolecule-inspired design drop the adsorption heat to 29.00 kJ/mol if secondary and tertiary amines are adopted, besides the primary one, a value that is one-third of the absorption heat of an industrially deployed, liquid absorbent of CO₂. The corresponding adsorption and desorption kinetics agree with an Avrami model, indicating that both processes involve multiple sorption pathways. Furthermore, PEI-purine-CNT maintains its adsorption capacity after 50 adsorption-desorption cycles, implying a great potential for carbon capture from smokestacks and air in a stable and cyclic manner.

Biography

Hyung Gyu Park is a Full Professor in the Department of Mechanical Engineering at Pohang University of Science and Technology (POSTECH), Pohang, Korea, where he leads the laboratory of Nanoscience for Energy Technology and Sustainability and directs Center for Low-Dimensional Transport Physics. He received PhD in Mechanical Engineering from the University of California, Berkeley, U.S.A., with pioneering research on mass transport through sub-2-nanometer carbon nanotubes. After a postdoctoral training in Lawrence Livermore National Laboratory, Livermore, CA, U.S.A., he joined the Swiss Federal Institute of Technology (ETH) Zurich, Switzerland, in 2009 and served as tenured faculty until 2018, before he is affiliated with POSTECH.

Amorphous Carbon Nanotubes as Efficient Remover of Heavy Metals and Textile Dyes

Diptonil Banerjee

Faculty of Engineering and Computing Sciences, Teerthanker Mahaveer University, Moradabad, UP, India

Abstract

Carbon nanostructure-based research has mainly been limited to crystalline carbon nanostructures like carbon nanotubes (CNTs) or graphene. However, these nanostructures though show excellent potential has inherent drawbacks regarding their costly, complex low yield synthesis process. That requires complex and costly experimental set up, suitable catalyst and inert atmosphere and even if one can achieve all these the yield of the synthesis is very low. Moreover, being inert nanostructures like CNTs it needs additional external functionalization in order to use it any particular application that needs development of carbon nanostructures-based hybrids. Amorphous analogue of all these established nanostructures is the best solution for such problem because it can be synthesized by simple and cost-effective process with very high yield and having a very defect rich structure it does not require any external functionalization for development of hybrids. It is an irony that from the very advent of scientific and technological development we always harnessed energy issue with the cost of environment. As we know that today we are standing

beneath a tremendous environment crisis in terms of air, soil, water, noise, and radioactive pollution thus a so potential field like nanotechnology should be used to address the problem. Keeping this in mind in this work I would discuss the use of amorphous carbon nanostructures in removing different pollutant from waters. The pollutants include heavy metals like arsenic, textile dyes like methyl orange or rhodamine B or organic molecules like resorcinol. Here the quantitative analysis has been done mainly from UV-Vis spectro-photometer. Investigation has been done in detail regarding the adsorption isotherm as well as reaction kinetics.

Biography

Diptonil Banerjee is currently working as Assistant Professor in Department of Physics, Teerthanker Mahaveer University. He has done his Doctorate from Jadavpur University in the year of 2012. He has around 9 years of Teaching Experience both in UG and PG in different fields of Physics and Materials Science. In his 14 years (including PhD tenure) research career he has published over 70 papers in different international journal of repute and around 15 conference proceedings. He also has written many book chapters and 2 books on basic Nanoscience and Technology. He has executed Government project successfully and delivered good many Invited lectures. He also has guided many PhD and PG students. His current research interest mainly includes carbon-based nanostructures and related composites and their electronic and optical properties. He has h-Index 19, i-10 Index 38 and cumulative citation over 1000 (Source Google Scholar).

Deep Eutectic Solvents as New Candidate for Dye Sensitized Solar Cell Electrolyte: Experiment and Simulation

Fatemeh Mohammadpour^{1*}, Maryam Heydari Dokoohaki² and Amin Reza Zolghadr²

¹Farhangian University, Tehran, Iran,

²Shiraz University, Shiraz, Iran.

Abstract

In the present study, we examined choline chloride-ethylene glycol (ChCl-EG) deep eutectic solvent (DES) mixed with different iodide salts as electrolyte in dye-sensitized solar cells (DSSC) by experiment and atomistic molecular dynamics simulations. The photovoltaic performance of DES based DSSCs revealed solar cells with inorganic iodide source shows higher performance than cells with organic iodide source. In this case, the influence of potassium (K⁺), and 1-Ethyl-3-methylimidazolium (Emim⁺) counter ions on the DSSC performance in DES-based electrolytes was studied. The photovoltaic and electrochemical properties reveal that the presence of KI salt in electrolyte solution considerably enhanced the DSSC efficiency. In this way, the effect of iodide sources on the viscosity, conductivity, and impedance spectra of DES electrolytes was investigated. Additionally, MD simulations of the TiO₂/DES electrolyte and Pt/DES electrolyte interfaces suggest that K⁺ cations cover the surface of anatase TiO₂, in contrast to Emim⁺. Furthermore, the dynamic of iodide anion in KI system is found to be higher than K⁺ cation, contrary to Emim⁺ in EmimI system. The diffusion coefficient of K⁺ in the DES was found to be systematically slower compared to the Emim⁺ due to the solvent effect and more strongly coordination with chloride atoms and also EG molecules of the DES.

Biography

Fatemeh Mohammadpour born in Isfahan, Iran, studied Physics at the University of Shiraz (M. Sc., 2009), and carried out her graduate studies "Optimization of TiO₂ and ZnO nanostructures to enhance conversion efficiency in dye-sensitized solar cells" (Ph. D. degree in 2014). From August 2013 to January 2014, she was

guest scientist at the materials science faculty, LKO lab, at the Friedrich Alexander University of Germany where her research focused on application of TiO₂ nanotubes in dye-sensitized solar cells. She joined to the Zolghadr group at the chemistry faculty at the Shiraz University, Iran, in the post-doc position in the fall 2016 where her research focused on the use of nanoporous materials as drug carriers. Now she is assistant professor of physics at the Farhangian University, Shiraz, Iran from winter 2017.

Carbon Fibres and Nanoparticles Impact on Advanced Phase Change Material Li₄Br(OH)₃ Synthesis Developed for the Thermal Energy Storage Applications.

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Abstract

The thermal energy storage is a key part for a successful set-up of a broad energy mix achievement. The choice of materials to be used in the storage units is directed to the phase change materials (MCPs) and mainly to the eutectic compositions due to their behavior close to the pure substances: their fusion is congruent and occurs at almost constant temperature. However, the stoichiometric peritectic compounds have energy densities two to three times, on average, higher than those of the standard MCPs due to a reversible chemical reaction occurring in addition to the solid/liquid transition during the thermal energy charge/discharge processes of the material. The first experimentations led to two components of interest according to the applied temperature programs: Li₄Br(OH)₃ reported in the LiBr/LiOH phase diagram ($T_m = 291$ °C, $\Delta H_f \sim 570$ J/g) and another structure, not reported this time, with the same composition ($T_m = 288$ °C, $\Delta H_f \sim 250$ J/g). Adding another component to improve the salt-based material's thermal conductivity is a common method but their presence can turn out to be another main criterion to take into account during the targeted material synthesis. The objective consists thus in seeing how the carbon fibers and nanoparticles can impact on the Li₄Br(OH)₃ formation process. To do so, in situ and real time experimentations at microscale have been performed to highlight the mechanisms involved in the formation of Li₄Br(OH)₃ and of its polymorph. The results are presented and discussed here.

Biography

Fouzia Achchaq is Associate Professor at the University of Bordeaux and Researcher at TREFLE Department (Fluids & Transfers) of the I2M Institute. She has expertise in thermal energy storage materials and systems used at low-medium and high temperatures and currently contributes to the ANR Project Pc2TES (National Project, 2017-2021) aiming at developing, studying and characterizing new advanced materials for the thermal energy storage applications at high temperatures (300 – 600°C).

Photo Assisted Regeneration of Activated Carbons: A Case Study on a WWTP

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Abstract

Current challenges in wastewater treatment are linked to the need for developing effective solutions to face emerging pollutants, capable of assuring a feasible economic upgrade of existing plants. Even though activated carbon is an excellent alternative, the cost associated to the regeneration of the spent carbon (energy consumption, transportation) still represents a major limitation. This work is a case study on the photoassisted regeneration of spent activated carbons from a wastewater treatment plant (WWTP) equipped with activated sludge technology and granular activated carbon in Almendralejo (Spain). Irradiation of the spent carbon from the WWTP resulted in a gradual regeneration, which efficiency depended on the saturation state of the carbon and the illumination time. A fraction of the components retained in the pores of the carbon are released into the solution upon illumination, and subsequently photodegraded. Long-term performance is discussed in terms of the quality of the reactivated carbon for further reutilization at the WWTP, and the quality of the effluent generated upon the treatment.

This project has received funding from the European Union's Horizon 2020 research and innovation program under the grant agreement N° 776816.

Biography

Conchi ANIA received her PhD degree in Chemistry in 2003; she is currently Research Director of CNRS at CEMHTI (Orléans, France), and Investigador Científico of CSIC (Spain; in leave of absence). She received the national L'Oreal-Unesco 2008 Research Fellowship "For women in Science", and the Excellence Research Award by University of Granada (2008). She is a grantee of the European Research Council (ERC) since 2016. Current research interests focus developing nanoporous materials with tailored surface chemistry and architectures for high-tech applications, covering energy storage and conversion, water treatment (photocatalytic, electroassisted processes), gas adsorption and separation, and solar energy conversion.

Carbon Properties Stimulating Microbial Extracellular Electron Transfer

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Abstract

The use of conductive carbon materials to speed up the extracellular electron transfer (EET) in certain bacteria, so-called electroactive, is essential for microbial electrochemical technologies (METs). Indeed, enhancing EET results in an enhancement for the biodegradation rate of pollutants, what converts

electromicrobiology in an emerging field for environmental applications, like wastewater treatment, bioelectrochemical desalination, and bioremediation of natural environments (soil and sediments). Despite this interest, the potential capability of these materials and the required properties that enable the optimization of these systems are still uncertain. Meanwhile, the development and full-scale application of certain METs, like METland® solution, currently demand massive amounts of microbially electro-active carbon materials. In this context, although the state-of-the-art METs are based on highly-conductive fossil-derived carbons, the availability, cost and environmental impact of these materials will be crucial for the feasible implementation of METs at large scale.

This work analyzes and evaluates the role of physicochemical and electrochemical properties of various carbon materials on promoting microbial EET. Special attention is paid on finding out properties-performance correlations. Particularly, various carbons including commercial graphite, coke, and different biochars have been thoroughly analyzed by several techniques. Then, the role of electrical conductivity, porosity and surface chemistry on microbial EET, biodegradation and/or bioelectricity production is studied and discussed. Examples on the application for cleaning-up urban wastewater or the amendment of soils are demonstrated. Our study concludes that electroactive biochar can be a good candidate for large-scale environmental applications of METs.

Biography

Raul Berenguer is Senior Researcher at the Institute of Materials Science of the University of Alicante (Spain). Graduated in Chemistry (2004), he got his PhD in Materials Science and Applied Electrochemistry (2010) at this institution. As Post-Doct researcher, he joined the Institute of Multidisciplinary Research for Advanced Materials at Tohoku University (Japan); the Chemical Engineering Department at the University of Malaga (Spain); and the Institute IMDEA Water (Spain). His research career has been mainly dedicated to the study and optimization of electrodes and electrochemical technologies for environmental applications, like wastewater treatment and energy storage/conversion.

Cement/Carbon Nanofiber Composites for Well Plug Integrity Sensing

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Abstract

All CO₂ storage wells will eventually need to be permanently plugged and abandoned. Subsidence, fault/fracture reactivation or chemical degradation can all possibly adversely affect well plug integrity leading to CO₂ leakages. Taking responsibility for the storage projects for posterity should not only rely on better understanding of leakage mechanisms but also on taking measures to detect and prevent any future leakage events. To this end monitoring of the well plug integrity in the long perspective would be needed. It is in vain to look for long-term monitoring technology in oil and gas industry. In contrast to CO₂ storage wells, the oil/gas wells are plugged when the reservoir has been depleted from gas/oil thus the pressure was reduced. Moreover, the long-term monitoring in oil and gas industry is a controversial topic as it requires difficult decision making on defining responsible authorities. At the early stage of laying down the CO₂

storage regulative laws, defining responsibilities should be relatively easier.

Cements with carbon nanofibers (CNFs) are materials whose electrical properties change upon application of mechanical stress or chemical alterations. As such the materials are good candidates for well plug integrity sensing. In this paper we summarize SEP FARAWELL project results that aimed on testing electrical response of conductive composites made of well cement and carbon nanofibers in response to load, carbonation, and water saturation changes.

The results show that bulk resistivity of well cement/CNF composites changes upon application of the three stimuli mentioned above thus the material proves promising for monitoring applications.

Biography

Kamila Maria Gawel present working as a research scientist in the petroleum unit of SINTEF Industry. Kamila Gawel research mainly focused on Hydrogel, Nanometer resolution, Antipoly electrolyte, Inclusion complex, Bio specific Hydrogel.

Bioactive 3D Printed Scaffolds Functionalized with Green Reduced Graphene Oxide: A New Strategy to Improve Bone Tissue Regeneration

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³ITQB – Institute of Chemical and Biological Technology, António Xavier, University Nova de Lisboa, Oeiras, Portugal

⁴CIEPQPF – Department of Chemical Engineering, University of Coimbra, Coimbra, Portugal

Abstract

Tissue Engineering arises as an emergent area aimed to produce three-dimensional (3D) structures, known as scaffolds. Recently, researchers have explored the incorporation of reduced graphene oxide (rGO) nanomaterials into scaffolds structure to enhance their properties for bone regeneration applications, namely the mechanical and osteogenic properties. However, rGO is generally obtained by treating graphene oxide (GO) with hydrazine hydrate, a highly hazardous reducing agent. Furthermore, rGO presents lower aqueous stability, which have hindered its incorporation in ceramic/polymeric blends to produce scaffolds through 3D-printing technique. To overcome this limitation, the main goal of this work was to develop a novel environmental friendly method to functionalize the 3D printed scaffolds incorporating rGO. To accomplish that, three different scaffolds formulations were produced: i) tricalcium phosphate/gelatin/chitosan (TGC), ii) tricalcium phosphate/gelatin/chitosan and GO (TGC_GO) and iii) tricalcium phosphate/gelatin/chitosan and reduced GO (TGC_irGO), which are obtained through the in-situ green-reduction of TGC_GO scaffolds mediated by L-ascorbic acid. The TGC_irGO scaffolds presented enhanced wettability and improved mechanical properties without impairing their porosity, when compared to their equivalents functionalized with GO and non-functionalized scaffolds (TGC_GO and TGC, respectively). Moreover, the TGC_irGO scaffolds exhibited improved calcium deposition at their surface and enhanced alkaline phosphatase activity (ALP), along 21 days of incubation with osteoblasts. Furthermore, the produced scaffolds also displayed antimicrobial activity since they are able to inhibit *S. aureus* and *E. coli* growth. Such features reveal the potential of the TGC_irGO scaffolds for bone tissue regeneration applications and also validate the developed in situ green reduction protocol of GO.

Biography

Catia S. D. Cabral received her B.Sc. in Bioengineering and M.Sc. in Biomedical Sciences from University da Beira Interior in 2016 and 2018, respectively. Currently, Catia S. D. Cabral is a Ph.D. student in Biomedicine at the same university. Her research interests focused on the development of new 3D composite biomaterials for bone tissue regeneration applications and characterization of the physicochemical and biological performance of biomaterials.

Enhanced Control of Recalcitrant Pharmaceuticals and Organic Matter in Urban Wastewater Treatment with Pine Nutshell CO₂ Activated Carbons

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Abstract

LIFE IMPETUS project (LIFE14/ENV/PT/000739) aimed to develop and test novel powdered activated carbons (PACs) for improved control of pharmaceutical compounds (PhCs) and organic matter (OM) in urban wastewater treatment plants (WWTPs) with conventional activated sludge (CAS) treatment. Several biomass precursors, activation agents and routes were explored at lab-scale pinpointing pine nut shell (PNS) as the most promising raw material: PAC steam activated sample PNS77/Steam performed similarly to the commercial golden standards (Cabot-Norit and Chemviron). PACs were tested in operational environment, i.e. under competitive adsorption of three PhCs in spiked (100 µg/L) WWTP mixed liquor and secondary effluent. PhCs were selected considering their worldwide occurrence and persistence in CAS-WWTP effluents (results validated in LIFE IMPETUS) and adsorption key-properties: carbamazepine (neutral, hydrophobic), diclofenac (anionic, relatively hydrophobic) and sulfamethoxazole (anionic, hydrophilic).

PNS-derived PAC production was scaled-up using CO₂ activation and results prove that, for similar burn-off degrees, steam and CO₂ activation attain similar and excellent textural properties. PNS72/CO₂ and PNS83/CO₂ outperformed PNS77/Steam for the removal of the three target PhCs and OM in spiked WWTP secondary effluent. Data modelling (HSDM – Freundlich isotherm) allowed estimating the PAC dose to the CAS bioreactor required for a given overall removal of the target-PhCs.

Acknowledgements

This work was supported by the European Union LIFE Programme under Grant Agreement LIFE14 ENV/PT/000739 - LIFE Impetus (<https://life-impetus.eu/>); Fundação para a Ciência e a Tecnologia (FCT, Portugal) grant UIDB/00100/2020 and Embrace Project (CEECIND/0137/2017).

Biography

Ana Sofia Mestre received her Ph.D. in Chemistry (2010) under the supervision of Prof. Ana Paula Carvalho from the Faculty of Sciences of Lisbon University (FCUL). She was a researcher on Water Cork project (2010-2012), in a project between REQUIMTE (FCUP) and CQB (FCUL) (2013-2019) and in the

LIFE Impetus consortium (2016-2019) coordinated by LNEC and recognized with two awards. Since 2019 Ana Sofia Mestre is Assistant Researcher at FCUL. Her research interests have been mainly focused on the development and characterization of new nano porous carbon materials from biomass and in advanced methodologies for emergent contaminants removal from water.

Graphene Based Nanostructured Materials for Water Remediation

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³CESAM, University of Aveiro, Portugal

Abstract

Worldwide, both freshwater and marine ecosystems are declining at alarming rates, causing the ecosystem and biodiversity to decay. Even Europe with its abundant freshwater resources is increasingly facing water scarcity. Actions are needed to avoid the growing level of water shortage. Horizon Europe includes the “Water challenges” in its mission. By 2030, it intends to reduce water stress, increase protection of water resources and ecosystems, enhance resilience, mitigation and adaptation of water systems to global changes. On December 2020, the European Parliament formally adopted the revised Drinking Water Directive 98/83/EC on the water quality for human consumption. The Directive entered into force in January 2021, and Member States have now 2 years to implement it in national law. Graphene based materials (GBM) are emerging as promising solutions to address water remediation. In this talk we aim to demystify the real efficiency of using GBM for water remediation. Several promising multifunctional nanocomposites based on graphene developed in our group for specific heavy metals decontamination in real waters will be presented. Also, dedicated research to determine possible harmful impact in the environment by the proposed GBM will be discussed. A comparison with alternative methods that constitute the current state of the art in terms of efficiency will be also given. Our ambition is to translate this knowledge into a high added-value product that can be exploited in water treatment plants.

Biography

Paula Marques (Principal Researcher) holds a PhD degree in Materials Science Engineering. Her research interests are the engineering and development of carbon-based nanostructured composites for health and environmental uses. She published +100 papers in international journals, 7 book chapters, 3 books, has 2 National and 1 European patents registered and 3 requested. The quality of her work is expressed by the number of citations (+3791) and h-index of 33. Paula participated in 25 R&D projects with 9 in progress, being presently the PI of a H2020-FETOPEN (A step forward to spinal cord injury repair using innovative stimulated nanoengineered scaffolds) and of a PTDC/NAN-MAT/30513/2017 (Graphene based materials and water remediation: a sustainable solution for a real problem?).

Graphene Based Aeromaterials: From High Performance Actuators to Air Sterilization

Rainer Adelung*

Chair for functional Nanomaterials, Kiel University, Germany

Abstract

The outstanding properties of graphene are based on its 2-dimensional character. But this creates a challenge to utilize the remarkable properties in 3D. The challenge is to transduce the properties from the surface plane to a bulk without losing 2D properties. This can be done by arranging graphite by following the structural concept we developed for Aerographite [1]. The arrangement in microscopic tubes with nanoscopic wall thickness doesn't create additional effects like in carbon nanotubes but allows mechanical stability and an interconnection between the tubes to create a three-dimensional tube framework of macroscopic expansion and extreme high amount of bottle neck free volume. This creates a material that is extremely lightweight with negligible masses of 1-10 milligram per cubic centimeters, but surprisingly robust mechanical features [1,2]. The negligible mass (and thus negligible heat capacity) in conjunction with high surface area enables new engineering possibilities like extremely rapid electrical heating with speeds of air explosions (heating rates of >100000 K/s) [3]. These opens up new possibilities in rapid pneumatic actuation with exceptional power to weight ratio (>10000) and air filtration that allows volumetric sterilization within less than a second. The talk reviews the past and recent findings in our graphene aeromaterials and demonstrates the latest experiments in ultra-rapid heating and actuation. [1] *Advanced Materials* 24, 3486 (2012); [2] *Nature Communications* 8, 14982 (2017); [3] *Materials Today* in press, doi: 10.1016/j.mattod.2021.03.010 (2021)

Biography

Rainer Adelung is Professor at the chair for Functional Nanomaterials in the institute for materials science at the Faculty of Engineering of the Kiel University (CAU Kiel), Germany. His scientific work includes various nanostructures, mainly on the synthesis and design of porous materials, nanostructured surfaces and nanowires including graphene and related Materials. Applications range from energy technology like batteries and supercapacitors to sensor devices and antiviral agents towards advanced adhesion technology in engineering technology. From 2013-2019 he was the spokespersons of the University focus on nano surface and interface science. Currently, he is speaker of the DFG Research Training Group RTG 2154 Materials for Brain.

Challenges in Biofuels Downstream Processing: Separation of the 1,3-Propanediol + Water Mixture

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Abstract

Current effort to reduce consumption of fossil fuels and to increase the use of renewable energy sources has raised a great interest in biofuels. Specifically, alcohols deriving from renewable sources (e.g., bioethanol and bio-butanol) can be regarded as excellent fuel substitutes or additives to raise the octane number, ensure a better combustion and, thus, reduce harmful exhaust pipe emissions. Nevertheless, even tiny amounts of water in the blend can lead to phase splitting, which in turn can cause engine troubles. Thus, alcohol

dehydration is essential and advanced separation methods have to be applied for an efficient purification, which is made complex by the formation of low-boiling azeotropes.

Moreover, heavy by-products, such as 1,3-propanediol, are often present in the aqueous mixture: their separation from water by distillation techniques is challenging due to the high energy consumption, leading to a high cost of the target product. This work focuses on the separation of the 1,3-propanediol + water mixture (required also in 1,3 propanediol production processes), which, to our knowledge, is poorly investigated in the literature. Different technologies may be applied for this separation, the major ones being reactive extraction, liquid-liquid extraction, evaporation, distillation, membrane permeation and ion exchange chromatography. The aim of this work is to simulate the removal of water and purification of 1,3-propanediol by distillation using the commercial process simulator ASPEN Plus® and, by means of a sensitivity analysis on different operating variables, to determine the optimal solution, which allows minimizing the energy requirements of the separation process.

Biography

Stefania Moioli is assistant professor (Ricercatore a Tempo Determinato B) at Dipartimento di Chimica, Materiali e Ingegneria Chimica “Giulio Natta” of Politecnico di Milano, where she is in charge of the courses “Process Plants” and “New Technology Frontiers in Gas Production, Transportation and Processing”. She is member of the “Group on Advanced Separation Processes & Gas Processing - GASP”, in which she studies the purification of acid gases, regarding in particular both thermodynamics and mass transfer with reaction modeling. Her research interests cover thermodynamics, kinetic modeling and steady state/dynamic process simulation.

Energy Storage Technologies: Synthetic and Catalytic aspects of Power-to-DME

Rosanna Viscardi^{1*}, Vincenzo Barbarossa¹

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Abstract

Energy storage has become a crucial technology in the energy transition from fossil fuel energy systems towards renewable electricity-based systems. Due to the various types in which energy can be stored, transported and consumed by society, it would be useful to identify which technology would be best for a given application. One subset of energy storage, called power-to-X (P2X), has been recognized by industry and governments as a fundamental point of technologies for obtaining net-zero emissions. P2X technology as a type of chemical energy storage transforms renewable electricity into useful chemicals for decarbonization of industrial sectors or for energy storage objectives. In many cases, P2X contains the class of energy storage vectors most closely mirroring the energetic and chemical properties of fossil fuels, and thus is well positioned to smooth the energy transition. Particularly, in this work the catalytic activity of a new class of materials for Power to DME is discussed and compared with others commercial catalysts. Alumina and zeolite-based catalysts are most widely investigated for methanol dehydration to DME, and commercial catalysts are typically g-alumina and H-ZSM-5 zeolite. Focus on catalyst development for P2DME process is predominantly related to the appropriate catalyst configuration, i.e., the combination of the catalyst for methanol formation with the one for the subsequent dehydration step, as well as utilizing new class of materials such as sulfonic resins-derived catalysts.

Biography

Rosanna Viscardi obtained a BSc in organic chemistry (2004) and a MSc in physical and analytical Chemistry (2006) from the University of Salerno. In 2009, she completed her PhD thesis in electrochemical chemistry at University of Salerno with a work developed in collaboration with ACTA S.p.A. From 2007 to 2012, she worked as researcher at ACTA. Major research interests involved the synthesis and characterization of electrocatalysts for alkaline fuel cells and electrolyzers. Since 2012, she works at ENEA Casaccia on the development and understanding of new processes and technologies for the capture and conversion of carbon dioxide into fuels and chemicals.

Phenazine analogues consist of chlorambucil and biotin moieties as new conjugates for anticancer therapy

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²Cytometry Laboratory, University of Lodz, Pomorska, Poland.

³University of Lodz, Poland.

Abstract

Phenazines (nitrogen-containing heterocyclic molecules) show a broad range of antiparasitic and antibiotic activities. They also indicate antimalarial, anti viral and anticancer effects thus, present a great potential for the discovery of new anti-infective agents. Therefore, this family of active compounds is valuable for chemotherapy leading to a decrease in the risk of resistance but is also capable of intercalating into DNA. The design of biotinylated prodrugs, which can accumulate in cancer cells rather than the normal ones, has great potential for the delivery of chemotherapeutics. We showed that phenosafranin (3,7-diamino-5-phenylphenazinum chloride, PSF) covalently bound to biotin allowed us to obtain the probe (Biot-PSF) with a high fluorescence intensity. Thus, a biotinylated conjugate can create a macromolecular bridge for different biomolecules e.g. avidin and can be used as a molecular recognition moiety. The Biot-PSF cytotoxicity towards three human colon cancer cell lines (COLO 205, HCT116, and SW620) was examined, and showed that the Biot-PSF conjugate can reduce non-specific charge-mediated uptake and increase specific SMVT-mediated uptake. Additionally, chlorambucil was attached covalently via amide bonds to the bifunctional fluorophore, which facilitates tracking with visible light. Our studies revealed that the new photosensitive compound exhibits improved intrinsic activity in vitro in HeLa cells culture experiments thus, it could be a potential anti-cancer candidate in theranostic drug-delivery systems. This strategy for the synthesis of innovative conjugates based on the phenosafranin backbone offers a promising possibility for drug control in anti-cancer therapy and diagnosis. This aspect makes the phenosafranin-chlorambucil conjugate unique among currently available biomarkers.

Biography

Beata Miksa has completed PhD Chemistry (Polymer department) at Centre of Molecular and Macromolecular Studies Polish Academy of Science. Beata Miksa worked as postdoctoral fellowship (Chemistry Department) at University of Memphis for 1 year and also worked as a postdoctoral fellowship (Chemistry Department) at Kansas State University.

Laser Synthesis of Hard Carbon for Anodes in Na-ion Batteries

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³CNRS ICMN, Université d'Orléans, Orléans, France

Abstract

Hard carbon becomes one of the most promising anode materials for sodium-ion batteries due to its high capacity, low insertion/reaction potential and low cost [1-2]. This carbon material is often obtained by heat treatment of nongraphitizable precursors such as sugar, biomass and some polymers. However, such heat treatments conducted in a furnace under vacuum or inert atmosphere are time and energy consuming. In this context, new heat treatment processes are highly sought after in order to develop eco-efficient synthesis approaches. Among these techniques, CO₂ laser irradiation can be used to produce locally ordered turbostratic carbon in a much faster and effective way compared to the conventional treatment in a furnace [3]. It appears important to optimize the synthesis protocol of hard carbons by CO₂ laser irradiation and provide a better understanding of the structural properties-electrochemical response relationships as a function of CO₂ laser heating parameters (temperature, exposure time). In the present work, a cotton fabric was used as a precursor and the structural modifications of the resulting carbon after the laser heat treatment were investigated by Raman spectroscopy and HRTEM.

Biography

Hbiriq Yassine was a Ph.D. Student at National Center for Scientific Research (CNRS), France. His present research mainly focused on Development of laser treatment within situ Raman spectroscopy monitoring on carbon materials for use in Sodium-ion batteries.

Cost Saving Schemes for Biomethanol Purification

Stefania Moioli^{1*} and Laura A. Pellegrini¹

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Abstract

Biosynthesis gas (bio-syngas) is a gas rich in CO and H₂ obtained by gasification of biomass, which can be used for the production of biomethanol, as substitute to the one produced from natural gas. Biomass sources are preferable for biomethanol than for bioethanol because bioethanol is a high-cost and low-yield product (Demirbas, 2008).

Bio methanol can be used as a clean biofuel or as a chemical feedstock. Its production process includes a section of its purification downstream the conversion unit, which is generally carried out by distillation, with relevant energy consumption that may significantly impact on the costs of the whole process.

This work aims at studying different configurations for the methanol purification section, so to determine the best one which allows for a reduction of the energy consumptions and thus of the operating costs.

The base scheme is composed of two main sections, one for removing the low boiling impurities present in the mixture mainly composed of methanol and water and the second one for separating water and other components so to increase the concentration of methanol to the required high purity.

Simulations have been carried out by using the commercial software ASPEN Plus®, by using the thermodynamic method Non-Random-Two-Liquid (NRTL), suitable for this system and for the low-pressure conditions, and by considering a rate-based approach for the simulation of the columns. On the basis of the obtained results, the scheme which favors a reduction of the operating costs of the plant has been determined.

Biography

Stefania Moioli is assistant professor (Ricercatore a Tempo Determinato B) at Dipartimento di Chimica, Materiali e Ingegneria Chimica “Giulio Natta” of Politecnico di Milano, where she is in charge of the courses “Process Plants” and “New Technology Frontiers in Gas Production, Transportation and Processing”. She is member of the “Group on Advanced Separation Processes & Gas Processing - GASP”, in which she studies the purification of acid gases, regarding in particular both thermodynamics and mass transfer with reaction modeling. Her research interests cover thermodynamics, kinetic modeling and steady state/dynamic process simulation.

Selection of the Proper Carbon-Based Working Electrode for the Catalytic Adsorptive Stripping Voltammetry

Agnieszka Królicka

Department of Building Materials Technology, Faculty of Materials Science and Ceramics, AGH University of Science and Technology, Mickiewicza, Krakow, Poland

Abstract

Working electrodes are the most important components of an electrochemical cell, which decide about the success of electroanalysis. The carbon-based materials can be easily machined and used in the form of discs, fibers, various types of paste, or carbon-filled polymers spread on the support by doctor blade or screen-printing method (SPE). Unfortunately, the binding polymers employed for the fabrication of inks for SPEs do not exhibit sufficient chemical resistance to oxidizing reagents. This factor strongly limits the applicability of SPEs in many applications, in particular in catalytic adsorptive stripping voltammetry (CAAdSV). In the present work, the usefulness of different heterogenous carbon electrodes (screen-printed carbon, mesoporous carbon, graphene, and reduced graphene oxide, boron doped diamond, and carbon paste) for the application in CAAdSV is discussed. Prior to application, the carbon-based supports were plated with bismuth, lead, tin, or tellurium to gain required sensitivity towards the analyzed ions. Then the catalytic systems involving chlorate, bromate, nitrite, hydroxylamine, and V(IV) complexes used to induce the catalytic reaction of metal complexes were tested employing electrodes of suitable electrochemical window. Voltametric studies, SEM imaging, and contact angle measurements were applied to evaluate the long-term stability and chemical resistance of the electrodes to the oxidizing action of catalytic agents.

Biography

Agnieszka Królicka, assistant professor, received her PhD in analytical chemistry from AGH-University of

Science and Technology (AGH-UST) in 2003. Since 2003 she has been a research scientist in the Faculty of Materials Science and Ceramics at the AGH-UST. Her current research interests are various aspects of electroanalytical methods and nanotechnology.

Graphene and Beyond Materials-Based Membranes to make Water Desalination more Fruitful and Efficient

Annarosa Gugliuzza*

Institute on Membrane Technology (CNR-ITM), Italy

Abstract

Water scarcity and pollution levels in water represent a real risk for human health and environment. Sustainable solutions to manage natural resources and protect environment are hence required. Membrane technology is a preferred choice for the production of drinking and reusable water. Green technologies such as membrane distillation and membrane crystallization are regarded as a real revolution in the way to manage seawater. However, their accomplishment on scale is severely dependent on presently available materials. There is hence urgency to design new advanced functional membranes in order to boost the production of larger amounts of better-quality water without affecting ecosystems. Herein, membranes filled with graphene and other 2D materials exfoliated via dispersant liquid phase are demonstrated to yield ultrafast production of freshwater from hyper-saline streams. These membranes take also the advantage of recovering better-quality salt crystals to be reused in various production chains. High productivity-efficiency trade-off is obtained exploiting the ability of 2D materials to accelerate water evaporation from saline solutions when a difference of temperature is applied across the membrane. Mass-energy transfer can be governed through the membrane, leading to amplified production of freshwater and less time-consuming formation of quality-crystals. It is demonstrated how the great potential of graphene flakes and beyond find new outlets in innovative water desalination.

Acknowledgements

We acknowledge financial grant from 'the Italian Ministry of Foreign Affairs and International Cooperation' within the framework of the Great Relevance International Project Italy (MAECI)-China (NSFC) 2018-2021 - New Materials, with particular reference to Two-dimensional systems and Graphene (2DMEMPUR)

Biography

Annarosa Gugliuzza is a Research Scientist at CNR-ITM. She received a Degree with honors in Chemistry and a PhD in Chemical Science from the University of Calabria, Italy. She worked abroad as a Visiting Researcher at the University of Ann Arbor (MI, USA) and POLYMAT Institute in San Sebastian (SPAIN). She is the scientific responsible for the Great Relevance International Project Italy-China 2DMEMPUR (MAECI-NSFC 2018-2020). She is editor of four books and co-author of more than 100 peer review publications and one patent. She served as a chair within International Conferences and continues to serve as an editorial boards member of repute.

Activated Carbon Fiber Cloth used as a Biomaterial to Improve Bone Regeneration

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²Univ. Côte d'Azur, CNRS, Inserm, Institut de Biologie Valrose, Nice, France

Abstract

This study is focused on the use of activated carbon fiber cloths (ACC) as biomaterials to be efficient in the field of bone regeneration. The commercial ACC used was selected after biological tests showing its good affinity with human osteoblasts. To improve the ACC biological properties, different treatments were performed. At first, the ACC surface was coated with biocompatible calcium phosphate (CaP) phases using a sono-electrodeposition process. A control of the process parameters allows getting a biomimetic calcium-deficient hydroxyapatite (CDA) coating. Then, the CDA coating was doped with bioactive strontium ions leading to biomimetic strontium-substituted CDA coating. We also took advantage of the ACC microporosity to adsorb bioactive molecules such as tetracycline. Finally, four types of ACC-based biomaterials were implanted in a bone defect performed in a femoral rat. After 1, 2 and 3 weeks of in vivo tests, the bone defects were investigated by X-ray micro-computed tomography to analyze the kinetic of bone regeneration. It is shown that the ACC use improves the bone regeneration and the kinetics are accelerated in the case of CDA and Sr-CDA coatings on ACC surface and in presence of adsorbed aspirin. The interest of ACC as efficiency drug delivery system is demonstrated.

Biography

Sylvie Bonnamy is Director of Research at CNRS (National French Center of Scientific Research). She is internationally renowned for her expertise in the multiscale characterization (HR-TEM) and the physicochemical studies of carbon materials (carbon biomaterials, nanotubes, porous carbons, carbon fibers, C/C composites). She was recipient of Carbon Schunck award in Berlin, 2000. She directed 18 PhD. A track-record of 80 publications in peer-reviewed journals, 5 patents, 9 book chapters, 28 invited lectures/keynotes and about 220 presentations in conferences. She participated to 60 international and national research programs. She is member of the director board of the French Carbon Group.

Stereolithography 3D Printing Technology as a Production Method to Generate 3D Porous Carbon for Electrochemical Capacitive Energy Storage

Babak Rezaei^{1*}, Anjali Achazhiyath Edathil¹, Jesper Yue Pan¹, Stephan Sylvest Keller¹

¹National Centre for Nano Fabrication and Characterization, DTU Nanolab, Technical University of Denmark, Denmark

Abstract

Electrochemical capacitors or supercapacitors (SCs) are typical energy storage devices that can store and release energy through physical adsorption/desorption of ions from an electrolyte (electric double layer capacitance) or electrochemical redox reactions (pseudo-capacitance) at the interface of electrode/electrolyte when voltage is applied. Among different types of materials, carbon materials with different

physicochemical properties have been widely employed as electrode materials for SCs due to their long-life cycles, electrochemical stability, high specific surface area and low cost. It is known that the overall electrochemical performance of the carbonaceous electrodes is largely dependent on the morphology and architecture of their materials. In this regard, employing permeable three-dimensional (3D) carbon architectures loaded with active materials offers higher energy density, shortened diffusion length for ions and higher charge/discharge rate capability, as compared with the same footprint area of 2D materials. In the past years, we have focused on expanding the toolbox for the micro- and nanofabrication to be able to prepare 2D and 3D pyrolytic carbon electrodes with dimensional features from macro to micro down to nano. In particular, stereolithography (SLA) as a cheap and accessible fabrication technique was employed to fabricate free-standing and on-chip carbon electrodes for supercapacitor application. In general, higher electrochemical capacitance was recorded due to the increased surface area of the carbonaceous electrodes and loading of the 3D complex carbon architectures with pseudocapacitive materials like crystalline hausmannite-Mn₃O₄.

Biography

Babak Rezaei is a senior Postdoc at DTU Nano lab, Technical University of Denmark. He received a Ph.D. in Nanotechnology at Tehran Polytechnique University, Iran. From 2015 until 2016 he worked as a visiting researcher in the group of Prof. Anthony P. F. Turner at Linköping University, Sweden. His main fields of investigation are electrochemical capacitors, biosensing, stereolithography and DLP 3D printing, pyrolytic carbon, enzymatic biofuel cells and wastewater treatment.

Preventing Degradation at Conducting Carbon Interfaces in Solid-State Batteries

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Abstract

Solid-state batteries (SSBs) are investigated with the goal to exceed the energy density of lithium-ion batteries. They consist of three cell components: a lithium metal anode, a thin solid electrolyte separator layer and a composite cathode layer. The solid electrolyte needs to have a high ionic conductivity for lithium transport, for example lithium-thiophosphates such as Li₆PS₅Cl. This solid electrolyte is often used in SSB research. However, it has a low electrochemical window of stability and decomposes at high and low potential. In order to increase the electronic conductivity in the composite cathode and to electronically connect all cathode active particles, carbon additives, such as vapor-grown carbon fibers, are added to the cathode composite mixture. As the conducting carbon additive is electronically connected to the cathode active particles, the solid electrolyte also decomposes when in contact with the carbon additive during cell cycling. The decomposition mechanism is investigated by cyclic voltammetry. The decomposition products are analyzed by SIMS and XPS. Inorganic and polymer coatings can reduce the interface decomposition, while maintaining the electronic connectivity with the cathode particles in the composite cathode. Non-conducting coatings on the carbon, such as alumina or polymers can reduce degradation and improve SSB performance.

Biography

Felix Richter is a junior research group leader in Physical Chemistry, Materials Science and Characterization at the Center for Materials Research of the Justus-Liebig-University Giessen. He works on concepts that link inorganic materials and polymers. Currently, the Richter workgroup specializes in analyzing the fundamental

transport mechanisms of ions across the interfaces of different battery components and the development of hybrid approaches for solid-state batteries. In March 2020, he received the NanoMatFutur funding by the Federal Ministry for Education and Research on the topic of Solid-State Batteries with Lithium Metal and Polymer Protective Coatings.

Silicon-Based Graphite Electrode Materials–Impact of Electrode Architecture on Electrochemical Performance and Cell Degradation

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Abstract

Graphite is commonly used as anode material in commercial lithium-ion-batteries (LIBs). Due to the demand for a significantly increased energy density for electrical vehicles, there is worldwide a strong effort in research and development to add silicon nanoparticles to composite electrodes. Pure silicon has the benefit to enable almost one order of magnitude higher gravimetric energy densities than graphite. Due to a huge volume expansion of silicon of about 300 % during electrochemical cycling it is so far most promising for commercialization to use silicon/graphite composites, instead of pure silicon. However, for silicon/graphite electrodes, the volume expansion during lithiation is still a problem regarding an enhanced cell degradation. Thick film electrodes are further concept to enable increased energy densities on cell level by avoiding inactive cell components namely separator and current collector materials. Due to limitations in diffusion kinetics in thick film electrodes and an increased diffusion overpotential at high charging/discharging currents, a significant drop in power density is observed. Material processing using ultrafast laser radiation provides now an exceptional approach to overcome power and lifetime limitations of thick-film and silicon/graphite electrodes. Laser structuring was applied on electrode materials without changing the electrochemical and material properties of the active material by maintaining mechanical integrity. Post-mortem studies using laser-induced breakdown spectroscopy were carried out. A reduced cell degradation was achieved with structured electrodes in comparison to unstructured ones. Laser structuring of electrodes offers a new manufacturing tool for next-generation battery production to overcome current limitations in electrode design and cell performance.

Biography

Wilhelm Pfleging is head of the group Laser Materials Processing at Karlsruhe Institute of Technology (KIT). He has more than 27 years of experience in laser technology and material science. He has published over 160 peer-reviewed articles in scientific journals, books and conference reports. He has six patents granted. He initiates and manages several industrial and academic collaborative research and development projects. Since 2008 his research is focused on the development of laser-assisted processes, analytics, and manufacturing of advanced lithium-ion batteries. He is Senior Lecturer at KIT for “Laser Technology” and “Laser-assisted methods and their application for energy storage materials”.

Adapting Carbons for Cathodes and Anodes in Lithium-Based Batteries

Susanne Dörfler* and Tom Boenke^{1,2}, Christian Kensy^{1,2}, Kay Schönherr¹, Benjamin Schumm¹, Paul Härtel^{1,2}, Thomas Abendroth¹, Holger Althues¹, Stefan Kaskel^{1,2}

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²Technische Universität Dresden, Anorganische Chemie I, Bergstr, Dresden, Germany

Abstract

In the last decade, electromobility and stationary energy storage have become more and more key issues of present science and development. Lithium-based batteries are energy devices that attract special attention. Generally, carbon materials are commonly used materials for this application due to their light weight, tunable microstructure, low resistance, and good polarizability. In addition, they are chemically stable, and the production techniques are mostly already up-scaled and not too cost-intensive. In state-of-the-art lithium-ion batteries, graphitic carbons take the role as anode active materials. In this work, new approaches in order to adapt carbon materials for anodes with advanced properties, both for liquid as well as for solid electrolytes, are discussed. Another energy storage application, especially for porous carbons, is the Lithium-Sulfur (Li-S) battery. In order to utilize the electronic inductive sulfur or Li₂S, electrons need to be transferred from a conductive carbon framework to the active materials. In this work, the impact of different carbon porosities and electrolyte formulations on the energy and power density of Li-S batteries are shown. In addition, a scalable nitrogen functionalization and its impact on Li₂S precipitation and cycle stability is discussed. Finally, a full cell with a pre-lithiated hardcarbon as anode for cyclestable lithium-sulfur batteries as next generation station energy storage concept is presented.

Biography

Susanne Dörfler studied chemistry and received her Ph. D. in the field of vertically aligned carbon nanotubes for supercap and lithium sulfur battery electrodes from the University of Technology Dresden in 2013. She then led a junior research group financed by the European Social Fund in the field of LiS batteries. Since 2016, she has been working as a group manager “Battery and Electrochemistry” at the Fraunhofer Institute for Material and Beam Technology in Dresden. Her main research topics are material development, establishing structure-property relations between the respective materials, electrolytes, and their electrochemical performance.

Electrochemically Enhanced or Inhibited Scale Deposition Inside Graphite Cylinders in Parallel Connection

Laura Edvardsen*, Malin Torsæter, Kamila Gawel, Sigrid Lædre, Paal Skjetne

SINTEF Industry, Trondheim, Norway

Abstract

Surface scaling of calcium carbonate, calcium sulphate and other minerals whose solubility is highly pH dependent can be either accelerated or inhibited by applying electrical polarization to the surface given that the surface is electrically conductive. This method can be utilized to both protect the surface from scaling but also to remove scaling ions from the solution in one place to protect other installation elements from scaling. Here we present the results of calcium carbonate deposition in a flow system of parallelly connected graphite tubes. Two of the three tubes are electrically polarized at the potential of 5 V. Scaling solution containing 45 g of $\text{CaCl}_2 \cdot 2\text{H}_2\text{O}$ and 0.84 g NaHCO_3 is circulated through the system with a flow rate of 1 mL/min. We show that the scaling is enhanced on the cathode and inhibited on the anode. We also show that the precipitate is mainly located in the space between the electrodes. When dielectric spacer is placed between the electrodes the electrochemical communication between the two electrodes is entirely blocked despite of large surface area of the electrode being exposed to electrolyte. We discuss the results in view of electric field distribution in the system. Our results are of importance for the design of electrochemical scale mitigation systems.

Biography

Laura Edvardsen did Master of Science in SINTEF Industry, focusing on geological storage of CO_2 and plugging and abandonment of oil wells. Leader of Green Team SINTEF Industry. Working to make SINTEF an even more sustainable corporation. She had MSc (sivilingenior) in Applied Theoretical Chemistry, specializing in computer simulations and Non-Equilibrium Thermodynamics. During her study of chemical engineering, she has also gained a broad training in laboratory work. She was a part of KONGSBERG's summer intern team (2018) for investigations of technological approaches to solve the marine plastic problem.

Functionally Graded Carbon Fiber-Reinforced Ceramics for Extreme Environments: Characterization and Numerical Assessment

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²Politecnico di Milano, Dept. of Aerospace Science and Technology, Via La Masa, Milano, Italy

Abstract

ZrB₂ is an ultra-high temperature ceramic (UHTC) possessing a melting point exceeding 3000°C and a combination of exceptional engineering and physical properties.[1,2] As such, ZrB₂ ceramics are potential candidates for space and hypersonic components. The main drawbacks that restrict the employment of ZrB₂ ceramics for a wider spectrum of applications are related to the low damage tolerance, poor oxidation resistance and relatively high density. However, the introduction of discontinuous C fibers can increase both ZrB₂ robustness and notably decrease the total weight.[3] Moreover, the addition of secondary phases, such as MoSi₂, can further improve the high-temperature strength and, most importantly, the oxidation performance of the boride matrix owing to an in-situ development of a complex multilayer oxide structure. [4] However, detrimental chemical reactions between Mo-compounds and C fibers occur during sintering at high temperature thus leading to degradation of the fibers and loss of their toughening function. Therefore, an accurate choice of the sintering additive is paramount to preserve the fiber structural function. Here we present a functionally graded (FG) composite made up of a ZrB₂-MoSi₂ outer scale, to provide oxidation and ablation resistance, and a progressively C fiber-rich body, to guarantee failure tolerance and lighten the whole structure. To define the best FG architecture and exploit residual stress toughening upon layering,[5]

thermo-elastic simulation by finite element modeling is adopted.

Biography

Laura Silverstoni obtained PhD of Industrial Chemistry from University of Bologna. Her field of expertise in design, processing and characterization of structural ceramics with emphasis on materials for severe environments. Lead author or co-author on more than 100 manuscripts published in peer-reviewed journals. Editor of the Journal of the European Ceramic Society. PI or co-PI on grants funded by the US Air Force Office of Scientific Research and US Army as well as other government agencies and companies.

Enhanced Hydrogen Storage Properties of NaAlH₄ Confined in Carbon Black

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¹University of Tartu, Estonia

²KTH Royal Institute of Technology, Sweden

Abstract

New efficient and economically feasible hydrogen storage methods are among the key enabling technologies for transitioning to a hydrogen economy. Although hydrogen is an excellent medium for energy storage with thrice the gravimetric energy density of gasoline, it suffers from low volumetric energy density. Chemical binding of hydrogen in complex metal hydrides, such as in the extensively investigated sodium aluminum hydride (NaAlH₄), offers high gravimetric energy densities for the total system. However, the system is hampered by slow kinetics, high required operational temperatures (≥ 183 °C), and poor reversibility demanding high hydrogen pressures for rehydrogenation.

The potential of mesoporous and nanoparticulate carbon materials in hydrogen storage applications in combination with solid-state H₂ storage mediums will be demonstrated. The commercial carbon black Vulcan XC72R (Cabot, USA) was used to synthesize composite materials with high NaAlH₄ loadings (50-90 wt%). The ball-milled composites exhibited improved H₂ release properties even at very high NaAlH₄ wt%. Hence, even relatively small amounts of carbon can significantly alter the hydrogen storage properties of NaAlH₄. Hydrogen evolution was noted even at near ambient conditions in the case of the composites with the lowest wt% of NaAlH₄. Furthermore, dehydrogenation/hydrogenation cycling experiments resulted in reversible storage over several cycles at remarkably low temperatures and pressures.

Biography

Kenneth Tuul (b. 1996) started his Ph.D. at the University of Tartu in 2021 on the project Nanoconfinement of complex metal hydrides in mesoporous carbon scaffolding materials for hydrogen storage. The primary focus of his research is applying carbons in improving the hydrogen storage properties of solid metal hydrides. In 2019, he was awarded 1st prize in the Estonian bachelor's thesis competition „Raven”, and in 2021, he received his MSc at the University of Tartu cum laude.

Optical Anisotropy Evolution of thin Porphyrin Films Grown on HOPG During the Molecular Oxidation in Acid Electrolytes

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²Istituto di Scienze e Tecnologie Molecolari of the CNR (ISTM-CNR), SmartMatLab Center, Italy

Abstract

Graphite electrodes still represent important devices for current batteries (e.g., lead-acid systems)¹, possible electrodes in Li- or Na-based batteries of next generation² and, in any case, a model-systems for studies and investigations of other stratified crystals (e.g., MoS₂, etc.)³. For these reasons, research and technology are involved in the graphite-electrode optimization in terms of chemical stability in acid environments⁴, surface protection⁵ and electrode performances⁴.

Recently, we proved that the graphite electrode surface can be protected by using a single molecular architecture without changing or altering the electronic performances⁵. It is now important to follow and monitor the stability of the deposited molecular film as a function of time and in real time during the electrochemical processes. This target can be reached by exploiting optical probes, which able to reach the electrode surface even when immersed inside a transparent electrolyte.

In this contribution, we show original results obtained by coupling a special optical spectroscopy system [namely reflectance anisotropy spectroscopy (RAS)]⁶ with a three-electrode electrochemical cell where the working electrode is a highly oriented pyrolytic graphite (HOPG) crystal covered by a thin film of free-base porphyrins (namely, H₂TPP). The latter can undergo an oxidation process at high anodic potential that is able to prevent the well-known graphite surface detriment in acid electrolytes⁴.

Biography

Gianlorenzo Bussetti is an Associate Professor at the Department of Physics, Politecnico di Milano at Milan, Lombardy, Italy.

He obtained PhD thesis with a study on the optical properties of organic films (“Thin and ultra-thin organic layers investigated by Reflectance Anisotropy Spectroscopy”). Currently he was working on the physical and chemical properties of electrified surfaces at the liquid/solid interface by means of electrochemical scanning probe microscopy (EC-SPM).

Amorphous Carbon Nitride Integration as Ultramicroelectrode in Microfluidics for Specific Nucleic Acids Capture and Detection

Claire Poujouly¹, Marie-Charlotte Horny^{1,3}, Florence Billon², Claude Deslouis², Alain Pailletet³, Jean Gamby^{1,3*}

¹Paris-Saclay University, France; ²CNRS, France; ³Sorbonne University, France.

Abstract

This paper reports a new method in microfluidics that integrates capture and detection modules for the analysis of circulating micro-RNA (miRNA) without a PCR amplification stage. The fabrication of the electrochemical detection module with channel microelectrode was reported in Lab chip 2016 [1], and an analysis of the increasing of the efficiency of DNA electrochemical hybridization detection using microelectrodes in droplets was reported at ECS 2016. [2] Here, a methodology is proposed to synthesize and integrate amorphous carbon nitride (aCN_x). Conversely to other carbon materials such as diamond like carbon, that are difficult to integrate in microfluidic devices due to their high temperature deposition, a-CN_x is easily synthesized at room temperature on various materials using sputtering techniques. The experimental set-up allows us to perform all stages of the analysis in 30 minutes with an attomolar detection threshold for miRNA-122 (DNA target mimicking the liver-specific micro-ribonucleic acid 122 (miR-122)), better than PCR, without amplification. One of the goals of our project is to further reduce this analysis time by two. This involves an incrementation of the technological process for the multiplexed measurements and an optimization of the aCN_x synthesis for a better efficiency of the steps of miRNA capture and detection.

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(2) Horny, M.-C.; Lazerges, M.; Siaugue, J.-M.; Pallandre, A.; Haghiri-Gosnet, A.-M.; Gamby, J. DNA Electrochemical Hybridization Detection in Droplets Using Gold Ultramicroelectrodes in a Two-Electrode Configuration. *ECS Meeting Abstracts* 2016, (39), 1973.

Biography

Jean Gamby received his PhD degree in Electrochemistry from Paris University in 2003 (LEM, Paris, France). During 2003–2005, he was in Postdoc position at EPFL (Switzerland) working on capacitive microchip devices in polyethylene for bioanalytical applications. He is CNRS researcher since 2007 where he focused his research activities on the development of microfluidic systems during the period stayed in 2007-2016 at the LISE (Sorbonne University, Paris). In 2016, he joined the Centre de Nano sciences and Nanotechnologies (CNRS Paris-Saclay University) to develop an activity “Electrochemistry in the MNBF Department. Since 2019, he is the head of the BioSys team at the MNBF department of C2N.

PANI/RGO Porous Ammonia Gas Sensor

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²Department of Bioengineering, University of California, Los Angeles, Los Angeles, CA

Abstract

There is a widespread notion that flexible carbon-based customized shape structures are advantageous for gas sensing purposes. The facile fabrication process and high sensitivity of resistive gas sensors make them a great candidate for monitoring hazardous gaseous substances such as ammonia [1], [2]. Resistive gas sensing depends on different factors such as the geometry of the sensing area, the chemical nature of the target gas, and sensing element and environmental condition. Graphene-based materials are vastly used

in ammonia detection applications. The highly conductive nature of rGO in a composition with a sensitive polymer such as polyaniline (PANI) provides a selective and sensitive platform for ammonia detection [3]. Using triply periodic minimal surfaces (TPMS) geometries allows us to fabricate customized geometries for gas sensing applications. Silicone rubber elastomer as a durable flexible material can operate in harsh environmental conditions and provides desirable physicochemical properties for gas detecting such as tunable flexibility, hydrophobicity, and chemical stability. In this direction, we present a flexible PANI-rGO based TPMS porous sensor for monitoring ammonia in a harsh environment.

Biography

Hamed Mirzaei is a Ph.D. candidate at university of British Columbia and his research is focused on development and fabrication of reliable porous-based gas sensor for detecting hazardous gases in room temperature.

Impact of Nanocarbon Dimensionality onto SNO₂-C Composite Used As Anode in Secondary Lithium Battery

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²MINES ParisTech, PSL University, Centre for processes, renewable energies and energy systems (PERSEE), France

³Safran Tech, SAFRAN, Rue des jeunes Bois, 78117 Châteaufort, France

Abstract

Tin dioxide (SnO₂) has been studied in a wide range of fields because of its nontoxicity, semi-conductor behavior associated to their good mechanical and thermal stabilities. In lithium-ion battery, when used as anode, a huge theoretical capacity up to 993 mAh.g⁻¹, 3 times that of graphite, is obtained. However, the electrochemical process implies huge volume changes and low cyclability. To limit the internal stress, a buffer matrix is needed, and nanocarbon-based ones appear as the bestii.

To do a smart composite, its synthesis, the dimensionality of the nanocarbon which will be coated by tin dioxide must be revisited. In this talk, mechanochemistry and solvothermal syntheses are implemented on mixtures of tin chloride with either graphene, MWCNT or carbon aerogel. Correlations between the characteristics obtained by a fine characterization of composite nanostructures by solid state NMR, SEM and N₂ sorption and their electrochemical properties are established. A 20 w/w % of MWCNT allows to increase by half the number of cycles and power density tests highlight the interest of solvothermal synthesis and sustainable 2C current density.

Biography

Katia Guerin Araujo da Silva is an associate professor at the Clermont Auvergne University. After getting the title of engineer from ENSCPB school, she received her Ph. D in chemical physics at Bordeaux University in 1999. She worked on lithium-ion insertion mechanism into graphite and hard carbons through solid state NMR and Raman spectroscopies.

Her research activities are now focused on solid-gas fluorine chemistry to discover new materials usable mainly in electrochemical energy storage materials in batteries, fuel cells and supercapacitors. She is leading a team of 20 persons on this topic.

Carbon Quantum Nanodots for Mercury Sensing

Douglas Austin and Yanfeng Yue

Delaware State University, Dover, Delaware

Abstract

The study of toxic heavy metals and their impact on the environment is closely watched to try and find ways of identifying contamination and mitigation of the pollution. The term 'heavy metal' refers to any metal and metalloid element that has a relatively high density ranging from 3.5 to 7 g/cm³ and is toxic or poisonous at low concentrations, such as mercury (Hg). Exposure to Hg is known to damage microtubules in platelets and red blood cells disrupting cell cycle of many organs leading to early cell apoptosis. This damage affects the nervous, cardiac, gastrointestinal, and renal systems in the human body. This research will involve microwave assisted hydrothermal synthesis of carbon nanodots and further used as a sensor for Hg detection or monitoring. Carbon nanodots which are luminescent in nature due free electrons in their structure will lose their luminescence in the presence of metals due to the charge interactions. The synthesis involves green chemistry that will keep waste down to a minimum and uses readily available carbon sources such as amino acids, and even waste from plant material. The end goal is to create carbon nanodot based sensors that can be applied to a device and used in the field to detect heavy metals in aqueous solutions. Currently dopamine hydrochloride and citric acid along with hexamethylenetetramine were used to create carbon nanodots with luminescent properties. These products were tested by adding metal salts and observing the quenching effect of the products. The materials being studied will help the world of science by finding ways to easily monitor heavy metal in aqueous solutions with a focus on water bodies in the environment.

Biography

Douglas Austin currently Working in Delaware State University.

None-Metallic Hermetic Fusion of Diamond Micro-Components

Melanie E.M. Stamp^{*1,2}, Alastair Stacey³, Kate Fox³, Steven Prawer² and David J. Garrett³

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Abstract

Permanent, implantable wireless devices that interact with neuronal systems are emerging in medical research, diagnostics, and therapeutics. They contain sensitive micro-electronics ranging from passive radio-frequency identification tags to active sensors and stimulators, requiring robust and biocompatible packaging. Hermetic sealing is one of the significant challenges for these prostheses, where a strong desire to reduce the size of such devices, enable wireless communication methods and protect these devices in the

body for many decades is required. Diamond as a material provides excellent biochemical stability, chemical inertness and mechanical stability. However, sealing diamond to diamond joints is a challenging task. We present a novel technology to hermetically fusing polycrystalline diamond using a thin silicon interlayer as a braze material in a hydrogen plasma for applications in biocompatible packaging of medical prostheses. This hermetic sealing is based on SiC formation at the interface of both materials and under a highly reductive atmosphere, where the plasma pressure controls the sealing temperature. Our results indicate a hermetic sealing of better than 2.2×10^{-9} cm³ atm/s of helium in a non-destructive optical methods, and excellent wetting of Si on smooth and rough diamond surfaces. The method is an industrially relevant route to forming long lived diamond bonding, in particular the incorporation of transparent ultrathin diamond windows to enable for optical power and data communication.

Biography

Melanie Stamp is a researcher at the Universite de Sherbrooke, Canada and honorary researcher at the Universite of Melbourne, Australia. With her background in Materials Science and Biophysics, her skillset is bridging the disciplines of science and medical technology, bringing together different research expertise to focus on new perspectives. Her experience ranges from studying interaction of cells with nanomaterials, acoustic and electrical manipulation. Her work has been recognised in stimulation of cells and tissue phantoms for designing life-on-a-chip systems and implant engineering. In her current research, she investigates the potential of diamond and carbon electrode arrays for neuronal stimulation.

Graphene/PDMS Touch Sensor Fabrication Using Sugar Cube Method

Sara Ghaderahmadi¹, Hamed Mirzaei¹, Mohammad Arjmand¹, Mina Hoorfar^{1*}

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Abstract

Flexible electronics have gained a lot of attention for application in wearable gadgets and transparent flexible sensors [1]. Due to the biocompatibility, durability, hydrophobicity, transparency, and flexibility polydimethylsiloxane (PDMS) is a great candidate for flexible sensors [2]. Among different types of wearable and flexible tactile pressure sensors such as capacitive, piezoresistive, piezoelectric, etc, the piezoresistive sensing method shows significant advantages in terms of sensitivity, design simplicity, and cost-effectivity. The sensitivity of the piezoresistive touch sensors depends on the resistance and the geometry of the sensor design. Graphene-based materials alone or in collaboration with other conductive materials have been widely used in pressure sensor fabrication to provide a superconductive network. A combination of flexible PDMS structure with graphene can build a robust conductive 3D network that is desirable for touch sensing applications. Herein, we present a study of a highly sensitive graphene-PDMS flexible touch sensor utilizing a sugar cube as a sacrificial porous template method. In addition, we will introduce a novel method for combining graphene-based material with PDMS to achieve a stable sensing platform.

Biography

Sara Ghaderahmadi received her B.A.Sc. Degree in Electrical Engineering from K.N.Toosi University of Technology, Tehran, Iran in 2019. She joined the Advanced Thermo-Fluidic Laboratory (ATFL) at the University of British Columbia as an M.A.Sc student in 2019. Her research is focused on Development a MOS-based gas sensor for self-powered applications.

Sara is an MSc student at NPPL. Sara received her B.Sc. degree in electrical engineering from K.N.Toosi

university of technology, Tehran, Iran. Her B.Sc. thesis was focused on PEDOT: PSS chemical treatment and its application in power generation. Her MSc thesis is on flexible electronics using engineered graphene. She is supervised by Dr. Hoorfar and co-supervised by Dr. Arjmand. in NPNL, Sara is working on the development of metal oxide gas sensors.

The Catalytic Effects of Iron on the Carbonization Process of Electrospun Carbon/Iron Nanofibers and their Utilization as Nanoadsorbents for Enhanced Cr (VI) Removal from Water

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Abstract

Electrospun polyacrylonitrile / iron nitrate (PAN/Fe (NO₃)₃) nanofibers are prepared and used as precursor nanofibers for the production of carbon/iron nanocomposite fibers via a carbonization process. The catalytic effects of the metallic iron on morphologies, chemical structures, graphitic carbon growth, and thermal behavior during and after the carbonization process are carefully investigated. The presence of iron nitrate can increase the fiber size and convert the non-woven morphology into a self-aligned assembly. The presence of catalytic iron facilitates the stabilization and the carbonization of the PAN fibers, resulting in an increased carbon yield along with more ordered and larger graphitic crystallites. The developed carbon/iron fibers can be used as an ultra-effective nanoadsorbent for removing toxic Cr (VI) in water. The nanoadsorbent shows a fast and powerful performance in Cr (VI) removal through reduction and adsorption (maximum removal capacity of 445.3 mg/g). The α -Fe nanoparticles on the carbon nanofiber surface are first oxidized to rapidly reduce the mobile Cr (VI) into the static Cr (III). Subsequently, the diffusion controlled redox reactions between the internal iron of the carbon matrix and the Cr (VI) achieve a sustained continuous Cr (VI) removal for 60 days. Furthermore, this versatile material is magnetic making processing of separation and recycling simple to perform.

Biography

Evan K. Wujcik is currently an Assistant Professor in the Department of Chemical and Biological Engineering and an Adjunct Professor in the Department of Civil, Constructions, and Environmental Engineering at the University of Alabama [Tuscaloosa, AL USA], where he directs the Materials Engineering and Nanosensor [MEAN] Laboratory. He obtained his Ph.D. in Chemical and Biomolecular Engineering from The University of Akron and his MBA, MS in Chemical Engineering, BS in Applied Mathematics, and BS in Chemical Engineering (2008) from The University of Rhode Island. His research interests include advanced materials, polymers, and sensors towards wearable and environmental applications.

Characterization of Carbon-Carbon Composite Wear Debris from Brake Applications

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Abstract

Carbon-carbon (C-C) composites are often used as friction and brake materials due to their high strength, low density, excellent frictional properties, high thermal conductivity and high heat capacity. When worn, C-C composites produce particulate wear debris. The fine wear debris particles then form a layer on the wear surface, known as a friction film layer, which has the potential to change the overall frictional performance of the system. The size, shape and chemistry of these wear debris particles and friction layers can give information about the mechanisms of wear in the composite and the effects of temperature, humidity, oxidation and other chemical modifications that can occur depending on the wear environment. However, this analysis is rather difficult to perform due to the wide range of particle size, from small primary particles to large aggregates. The chemical and material similarities of the carbon fiber and matrix further complicates decoupling the effects of the different components of wear debris on performance. This research explores particle separation and characterization techniques to obtain information about the C-C wear process. The principle technique for particle separation is density gradient ultra-centrifugation (DGU) in which fibrous and matrix-rich particles are separated based on their density. Orthogonal analysis with Raman and UV-vis spectroscopy, optical and electron microscopy, and X-ray Photoelectron spectroscopy can then be made on separated aliquots. Understanding the properties of the wear particles and friction film gives information about the wear process and can help inform future design and material considerations.

Biography

Matthew Noor is a post-doctoral researcher at the National Institute of Standards and Technology (NIST). Matt earned his PhD in Chemical Engineering from Auburn University in the laboratory of Dr. Virginia A. Davis. His PhD work focused on interactions in anisotropic nanomaterials dispersions. As an associate of the Particles, Tubes, and Colloids project at NIST, he is working to characterize particle size and composition distributions in complex mixtures that result from the wearing of composite materials. These particle populations can contain a wide range of sizes, shapes, and chemical functionalization, which make them particularly difficult to characterize.

DAY-3

Detection to Polar and Non-Polar Organic Solvents by Flexible Gas Sensor Based on Multi-Walled Carbon Nanotube Paper

Mengli Zhang^{1*}, Shuhei Inoue², Yukihiro Matsumura³

Hiroshima University, Japan

Abstract

High structural porosity and high specific surface area make Carbon nanotubes (CNTs) to be the potential material for gas sensors. In previous study, Spin-coating method was developed to make gas sensor based on multi-walled carbon nanotube (MWCNT) film. MWCNT film with substrate increased the weight of gas sensor and limited the flexibility. Therefore, we considered to fabricate MWCNT paper for removing the substrate and increasing the flexibility.

In this study, multi-walled carbon nanotube (MWCNT) paper-based gas sensor is developed by a low-cost solution called filtration method. And the characteristics of MWCNT gas sensor are investigated at room temperature. The uniformity of MWCNT paper is measured by four probes method, which checking the resistance of 5 points for each CNT papers. Then, we developed the experiments under room temperature to observe the sensor response of MWCNT paper-based gas sensor. The target gases are polar organic solvents (Ethanol, Acetone) and non-polar organic solvents (Benzene, Cyclohexane), And the sensor response defined by equation (1).

$$S=R-R_0R_0 \quad (1)$$

where S denotes sensor response, R represents the sheet resistance after the reaction gas was introduced, and R_0 represents the sheet resistance under the vacuum condition.

Results show that MWCNT paper gas sensor has stable repeatability, the response of MWCNT paper gas sensor response to polar organic solvents (Ethanol, Acetone) fit to the Langmuir isotherm, and the response of MWCNT paper gas sensor response to non-polar organic solvents (Benzene, Cyclohexane) fit to the VI Isotherm.

Biography

Mengli ZHANG is a Phd student at Hiroshima University, Japan. Her research focuses on multi-walled carbon nanotube paper gas sensor, identifying and understanding the process of adsorption of gas molecules is key to the development of gas sensor with faster and higher response. Ms. Mengli ZHANG has received Chinese Government Scholarship (CSC NO. 202008050230). And she got the Best Presentation Award at the 4th International Symposium on Fuels and Energy (ISFE2020), Best Oral Presentation Award and Outstanding Oral Presentation Award at the 9th Joint Conference on Renewable Energy and Nanotechnology (JCREN 2020).

CNT Gas Sensor: Detection Mechanism and Physisorption

Shuhei Inoue^{1,*}, Mengli Zhang¹, Yukihiro Matsumura¹

Hiroshima University, Japan

Abstract

Carbon nanotube (CNT) thin film is expected to be a next-generation gas sensor owing to flexibility and room temperature operation unlike present gas sensors. Here, it is important to understand the detection mechanism for practical use. Regarding a detection mechanism of gas sensor using isolated CNT, two mechanisms have been suggested; modification at CNT/electrode contact interfaces and charge transfer between CNT and adsorbed gas. Based on previous studies, it can be expected that CNT junctions play an important role in gas detection of CNT gas sensor, especially CNT film gas sensor because it has a great number of junctions. In our previous study, we found that the electric resistance changes were explained by Fluctuation Induced Theory that originally explained the electric resistance of conductive materials with a lot of very small insulation parts. CNT film was fabricated by spin coating method using a dispersed CNT solutions on the glass substrate. This substrate was equipped 4 electrodes to measure its sheet resistance. With respect to the microscopic cross section view, the thickness might be not the same, but it showed macroscopically uniform. When the adsorbed gas was not so reactive i.e. physisorption was shown, the change of the sheet resistance showed Langmuir isotherm under some assumptions. At first, we could not explain those assumptions were appropriate or not, but we finally understood the mechanism for the change of the sheet resistance. These assumptions were correct and their details will be presented in the conference.

Biography

Shuhei Inoue earned Ph. D (mechanical engineering) at the University of Tokyo in 2003. He was a postdoctoral fellow (JSPS) under the supervision of Prof. Maruyama in the University of Tokyo. He became an assistant professor in the School of Engineering, Hiroshima University, Japan; and currently he is an associate professor in the Graduate School of Advanced Science and Engineering, Hiroshima 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.

Asymmetric IR-Catalyzed Carbene C–H Insertion

Tatsuya Uchida^{*}, Keigo Hashimoto, Yuki Yamakawa, Takashi, Ikuta

Kyushu University, Japan.

Abstract

Asymmetric carbene C–H insertion is an important and strong tool for the construction of chiral carbon framework. Although, various methodologies have been reported in this field, however, stereoselective C–C bond formation via C–H bond activation has been limited. Among them, transition-metal catalyzed carbene C–H insertion would be becoming one of ideal and versatile tools for the formation of C–C bond,

if C–H bond, even stable C(sp³)–H bond, could be transformed with high chemo-, site-, and stereoselective manner. Herein we described the high catalytic utilities of iridium-salen complex in site-selective asymmetric carbene C–H insertion using α -aryl- α -diazoacetates as carbene precursor.

Iridium-salen complex-catalyzed carbene C–H insertion reaction using various α -aryl- α -diazoacetates as carbene source underwent at benzylic, allylic, and propargylic carbon with excellent diastereo-, enantio-, and site-selectivity. Based on the mechanistic studies such as kinetic and computation, it was thought that the reaction includes rate-determining asynchronous insertion process.

Biography

Tatsuya Uchida graduated from Kyushu University (KU) in 1999, where he received his doctoral degree in 2004 under the direction of Professor Tsutomu Katsuki. In 2002, he was adopted as DC2 of a Research Fellowship for Young Scientist from JSPS. In 2004, he joined the Department of Chemistry, Graduate School of Science, KU, as a Research Associate and was promoted to Assistant Professor in 2007. He was promoted to Associate Professor in that department in 2012 and moved to the Faculty of Arts and Science at that University in 2014. He took an additional position at WPI-I2CNER, KU, in 2010

Superdense Hydrogen Adsorption on Carbon Materials at 20K

Takayuki Ichikawa*, Hiroyuki Gi, Hiroki Miyaoka and Norio Ogita

Graduate School of Advanced Science and Engineering, Hiroshima University

Abstract

Hydrogen adsorption on the surface of porous materials, such as carbon nanotubes, metal organic frameworks, and activated carbon, has been widely investigated. In this study, the measurements of adsorbed hydrogen density at 20 K were carried out for the super activated carbon with more than 3000 m²/g surface area. The density of adsorbed hydrogen was found to be much higher than that of liquid hydrogen and comparable to solid hydrogen density. Generally, when estimating the surface area, the assumption that the adsorption state is a liquid state at the boiling temperature of the adsorption medium has been adopted. However, this result shows inconsistency with this assumption. This superdense state of adsorbed hydrogen is not understood well. Therefore, more detailed analyses are necessary for estimation of the density of adsorbed hydrogen on the super activated carbon and graphene as a reference material. As a result, the adsorbed hydrogen on graphene did not show the superdense state that was observed only on the activated carbon. This result suggests that presence of pores is one of the important factors to form the superdense adsorbed hydrogen.

Biography

Takayuki ICHIKAWA is a professor of materials engineering for energy conversion and storage in Hiroshima university, Japan. He studied theoretical physics at Hiroshima univ. and received his Ph. D in the field of low temperature physics at Hiroshima univ. in 2002. After that he slightly changed his field to experimental material research. He is focusing mainly on inorganic hydrogen storage materials, such as amide-imide systems, magnesium hydride, ammonia, titanium hydride, ammonia borane, and carbon materials. He now investigates the economic evaluation of hydrogen production as well.

High-Throughput Screening of 2D Materials for Hydrogen Evolution

Lei Shen* and Tong Yang

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Abstract

Two-dimensional (2D) materials with intrinsically active basal planes are promising alternative catalysts to the Pt-group noble metals for large-scale hydrogen production. Herein, we perform a comprehensive screening of a 2D materials database (2DMatPedia) to identify such 2D catalysts for hydrogen evolution reaction (HER). Using the differential hydrogen adsorption Gibbs free energy as the thermodynamic descriptor, we report nine conducting, synthesizable, and exfoliable 2D catalysts with active basal planes (C8, NbS₂, NbSe₂, TaSe₂, IrTe₂, Ti₂Se₂, Ba₂Cu₂, Pr₄C₂Cl₅, and Ce₄C₂Br₅), which may have an HER performance comparable to that of Pt-based catalysts. These 2D catalysts screened with high-throughput calculations provide a useful data set for further machine learning model construction or experimental examinations.

Biography

Lei Shen is a Senior Lecturer in Department of Mechanical Engineering at National University of Singapore. His research interest lies in computational materials, physics and chemistry, focusing mainly on the understanding of fundamental properties of materials for advanced technologies, and prediction of advanced materials based on materials genome, high-throughput calculations, and machine learning. In recent years, he has studied various advanced materials including spin-orbitronic materials, topological materials, low-dimensional materials, battery electrode materials, and electro-catalysts for the applications of clean energy, batteries, and quantum devices.

C Deposited 2D LDH to Promote Formation of Plated Black Mg Alloy on AZ31

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Abstract

Black photothermal materials have attracted much attention owing to its broadband solar absorption properties for efficient heat harvesting, which are usually synthesized in powder form, such as black semiconductors, aluminum nanoparticles, and carbon materials. However, due to the limitations present in powder forms, in this study we report a novel preparation method of black color Mg-Al-Zn two-dimensional

layered double hydroxide (2D LDH) film on Mg alloy AZ31 substrate by a unique steam coating technique. The prepared films were characterized by SEM, AFM, XRD, XPS and FTIR analysis. Preliminary results show that the 2D LDH coating displays a vertical nano- flake micro/nano structure. After steam coating, the presence of C was detected on the film surface and the molar percentage of C, and O increased with longer treatment time. This may originate from the reaction with CO₂ in the air, trapped by defects created by oxygen vacancies in metal complexes, or through adsorption on Mg (OH)₂ leading to the formation of MgCO₃, which was also detected by XRD. Hence, the gray and black colors may be due to metal carbonates and oxygen deficient-type Metal-C-O complexes, respectively, which traps visible light [1]. This metallic surface plated with a thin black film may open a novel avenue for developing different shape structures with high mechanical stability for solar thermal applications.

Biography

Vishakha Weerasinghe is a 2nd year PhD candidate in Singapore University of Technology and Design majoring in 2D nanomaterials synthesizing using novel techniques. She completed her M.Sc. and BSc in University of Moratuwa, Sri Lanka. She has been working nanotechnology based individual research and commercial projects in Sri Lanka Institute of Nanotechnology for 2 years.

Advanced Carbon Film on Bipolar Plate for Proton Exchange Membrane Fuel Cell

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Abstract

Advanced carbon films have been successfully deposited on SS316 substrate and bipolar plate by sputtering and vacuum arc deposition method respectively. For sputtering deposition, the effects of different deposition conditions or parameters such as sputtering targets made by different companies, substrate chemical cleaning and Ar⁺ plasma cleaning on the film properties have been investigated. Film properties like the Interface Contact Resistance (ICR) and anti-corrosion property have been characterized. The results showed that carbon film deposited by the vacuum arc method has a very good contact resistance and excellent anti-corrosion property, which meets the US Department of Energy (DOE) requirements and can be applied to the coating process of bipolar plate production. For the carbon films deposited by in-house sputtering machine from different sputtering targets all have high ICR and high corrosion current. Among the 3 different targets (US graphite, Japan graphite, US pyrolytic graphite target), the US graphite target gives the relatively good results. It is also found that the cleaning of the SS316 surface by normal cleaning of HCl acid is not enough, while 250W, 10min Ar⁺ plasma cleaning is also necessary to remove the oxide layer. The fuel cells with bipolar plates deposited with carbon films by vacuum arc method and sputtering method have been assembled to test the performance of fuel cells. It is found that the bipolar plates with the carbon films deposited by the vacuum arc technology shows the best performance among the films we experimented with.

Biography

Hong Zhu works as a senior research scientist in healthcare engineering center, school of engineering, Temasek polytechnic. He graduated from Chinese Academy of Sciences. Dr. Hong Zhu has many years of experience in semiconductor industry and is good at micro fabrication technology and process. His current research work focuses on thin film deposition, sensor fabrication and wearable electronics.

Critical Analysis of the Heat Capacities of Diamond and Graphite

Valery P. Vassiliev

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Abstract

The investigation of the heat capacities of systems based on light elements such as lithium, beryllium, boron, and carbon is an extremely complex experimental task. The presence of impurities or variations in the isotopic composition has a stronger effect on the physicochemical properties than on the heavy elements. In accordance with our proposed concept of similarity put forward by us, isostructural substances with the same sum of atomic numbers have the same heat capacities per $J \cdot (\text{mole-atom})^{-1} \cdot K^{-1}$ [1, 2].

Diamond and cubic boron nitride have the same crystal structure of the type ($Fd3m$). Both substances are in a metastable state under normal conditions. Synthetic diamond and various modifications of boron nitrides contain various impurities due to the specifics of their synthesis. Consequently, cubic boron nitride must have the same heat capacity as the diamond.

Similarly, we can compare the isostructural phases of graphite and BN with a hexagonal structure. All deviations from this rule are caused by the presence of impurities in the final product.

The functions C_p and C_v using both the Debye models and the Maier-Kelley equation are proposed to describe the heat capacity of substance in solid state using the in-house software on the base of commercial one DELPHI-7. They make it possible to calculate the heat capacity values equal to the experimental data within the range of the deviation.

Biography

Valery V. Vasiliev was faculty of chemistry in Lomonosov Moscow State University|MSU. He was the Corresponding Member of the USSR (Russian) Academy of Sciences, 1984. He was the Membership on Editorial Boards and Committees of Problems of Defence Technology (1973-present), Mechanics of Composite Materials and Structures, (1998-present).

He was expertise in the fields of Optimization, DSC, Materials Science, Materials, Thermal Analysis, Material Characterization, X-ray Diffraction, Nanomaterials, Physical Chemistry.

On the Role of Impurities on Spheroidal Graphite Degeneracy in Cast Irons.

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Abstract

Though manufacturing spheroidal graphite cast irons is a well-established industrial process, good nodularity which is essential for mechanical properties may be hampered by several factors. Amongst them is the presence of impurities at trace level which lead to the growth of protrusions and the question is how they can destroy the spheroidizing effect of magnesium. For the first time, it is shown that such impurities are present together with magnesium at the interface between spheroid and protrusion. For getting this result, site-specific electron transparent lamellae were prepared using Focused Ion Beam and characterized at nanometric scale using atomic resolution scanning-transmission electron microscope. It is also shown by automatic crystal orientation mapping that there is no definite crystallographic relationship between protrusions and underlying spheroids

Biography

Mayerling Martinez Celis is faculty of Mathematics and Physics Department of Condensed Matter and Physics in Charles University. She got her PhD diploma in Toulouse (France), she has been working in different laboratories in France and Luxembourg. Now she was in sabbatical leave in Prague (Charles University). Her research interest could be summarized as: study of the relationship between mechanical properties and microstructure of metallic alloys. Microstructure will be the key word of his talk.

Probing the Nature of Defects in Polished Sp² Carbons by Polarized Raman Spectroscopy

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Abstract

Carbon-based materials are of great interest in various domains such as aeronautics, electronics and energy storage. Their accurate structural characterization is of crucial importance and Raman scattering spectroscopy becomes nowadays an essential technique for this purpose. The structural study is usually achieved by the well-known *IDIG* parameter which informs about the defect density. The latter may be for example boundary defects present during the transformation of some precursors into sp² carbon, or point defects created by neutron or ion beam irradiation. Both types of defects produce changes in the Raman spectrum and can be separately identified. However, where it becomes more intriguing is when the carbon material is polished. The behavior of Raman spectra is completely different and seems to suggest the presence of other types of defects.

Here, polarization Raman-dependent studies, in the back-scattering configuration, were performed on polished anthracene-based coke heat-treated at 2000 °C. Fixed polarization directions of the incident and the scattered light combined to the sample rotation allow providing a better understanding of the nature of defect induced by polishing. These experimental results have been confirmed by theoretical calculation

Biography

Mohamed-Ramzi AMMAR was graduated from Maine University of Le Mans-France in drug delivery systems and Habilitation from Orleans University (France) for Raman spectroscopy of carbon materials under extreme conditions. Dr. M.-R. AMMAR is an associate professor in the institute of Orleans ICMN

« Interface, confinement, Materials and Nanostructures » affiliated to the French National Centre of Scientific Research CNRS (UMR-7374). The main research areas are devoted to the optical properties of nanostructures materials. M.R. AMMAR is author and co-author of more than 70 scientific peer review articles and refereed proceedings, 2 patents, contribution of an invited book and more than 160 national and international conference communications.

Recent Advances in the Synthesis of Graphite Intercalation Compounds

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Abstract

Graphite Intercalation Compounds (GIC) are a specific class of two-dimensional materials resulting from the stacking of graphene planes and various kinds of intercalated species (atoms, ions, molecules). From the well-known LiC₆ compound used in the Li-ion battery technology to CaC₆, a superconducting material exhibiting the highest critical temperature ($T_c = 11.5\text{K}$ at atmospheric pressure) for this class of material, numerous GIC have been the subject of extensive studies and the preparation of novel compounds remains an interesting challenge.

In this presentation, we will describe a large overview of the past and current ways of synthesis used in order to prepare GIC. From the classical solid-gas and solid-solid intercalation reactions, we will shift to the solid-liquid reactions which allow the preparation of a large variety of binary and ternary compounds. Especially, we developed in our group intercalation protocols in order to perform reactions in alkali metal-based molten alloys or molten salts. Such ways of synthesis lead us to the preparation of homogeneous binary GIC intercalated into the bulk and of course novel ternary phases.

Biography

Sebastien Cahen is assistant professor at the department of chemistry of the Faculty of Science and Technologies (University of Lorraine) and is head of the master's degree "Solid-State Chemistry for Energy". His research activity is realized at the Jean Lamour Institute of Nancy, France. He is member of the advisory board of the International Symposium on Intercalation Compounds. His work is focused on low dimensional carbon-based materials and especially intercalation chemistry. He investigates new synthesis routes for graphite intercalation compounds, and is involved in research dealing with the preparation of new carbon materials for energy storage.

Isotopic Exchange Inside Impregnated Activated Carbons

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Abstract

Activated carbons (AC) have been used for the removal of iodine within ventilation networks of nuclear facilities. More particularly, the commonly used nuclear grade AC are co-impregnated with potassium iodide (KI, 1 wt%) and triethylenediamine (TEDA, < 5 wt%) [1]. The present study aims to gain insights on the importance of isotopic exchange reaction resulting from KI as a comparison with other mechanisms (physisorption and chemisorption).

On the one hand, an increase in decontamination factor (DF) up to about 104 is observed for KI contents ranging from 0 to 0.5 wt% at {R.H. = 40% at 20 ° C} (Fig. 1). This increase could be attributed to isotopic exchange between CH₃I₂ and K¹²⁷I still accessible by physisorption [2]. On the other hand, a drop in microporous volumes of 20% is observed from 0.5 to 5% wt% in KI, leading therefore to a significant decrease in DF until 600. At 90% R.H., the increase in DF followed by a plateau obtained for those same AC constitutes qualitative proof of the occurrence of isotopic exchange between K¹²⁷I sites on the external surface and CH₃I₂ molecules [3]. The low DF values between 10 and 20 can be attributed to competitive adsorption between CH₃I molecules and water [3].

The presence of isotopic exchange in some configurations has been qualitatively proven. However, the quantification of this reaction must be evaluated by comparing the breakthrough curves in active and inactive. Hence, a specific test bench allowing the determination of breakthrough curve in active is under validation.

Biography

Hantao Lin, 3rd year PhD student of the IRSN Institute, previously studied in Chinese French institute of the nuclear energy. He is now specialized in the adsorption of the methyl iodine towards porous material.

Laser-Induced Graphitization and White Light Emission of Microdiamonds

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Abstract

Recent experiments by Strék et al. have shown intense, anti-Stokes laser-induced white light emission (LIWE) from graphene-based materials: graphene ceramics [1] and graphene foam [2] after the excitation of samples with a continuous wavelength (CW) laser from the near infra-red (NIR) range. It is particularly interesting since all materials for which LIWE was observed previously were large bandgap insulators. A number of possible application areas of LIWE were proposed including white-lighting, telecommunication or Li-Fi. However, a true nature of LIWE is still under debate. The subject of this work [3] was to investigate the co-occurrence of LIWE and structural changes in diamond after CW NIR laser excitation. For this study, HPHT produced micrometer sized diamonds were investigated. Broadband, intense, anti-Stokes LIWE with very low threshold were observed. LIWE resulted in the graphitization of the diamond grain surface with different stages of graphitization depending on the excitation time. The model of defect mediated multiphoton electron ionization and free to bound recombination resulting in the continuous spectra of the emitted photons was presented. It was proposed that, the sp³-sp² hybridization switch of two carbon atoms occurs simultaneously with every ionization recombination pair. When excitation follows sp²-defect group can spontaneously collapse to the graphite structure.

Biography

Adam Olejniczak graduated at the Faculty of Fundamental Problems of Technology, Wrocław University of Science and Technology in 2016 and he received the MSc degree in Technical Physics. After graduation he started PhD study at Institute of Low Temperature and Structure Research, Polish Academy of Sciences. He specializes in computational physics in atomic scale, especially in calculations from first principles.

Adam Olejniczak current research interest are optical properties of carbon (nano)structures as well as semiconductor nanostructures with quantum-confinement effect (quantum dots).

TiO₂/AC Composites for Methylene Blue Removal Over Solar Light

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Abstract

The quest for new advanced technologies to ensure safe and sustainable water supply is growing at an accelerating pace, being one of the grand global challenges of the nearest future. Photocatalysis harnessing solar energy has emerged as a promising method for mineralization of non-biodegradable pollutants under mild and environmentally benign conditions.

Methylene blue (MB), extensively used in textiles and printing industries, was chosen as model compound of non-biodegradable dye and its photocatalytic oxidative degradation was studied. A biomass-derived activated carbon (AC) from spent coffee grains was used to support TiO₂ nanoparticles. Composites prepared by in situ sol-gel method in different TiO₂:AC weight proportions were tested as adsorbents and photocatalysts for MB removal from water. The materials were characterized by XRD, N₂ adsorption, SEM, UV-VIS diffuse reflectance, FTIR, TPD, and TGA. The higher MB adsorption efficiency (dark experiment) was found for 50TiO₂:50AC composite. The adsorption process followed pseudo-second-order model and intraparticle diffusion, with film diffusion playing a significant role in MB adsorption. In photocatalytic MB degradation, the TiO₂:AC composites showed better photocatalytic response than bare TiO₂ or AC, under simulated solar light irradiation. The 50TiO₂:50AC photocatalyst promoted 98% MB degradation during 90 min light irradiation. The photocatalytic behavior of the composites tested was described by the first-order kinetic model. The rate constants of photocatalytic MB removal for 50TiO₂:50AC ($k=1.01 \cdot 10^{-1} \text{ min}^{-1}$) were 1.8, 2.3, 2.7 and 9.7 times higher than those of 25TiO₂:75AC, AC, 10TiO₂:90AC, and TiO₂ materials, respectively, after 90 min of visible light irradiation, and reuse was assessed.

Acknowledgements

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Embrace Project (CEECIND/0137/2017), by CP for FCT Investigator contract IF/01080/2015, and by IKB for funding through program DL 57/2016 – Norma transitória REQUIMTE/EEC2018/14.

Biography

Ana Paula Carvalho has a PhD in Chemistry (1996) by the Faculty of Sciences of Lisbon University (FCUL) being Associate Professor at FCUL. In parallel with the academic career Ana Paula Carvalho have developed and supervised several studies in the field of material science, adsorption, and catalysis. Her present research interests are mainly centered in the development of carbon materials to be applied as adsorbents in liquid phase process, as well as catalysts supports. The catalysis studies are made in collaboration with colleagues of from FCUL, and from REQUIMTE (FCUP), IST (UL) and ISEL (IPL)

Langmuir Layers of Fullerene C60 and its Mixtures with Amphiphilic Polymers

Boris Noskov*, Kirill Timoshen, Alexey Bykov

St. Petersburg State University, Russia

Abstract

The interest in fullerene monolayers at the liquid – gas interface appeared just after the discovery of the methods for preparing macroscopic quantities of fullerene C60. Most attempts have been unsuccessful and spreading fullerene solutions in a volatile solvent onto the water surface resulted in the formation of heterogeneous surface films of variable thickness due to strong hydrophobic attractions between the molecules. At the same time, these heterogeneous fullerene films proved to be highly stable, displayed the high surface elasticity and sustained the surface pressure up to 70 mN/m. To elucidate the causes of this high stability the methods of dilational surface rheology and optical microscopy combined with the more conventional methods of surface tensiometry, ellipsometry and atomic force microscopy have been applied to fullerene C60 layers and to mixed layers of the fullerene with amphiphilic polymers [1]. The mixed layers consist of two separate phases at low surface pressures below the characteristic value of the polymer displacement from the interface. Although the collapse of the fullerene layers starts at surface pressures of far less than 70 mN/m, some patches of the layers sustain high surface pressures. The high stability of the spread layer and its strong adhesion to water can be explained by the partial hydroxylation of the fullerene molecules.

[1] B. A. Noskov, K.A. Timoshen, A.G. Bykov, J. Molecular Liq. 320 (2020) 114440.

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Biography

Boris Noskov is a professor at the Institute of Chemistry of St. Petersburg State University and head of the Laboratory of Surface Phenomena (LSP). He obtained PhD in 1979 under supervision of academician A.I. Rusanov and his Doctor degree in 1999. In 2012 B. Noskov gained the first prize of Vinogradov Rheological Society for the development of new approaches in surface rheology. The main subject of LSP is spread and adsorption layers of biomacromolecules but since 2012 it is also active in the field of surface properties of solutions of fullerene derivatives and fullerene spread layers.

Comparative Microstructural Analysis of Non-Graphitic Carbons (Ngcs) Based on Wide-Angle X-Ray (Waxs) / Neutron (Wans) Scattering as Well as Pair Distribution Function (Pdf) Analysis

Bernd Smarsly* and Oliver Osswald

Justus-University-Giessen, Institute of Physical Chemistry, Germany

Abstract

Non-Graphitic Carbon (NGC) is the most abundant type of sp²-hybridized carbon materials and is composed of small graphene layer stacks possessing significant structural disorder in the single graphene sheets as well as the stacking. A quantitative description of this disordered sp² polyaromatic microstructure is frequently performed by WAXS, but challenging, as the signals are quite broad.

In 2002 we introduced a novel evaluation approach for WAXS/WANS data of NGCs, in which the data are fitted by theoretical function [1]. As particular feature, the fitting parameters are structural parameters such as disorder in the stacks and within the graphene layers, stack height, graphene extension, etc., providing a meaningful structural characterization. However, WAXS suffers from experimental and physical limitations diminishing the general validity of the NGC analysis by WAXS.

In this study first the aforementioned evaluation approach we performed WANS and WAXS experiments and applied the Ruland/Smarsly analysis to several different NGC samples [2]. A good agreement within the error margin was found proving the model's validity for quantifying the structure on the atom dimension. Furthermore, PDF analyses on suitable WAXS data were carried out, obtained from a synchrotron facility, from which we examined the disorder degree in NGCs on a local scale. Interestingly, as a major insight, we found a high degree of order within the first few benzene rings, i.e. ordered aromatic core(s) surrounded by a less ordered shell. Such high degree of order for "disordered" NGC is unexpected and reshapes the general view on the structural make-up of NGCs

Biography

Bernd Smarsly is a professor in the Department of Biology and Chemistry, Physico-Chemical Institute, at Justus Liebig University Giessen (Germany) since 2007- PRESENT. From 2003-2007, he acts as a Group leader at the Max-Planck Institute of Colloids and Interfaces (MPI KGF), Potsdam (Department of Colloid Chemistry).

Ni-Decorated Highly Nitrogen Doped Carbon Electrocatalysts for Unconventional CO₂ Reduction Reaction to Formic Acid

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Abstract

Metal single atoms dispersed into carbon-based materials have emerged recently as very promising systems in different fields such as heterogeneous catalysis, electrocatalysis or batteries.¹ However, new strategies to prepare such materials and more control over carbonization is still needed. In 2018, Antonietti et al. reported

that by smart selection of the starting organic precursors, "noble" carbons with astonishing and predictable physico-chemical properties (e.g., electron density, heteroatom doped, highly stable upon oxidation) could be obtained.² Herein, we have prepared noble carbons using nucleobases as precursors in the presence of melting salts. The as prepared noble carbons exhibit surface areas of ~ 1500 m²/g, high nitrogen content (up to 15wt.%), high stability upon oxidation (ca. 600 °C) and high affinity towards CO₂ sorption.

Their very high resistance upon oxidation allowed us preparing Ni single atom decorated carbonaceous electrocatalysts by simple impregnation with an organic Ni salt and subsequent calcination in air. Figure 1a and b show the XRD patterns of the samples with nanoparticles emerging only at high loadings and HRTEM micrographs. Their electrocatalytic performance for the CO₂ reduction reaction (CO₂RR) was tested. Contrary to the state-of-the-art, where Ni single atoms coordinated to nitrogen supported on carbon-based materials exhibits near 100 % selectivity towards H₂/CO, the materials show remarkable Faradaic efficiency towards HCOOH (Figure 1c and d, ≈ 30 % at -0.94 V) due to the first coordination of nickel being mainly oxygen.³

Biography

Nieves Lopez studied Chemical Engineering at the University of Murcia (Spain). Then she joined the Group of Bioinspired Materials at the Institute of Materials Sciences of Madrid to carry out her PhD studies under the tuition of Francisco del Monte. After finishing her PhD studies she joined the team of Prof. Markus Antonietti at the Colloid Chemistry Department of the Max Planck Institute of Colloids and Interfaces where she works now as Group Leader. Her current research interests are the preparation of carbons at low temperature and noble carbonaceous structured materials and their use as carbo- and electrocatalysts.

Inspired by Nature: Controlled Condensation of Nucleobases to Functional Materials

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Abstract

Developing carbonaceous materials is of great interest for several applications including gas adsorption, electrochemical energy storage and conversion or heterogeneous catalysis among others.^[2] The choice of the carbonaceous precursor plays a key role in the design of the final carbonaceous product and on its properties. Inspired by the concept of noble carbons introduced by Oschatz and Antonietti^[1], and nature's choice of molecules, nucleobases appear to be very promising noble carbonaceous precursor. Moreover, their high nitrogen content facilitates the production of highly heteroatom doped carbonaceous networks.

In this work, several carbonaceous materials were obtained by condensation of guanine, uric acid or uracil. Investigations on different condensation temperatures (from 500 °C to 800 °C) and the influence of different salt mixtures as solvent and porogen were performed. Systematic analysis of the results provided us tools to control the carbonization process and design the final carbonaceous materials for different applications. For instance, guanine or uric acid heat treated up to 700 °C in N₂ atmosphere exhibit a C:N ratio of 1:1 (i.e., they are C₁N₁ networks) and show an ultrahigh CO₂/N₂ selectivity.^[3] When heating the precursors up to

800 °C in the presence of salt melts as porogens, highly porous carbonaceous materials with up to 20 at% of nitrogen content were obtained. Their tunable porosity and composition make them excellent candidates for heterogeneous catalysis.[4] Interestingly, using these simple designing tools (i.e., temperature and porogen) the hydrophilicity of the carbonaceous materials was tuned from very hydrophilic to very hydrophobic.

Biography

Janina Kossmann studied business chemistry at the Heinrich-Heine-University in Dusseldorf. She wrote her bachelor thesis in the department of Organic Chemistry and Macromolecular Chemistry with Prof. Thomas J. J. Muller and finished her studies with a master thesis in cooperation with Evonik Resource Efficiency GmbH. In 2019 she joined the Colloid Chemistry Department of the Max-Planck Institute under Prof. Markus Antonietti in the group of Nieves Lopez-Salas where she is now working on the synthesis, characterization and application of noble carbonaceous (C1N1) materials with a focus on the gas sorption behavior.

Non-Covalent NIDO-CAGE...PI-Ring Interaction

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Abstract

To date, non-covalent interactions involving multicenter multielectron skeletons like boron clusters is rarely reported. Here, a non-covalent interaction, nido-cage $\times\times\times$ p bond, is discovered based on the boron cluster C₂B₉H₁₂⁻ and an aromatic p system [1]. The X-ray diffraction studies indicate that the nido-cage $\times\times\times$ p bonding presents parallel-displaced or T-shaped geometries. The contacting distance between cage and p ring varies with the type and the substituent of the aromatic ring. The theoretical calculations reveal that this nido-cage $\times\times\times$ p bond shares a similar nature to the conventional anion \cdots p or p \cdots p bonds found in classical aromatic ring systems [2-4]. Besides, such a nido-cage $\times\times\times$ p interaction induces variable photophysical properties such as aggregation-induced emission and aggregation-caused quenching in one molecule. This work offers an overall understanding towards the boron cluster-based non-covalent bond and opens a door to investigate its properties.

[1] D. Tu, H. Yan, J. Poater and M. Sola, *Angew. Chem. Int. Ed.* 2020, 59, 9018-9025.

[2] J. Poater, M. Sola, C. Viñas and F. Teixidor, *Chem. Eur. J.* 2016, 22, 7437.

[3] J. Poater, M. Sola, C. Viñas and F. Teixidor, *Angew. Chem. Int. Ed.* 2014, 53, 12191.

[4] J. Poater, M. Sola, C. Viñas and F. Teixidor, *Chem. Eur. J.* 2013, 19, 4169.

Biography

I got my PhD in Chemistry in 2003 at the Universitat de Girona (UdG) with a thesis on the analysis of

chemical bonding and aromaticity of organic systems with tools based on the electron-pair density. Next, I moved to the Vrije Universiteit Amsterdam (VUA), where I carried out research on the DNA replication mechanism by means of Kohn-Sham molecular orbital theory complemented with quantitative bond energy decomposition analyses. In 2016, I was appointed ICREA Research Professor at Universitat de Barcelona. I have published more than 150 scientific publications in peer-reviewed journals, which have received more than 5.700 citations.

Reversible Formation and Disappearance of Graphitic Domains in Carbide-Derived Carbons under H₂ Loading

Rasmus Palm^{1*}, Miriam Koppel², Riinu Harmas², Margarita Russina³, Nami Matsubara¹, Martin Mansson¹, Veronika Grzimek³, Maarja Paalo², Jaan Aruval², Tavo Romann², Ove Oll², Enn Lust²

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Abstract

Control of carbon structure, e.g. from highly ordered graphitic domains to non-graphitic and amorphous carbons, is of high interest for the use of carbon materials in different applications. Modifications to carbon structures, e.g. graphitization through heat-treatment, physical and chemical activation etc., have thus far been irreversible or achieved under extreme pressure conditions. The formation and disappearance of graphitic domains in an otherwise non-graphitic carbide-derived carbon will be shown to be possible under a hydrogen loading and during a temperature increase from 40 K to 60 K. In situ neutron diffraction and quasi-elastic neutron scattering methods are used to show the development and disappearance of the carbon structures and the changes in the self-diffusional capability of the adsorbed hydrogen during the temperature increase routine. An explanation to the formation and disappearance process of the graphitic domains is given and the requirements for suitable carbon materials for the process are presented.

Biography

Rasmus Palm defended his Ph.D. thesis in 2018 at the University of Tartu, Estonia, on the application and optimization of carbon materials in different energy storage applications. From his doctoral studies Dr. Palm attained experience in electrochemistry, gas adsorption methods and with hydride-based hydrogen storage materials. From 2020 Dr. Palm is a postdoctoral researcher at Royal Institute of Technology, Sweden, and focuses on application of in situ neutron scattering methods to study hydrogen storage and carbon materials.

The Mobility of H₂ Adsorbed in Mo₂C Derived Carbon Materials with Different Porous Structures Studied with Quasi-Elastic Neutron Scattering

Miriam Koppel^{1*} and Rasmus Palm², Riinu Harmas¹, Maarja Paalo¹, Indrek Tallo¹, Veronika Grzimek³, Ove Oll¹, Heisi Kurig¹, Enn Lust¹

¹University of Tartu, Estonia.

²KTH Royal Institute of Technology, Sweden; ³Helmholtz-Zentrum Berlin für Materialien und Energie, Germany

Abstract

H₂ is a promising energy vector since the oxidation of H₂ produces no pollutants. However, the current methods for transportation and storage of H₂ are not very efficient. One method for storing H₂ is physical adsorption on porous carbon adsorbent. Carbide derived carbons are good model materials for investigating the influence of porosity on H₂ storage capability. The porous structure of three Mo₂C derived carbon materials synthesized at 700 °C, 800 °C and 900 °C (denoted as C700, C800 and C900) has been characterized with N₂, Ar, CO₂ and H₂ adsorption methods. With increased synthesis temperature, the pore volume and specific surface area decrease. Accurate confirmation of the pore volumes enables to investigate how the porous structure influences the mobility of H₂ adsorbed in the ultramicropores (width < 7 Å), micropores (7 < width < 20 Å) and mesopores (width > 20 Å) of the samples. The mobility (self-diffusion) of H₂ adsorbed in the samples was determined with quasi-elastic neutron scattering method at conditions where different volumes of pores were filled with H₂. A strong confinement of H₂ adsorbed in the ultramicropores of C700 and C800 at 50 K is shown. It is evidenced that the confinement of H₂ is controlled by the volume of ultramicropores present in the sample. At moderate and high loading pressures, H₂ diffusion in two timescales can be distinguished. It is evidenced that micropores in addition to ultramicropores help to confine H₂, but mesopores do not have a noticeable effect on the H₂ confinement.

Biography

Miriam Koppel is a PhD student in University of Tartu in Institute of Chemistry where she also works as a chemist. Her research interests focus on material characterization and H₂ storage methods, more precisely on physical adsorption on porous carbon adsorbents. She has experience in multiple gas adsorption methods and quasi- and inelastic neutron scattering methods, which includes sample preparation, planning and conducting the experiment and data analysis. Miriam has a publication list including one first and six co-authorships and her previously defended bachelor's thesis has been awarded in two national-level competitions.

Carbide-Derived Carbons: WAXS and Raman Spectra for Detailed Structural Analysis

Riinu Harmas^{1*}, Rasmus Palm¹, Heisi Kurig¹, Laura Puusepp¹, Torben Pfaff², Tavo Romann¹, Jaan Aruvali¹, Indrek Tallo¹, Thomas Thomberg¹, Alar Janes¹ and Enn Lust¹

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Abstract

Quick characterization methods are necessary to improve the characterize the synthesized porous carbon materials accurately. Carbide-derived carbons (CDC) are excellent carbon materials for many applications (supercapacitors, PEM fuel cells, etc). The properties of CDCs, like pore size distribution and level of graphitization, depend drastically on the precursor carbide and the synthesis conditions. In this study, the combined analysis of the structure of carbide-derived carbons (CDCs) with Raman spectroscopy and wide-angle X-ray scattering (WAXS) methods is presented. The optimal deconvolution method to be used for the detailed analysis of Raman spectroscopy data of CDCs is found and comparison to corresponding WAXS results is made. For a broad set of CDCs both WAXS and Raman spectroscopy data showed that

the average graphene layer extent increases with the increase in synthesis temperature of CDC, while the coherent domain lengths obtained from Raman spectroscopy, in comparison to WAXS, was higher by an average of 4.4 nm. In addition, the presence of correlations between the parameters (D-band width and the parameter $S\Sigma D/S\Sigma G$) from Raman spectroscopy and the synthesis temperature are established. Based on the WAXS and Raman spectra data analysis the strong influence of the precursor carbide structure on the graphitization pathway is presented.

Biography

Riinu Harmas is a PhD student at the Institute of Chemistry in the University of Tartu. She has studied porous carbons with gas sorption, Raman spectroscopy, XRD and neutron scattering methods and is a co-author to twelve research papers, mostly in the field of electrochemistry. With an honest, but friendly manner, she is a supervisor to three students and currently amid writing her final thesis.

The Role of Carbon and Vacancy Defects in the Myricetin Functionalization of $MnFe_2O_4$ Nanoparticles

Oscar E. Cigarroa-Mayorga*

UPIITA-Instituto Politecnico Nacional, Mexico City, Mexico.

Abstract

In this work, was used the Myricetin flavonoid to functionalize $MnFe_2O_4$ nanoparticles. The nanoparticles were synthesized by the hydrothermal method. Thus, sodium dodecyl sulfate, sodium hydroxide, iron chloride, and manganese chloride were mixed, and the solutions were introduced into a cylindrical stainless-steel vial cover inside with Teflon. A rate of 2:1 in Fe-Mn (atomic weight percentage) was used in the synthesis. The synthesis was carried out under an isothermal process from 80 °C to 200 °C from 4 h to 24 h. Afterward, the samples were cleaned into an ultrasonic bath of deionized water. To bound the Myr to the nanoparticles, a layer of Si was coated in the surface of $MnFe_2O_4$ nanoparticles. Thus, ethanol, deionized water, and ammonia were mixed. Then, the $MnFe_2O_4$ nanoparticles and tetraethyl orthosilicate were added, and the mixture was agitated for eight hours at room temperature (RT). The samples were characterized by X-ray diffraction (XRD), field-emission scanning electron microscopy (FE-SEM), energy-dispersive X-ray spectroscopy (EDS), Raman spectroscopy performed (into an INTEGRA Spectra equipment with wavelength excitation of 633 nm), selected area electron diffraction (SAED), transmission electron microscope (TEM), dynamic light scattering (DLS), and X-ray photoelectron spectroscopy (XPS). The implications of the carbon atoms (inner the myricetin molecule) and the oxygen vacancies (in the surface of $MnFe_2O_4$ nanoparticles) toward the myricetin binding are discussed in the functionalization process.

Biography

Oscar E. Cigarroa-Mayorga holds a Ph.D. in nanoscience and nanotechnology from the CINVESTAV. Currently, he is a full-time professor at the Mexican National Polytechnic Institute (IPN). He has published fifteen research works in international journals such as Applied surface science, particularly in the solid-state physics field. Because of his scientific carrier, he has awarded distinctions such as the best master dissertation work from the Mexican National Institute of Electricity and Clean Energies (INEEL), Youth price of Mexico City in the academic merit from the Youth Institute.

Quantum Monte Carlo Approaches to Molecules and Solids with Dispersive Interactions

Olle Heinonen*, Hyenondeok Shin, and Anouar Benali

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Abstract

Dispersive interactions, such as Van der Waals interactions, play a crucial role in a number of interesting carbonic compounds. Examples range from layered two-dimensional compounds such as graphene and graphyne, to important organic molecules such as amino acids and DNA base pairs. While density functional theory (DFT) is usually the workhorse for electronic structure calculations and structural optimizations, dispersive interactions are difficult to accurately capture with DFT, although great progress has been made over the past decade. Quantum chemical methods such as Coupled Cluster methods are typically used for “gold standard” calculations on benchmarking test sets, which are used as reference. However, quantum chemical methods are very expensive with poor scaling with electron number, and dependencies on basis sets that make extrapolation to the complete basis set limit difficult. We used Diffusion Monte Carlo (DMC) methods on a number of layered compounds and molecular systems. In contrast with quantum chemical methods, DMC is relatively insensitive to basis sets, scales very well on leadership computing platforms, automatically includes all electron-electron interactions to all orders and has been shown to reach chemical accuracy. In this presentation, I will present results on layered graphyne [1] and on the L7 molecular benchmark set [2,3], and discuss outlooks for the future

Biography

Olle Heinonen is a Sr. Materials Scientist in the Materials Science Division. His research is in the areas of condensed matter theory and computational materials science, and includes magnetization structures and dynamics in magnetic nanostructures, electronic structure and transport in oxide nanostructures, and mesoscale computational materials sciences approaches to structure and microstructural evolution. He is a Thrust leader in the Center for Predictive Simulations of Functional Materials, deputy director in the Engineering Frontier Research Center “Center for the Advancement of Topological Semimetals”, and he leads strategies for artificial intelligence in science in the Physical Sciences and Engineering Directorate.

Synthesis, Characterization, and Mechanical Properties of Lightweight Boron-Carbon Based Composites

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²Department of Mechanical and Industrial Engineering, Tallinn University of Technology (TalTech), Tallinn, Estonia.

³Department of Chemical and Materials Engineering, Complutense University of Madrid, Madrid, Spain.

Abstract

This work studied the mechanical and physical properties of ceramic-ceramic composites with a carbonboron-nitrogen based system. Initial materials for composites processing were composed of boron carbide (B₄C) and aluminum powders. The composites were fabricated by self-propagating high temperature synthesis (SHS), attrition milling, and chemical leaching followed by spark plasma sintering (SPS) under nitrogen gas pressure. In the first step of processing by SHS, boron carbide-aluminum based composite with relatively soft, as well as superhard, compounds were formed. Using the attrition milling technique, a fine-grained powder was achieved, then using the chemical leaching technique, the relatively soft phase (Al-based) was leached out. The produced compound was purified from the soft phase in HCl and HNO₃ acids and then was compacted by the SPS technique. The achieved ceramic-ceramic composite was a lightweight carbon-boron-nitrogen compound that contained superhard chemical compounds including B₁₃C₂, B_{11.7}C_{3.3}, c-BN, and c-BC₂N. The composition of the composites was studied by X-ray diffraction patterns, scanning electron microscope as well as energy-dispersive spectrometry facility (SEM-EDS). The micromechanical properties, including Vickers nano-hardness and Indentation modulus, were studied by a nanoindentation instrument using Berkovich indenter. Results of materials characterization showed that the composite materials had Ultra-Fine Grain (UFG) microstructure with nanocrystalline particles. Results of hardness testing revealed that the materials held different values of hardness due to the variation of the chemical composition. The following hardness results were achieved from the nanoindentation testing. B₁₃C₂: 43 GPa, c-BN : 65 GPa, c-NC₂N: 87 GPa.

Biography

Babak Omranspour Shahreza had doctor's degree in 2019 from Tallin university of technology and school of engineering in department of mechanical and industrial engineering. He was a Researcher-nanostructured metals, Mechanical properties, microstructure and alloys, he was the Member of the R&D department of SANDVIK coromant, ITALY. He Qualified TEM operator for the investigation in bulk nanostructured materials.

Soft-Metamaterials: Cd Responsive Liquid Crystal-Gold Nanoparticles

C. V. Yelamaggad*

Centre for Nano and Soft Matter Sciences (CeNS), India

Abstract

Several monodisperse liquid crystal (LC) gold nanoparticles (LC-GNPs) self-assembling into a fluid/frozen periodic structure in the form of a lamellar phase and exhibiting CD activity have been prepared and fully characterized. These LC-GNP (soft-nano) composites have been prepared by simple, hassle-free protocols that involve the room temperature addition of chiral (cholesterol-based) dimer-like/dimeric LC arylamines to Au (III). Three types of soft-nano composites have been prepared using chiral LC arylamines wherein the cholesterol is covalently linked to either a benzene ring or biphenyl unit or photoactive azobenzene core via a flexible spacer of varying length and parity. In the case of photo-responsive LC-GNPs, it is evidenced that the localized surface plasmon resonance (LSPR) peak wavelength of gold can be modulated effectively. The amplitude (ψ) and phase (δ) values of the reflected light from the surface of the photoactive sample recorded during the ellipsometry experiments have been fitted to an effective medium model to extract the real and imaginary permittivity values. The data clearly shows the evidence of epsilon dropping below zero (ENZ) behavior, indicating that the material has the characteristics of a soft metamaterial. Thus, the photoactive soft-nano composite realized is a soft-metamaterial with a layered superstructure exhibiting

ENZ property in the optical regime at room temperature.

Biography

C. V. Yelamagad is a research scientist in Centre for Nano and Soft Matter Sciences (CENS). He done his Ph. D in organic chemistry from Karnataka University, Dharwad in 1991. He was a Senior R & D Scientist (1995-1996), Recon Ltd., Bulk Drug Industry, Bangalore and Postdoctoral Fellow (1996-1997), Dept. of Appl. Chem., NCTU, Taiwan. he was a research experienced Scientist at Centre for Nano and Soft Matter Sciences. He published more than 4000 citations and H-Index is 36.

POSTERS

Structural Evolution and Stability Behavior of Functionalized Nano Diamonds

Sepehr Yazdani^{1*}, Veronique vitry¹

¹Mons University, Belgium

Abstract

Diamond nanoparticles have a strong tendency to agglomerate in solution, based on electrostatic attraction between facets with positive and negative potential. This limits their applications especially when a homogeneous distribution is needed. Therefore, a simple and effective strategy for producing novel functionalization routes is needed as prerequisite to promote the increment of functional groups on the internal and external surface of nano diamond (ND) particles. In this study we have compared the structural and stability behavior of nanodiamond functionalized by air annealing and acid treatment method. Using FTIR and XPS analysis, it was demonstrated that ND aggregates of different sizes, separated from the same pristine ND, have different surface compositions of active surface groups, particularly oxygen-containing groups, which finally influence their zeta potential values and colloidal stability. The results show acid treated nanodiamonds have better stability due to the repulsive force between carboxylate group and presence of more Oxygen-free carbon sites.

Biography

Sepehr Yazdani is currently a PhD at University of Mons in Belgium. He received his MSc at the Amirkabir University in Iran. He has extensive experience in coatings and deposition techniques and analyzing film properties, including characterization (SEM, EDS, ICP, XRD, FTIR) and electrochemical behavior (linear polarization (LP), cyclic voltammetry (CV), electrochemical impedance spectroscopy (EIS), and electrochemical noise (EN). His recent research focuses on the stabilization of nano diamonds in Ni-B electroless bath. He is author of 6 refereed publications and has presented numerous talks at national meetings

Functionalization of ZNO Nanostructures with Carbon Arrays for Gas Sensing

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Abstract

The Zinc oxide (ZnO) is an n-type metal oxide semiconductor (MOS) that has been widely used for gas sensors along many years because of their chemical response to different adsorbed gases, high chemical stability, amenability to doping, non-toxicity, affordability, and relative fabrication simplicity. It has a wide range of electronic, chemical, and physical characteristics and has become a well-known commercial sensor because of the sensitivity of its properties to variations in its chemical environment, exploration into surface modification is a real need to increase application-oriented properties in gas sensing. In this work ZnO films are deposited by a Sputtering system using radiofrequency (RF), on substrates of silicon (001) p-type, quartz and glass with a size of 1.5 x 1.5 cm², the substrates were washed using a conventional washing method. ZnO was deposited on the substrate during a fixed deposit period of 45 minutes with a thickness of approximately 150 nm, the deposit was made at room temperature. After the deposit of ZnO films, a carbon layer was placed with different deposit times. The degree of graphitization in carbon materials can be clarified by Raman spectroscopy. The Raman spectra is well-known, the prominent peaks appear at 1350 cm⁻¹ and 1598 cm⁻¹ can be defined as the D band and G band. The D band is caused by defects exist in graphene or at graphene edges, the G band is associated with the vibrations of sp² hybridized carbon atoms. In the case of the samples deposited on Si substrates, these present a substantial increase in the G band with respect to the other two substrates.

Biography

Yazmin Mariela Hernandez Rodriguez is studying the PhD in nanoscience and nanotechnology at CINVESTAV, in Mexico City, has a master's degree in Materials Science from the UAEH, has published articles about synthesis and characterization of metallic and semiconductor materials.

One-Step Template-Synthesis of Fe_{1-x}S/Nitrogen-doped Porous Carbon Membranes from Poly(Ionic Liquid)

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Abstract

This study was designed to develop a novel nitrogen (N) and iron sulfide (Fe_{1-x}S) co-doped porous carbon membrane and study its application as a sulfur host material to decrease the shuttle effect in lithium-sulfur (Li-S) batteries. N-doping can sufficiently enhance the conductivity and electrochemical stability of carbon materials, on the other hand, the Fe_{1-x}S nanoparticles effectively improve the utilization of sulfur in Li-S batteries. The straightforward synthesis of Fe_{1-x}S/nitrogen-doped porous carbon membrane (Fe_{1-x}S/N-PCMs) directly via vacuum carbonization of ferrocene-bearing hybrid porous poly (ionic liquid) (PIL) membrane that worked as both template and iron source, is novel. The porous polymeric membranes as the sacrificial template were prepared via ionic crosslinking of a cationic PIL with base-neutralized 1,1'-ferrocenedicarboxylic acid so that the iron atoms were molecularly incorporated into the entire template. The Fe_{1-x}S/N-PCMs pyrolyzed at 900 °C demonstrated a promising hierarchical pore size distribution with a reasonably high surface area and well-dispersed iron sulfide nanoparticles to physically and chemically limit the lithium polysulfides (LiPSs). The sulfur/Fe_{1-x}S/N-PCMs-900 composites were then tested as a cathode in Li-S batteries, showing superior capacity, rate performance, and cycle stability compared to iron sulfide-free nitrogen-doped porous carbon membranes. Moreover, the embedded Fe_{1-x}S nanoparticles acted as efficient adsorbent and active site for conversion of LiPSs.

Biography

Sadaf Saeedi Garakani studied chemical engineering at the University of Tehran and completed her master's degree in 2019. She then moved to Sweden and started her Ph.D. degree in materials chemistry in 2019 at Stockholm university. The main research focus is currently on Heteroatom-doped porous carbon materials derived from poly (ionic liquid)s and their application in the energy field.

The Synthesis of Free-Standing Carbon Pellicles and Application for Energy Storage

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Abstract

Carbon-based anode materials for sodium-ion batteries (SIBs) had raised a great deal of interest due to their low-cost, high stability, and lightweight (i.e., high energy density). Among these carbonaceous materials, porous carbon pellicle was a potential anode material with the advantages of high specific strength, high temperature resistance, and high conductivity; especially not needing any binders or additives. Here, N-doped hierarchically structured carbon pellicles were prepared by the carbonization of zeolitic imidazolate framework/polyacrylonitrile (CZIF-8/PAN) composite fibers which were fabricated by an electrospinning technique. As an anode for SIB, the CZIF-8/PAN fabric carbon pellicles showed superior reversible capacity (186.2 mAh g^{-1}) at a current density of 1.0 A g^{-1} with an excellent cyclic stability. The increased electrochemical performance of fabric anodes also benefit from the doping of nitrogen atoms which enhance the conductivity and increase the active sites. These results indicated that self-supporting porous pellicles obtained by a simple electrospinning technique are promising anode materials for development of various porous conductive carbon nanomaterials of interest for energy storage devices.

Biography

Yanfeng Yue currently is an assistant professor of chemistry from Delaware State University, USA. After he received his Ph.D. in Inorganic Chemistry from Peking University in 2008, he started working in functional porous materials including porous metal-organic frameworks (MOFs), Prussian blue analogues, and carbon materials for gas storage, heavy metal adsorption, and energy storage.

Sustainable Conversion of Corncob Biomass Waste into Economic, High Performance Carbon Materials

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Keywords: Corncob, Porous Carbon, K_2CO_3 Activation, Gas Sensors

Abstract

The development of reliable and affordable gas sensors with short response times, excellent sensitivity, and selectivity has become an area of interest over the past years due to an increasing demand in areas such as environmental monitoring, biomedicine, and pharmaceuticals. Carbon materials show unique electrical, optical, and mechanical properties, which make them very interesting for developing a new generation of miniaturized, low-power, ubiquitous sensors. Further, the conversion of agricultural waste materials into high performance carbon materials has great environmental and economic impacts. Herein, corn cob residue was used to fabricate porous carbon structures by means of a simple one-step activation method using varied impregnation ratios of potassium carbonate for application in room temperature gas sensing devices. The prepared porous carbon structures were characterized using scanning electron microscopy, X-ray diffraction, Fourier transform infrared spectroscopy, and Brunauer-Emmett-Teller (BET) surface area analysis. The synthesized carbon materials exhibit high specific surface areas and large pore volumes. The porous carbon materials were further applied in room temperature sensing of volatile organic compounds.

Biography

Lindokuhle Magagula is a postgraduate student pursuing her Master of Science degree at the University of the Witwatersrand, Johannesburg, South Africa. She has special interest in engaging in projects that have economic and societal impacts. She was recently awarded a prize for a favourite oral presentation during the 2021 SANI symposium.

Effect of Reinforcement of Carbon Foams with Graphene Structures on Morphology and Mechanical, Thermal and Tribological Properties of Epoxy-Carbon Composites

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Abstract

Rapid development of new technologies requires complex multifunctional materials with good mechanical parameters, thermal resistance, advantageous tribological properties and low density at the same time. Application of carbon foams with specific structure and properties as a particulate filler of epoxy matrix gave the opportunity to develop new multiphase polymer/carbon materials. They are easy to process and characterized by good thermal stability, tribological properties, and ability to absorb different types of energy while maintaining good mechanical strength and relatively low density, compared to the pure epoxy matrix. It is known that the properties of carbon foams and in a consequence their composites, can be changed in relatively wide range by controlling of graphitic to amorphous structures ratio in carbon skeleton.

Thus the main purpose of this study was to determine the effect of reinforcing of carbon foam skeleton with graphene nanoplatelets on carbon foam properties and interaction with polymer matrix, and consequently on properties of polymer-carbon composites. Reinforced carbon foams containing graphene material (0.1 to 2% by mass) in amorphous carbon skeleton was produced by carbonization of epoxy/novolac precursors with uniformly dispersed graphene nanoplatelets. Characterization of composites with carbon foam particles of different skeleton structure and chemical nature of the surface was carried out. Carbon foams enriched with graphene materials contain the areas of ordered arrangement of graphene layers in the generally

amorphous carbon phase, which affect the key parameters of epoxy-carbon composites. Especially mechanical and thermal parameters, and tribological properties of epoxy composites were improved.

Biography

Karolina Olszowska has received master's degree in the Faculty of Mechanical Engineering of Silesian University of Technology in Gliwice, Poland (2015). The title of master's thesis was "Epoxy composites with porous carbon materials as fillers" in the field of Nanotechnology and Material Process Technologies. Currently she is working as an assistant in Centre of Polymer and Carbon Materials Polish Academy of Science. Her research interests are focused on preparation and functionalization of graphene materials and porous carbon materials, as well as the development of preparation procedures and characterization of polymer-carbon composites. She published 6 articles in peer-reviewed journals.



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