



## ABSTRACT BOOK

2<sup>nd</sup> International Conference on

# Carbon Chemistry and Materials

October 10-14, 2022 | Roma RM, Italy | Hybrid





## MONDAY, OCTOBER 10, 2022 IN-PERSON

## **Plenary Presentation**

Synthesis and Applications of Carbon Dots

## Maurizio Prato

University of Trieste, Italy

Abstract Not Available!!!

## **Keynote Presentations**

## Novel Carbon Fiber Precursors Based on Polyethylene Copolymers

## T. C. Mike Chung\*, Houxiang Li, Joseph Sengeh, Matthew Agboola, and Wei Zhu

The Pennsylvania State University, USA

## Abstract:

High strength carbon fiber (CF), offering a combination of light weight, high tensile strength, good thermal and dimensional stability, etc., is currently produced from polyacrylonitrile (PAN) polymer precursor. The conversion process is very expensive due to a combination of high precursor cost, complex fiber wet-spinning process, long thermal conversion process, and low C-yield ~50%. In this study, we present a new class of low-cost CF polymer precursor called <sup>2</sup>PE-g-Pitch<sup>2</sup>, having a semi-crystalline polyethylene (PE) backbone and several Pitch (polyaromatic) molecules in the side groups. This PE-g-Pitch precursor can be prepared by using a PE copolymer with several reactive diphenylacetylene moieties that show effective thermally induced cycloaddition (coupling) reaction with Pitch polyaromatic molecules. The resulting PE-g-Pitch precursor is melt and solution processable. With the presence of some free Pitch molecules serving as plasticizer and precursor, we have successfully prepared the corresponding PE-g-Pitch precursor fibers with diameter of ~80 um using melt-spinning process. The combination of thermogravimetric analysis (TGA), mass spectroscopy (MS), X-ray diffraction (XRD), Raman spectroscopy, and scanning electron microscope (SEM) was used to monitor the thermal conversion from PE-g-Pitch precursor into graphitic structure. Evidently, this PE-g-Pitch precursor can engage in an effective thermal transformation to C structure in one-step heating process under inert atmosphere (no oxygen requirement during the stabilization reactions), which results in the polymorphous morphology like those in current PAN-based CFs and a high C-yield >70% (>20% higher than PAN precursors).

## **Biography:**

Chung is a Fellow of the USA National academy of Inventors. He obtained his Ph.D in Chemistry from University of Pennsylvania in 1982 on conducting polymers (Adviser: Professor A. J. Mac-Diarmid, Nobel Laureate). He spent two years as a Research Associate at University of California, Santa Barbara (with Professor Alan J. Heeger, Nobel Laureate). In 1984, he moved to Exxon Mobile Company, Cooperate Research as a research staff. In 1989, he joined the faculty of the Pennsylvania State University, as an associate Professor in the Department of Materials Science and En-

gineering. In 1992, he was promoted to Full Professor. He has published 2 books, 235 papers, and 45 US and 10 international patents.

## **Tailored Graphene Functionalization to Better Device Performance**

### Martin Kalbac\*

J. Heyrovsky Institute of Physical Chemistry of the Czech Academy of Sciences, Dolejškova 2155/3, 182 23 Prague, Czech Republic

## Abstract:

It is often suggested that functionalization of graphene dramatically enhance potential for application of this material. However, so far realized strategies do not typically allow to control the functionalization process in terms of localization of the functional groups and mutual interactions with the graphene. Also appropriate strategy for the identification and full characterization of functional groups on graphene is rarely adopted. Mastering of these processes pave the way to not only give graphene new functionality but also to precisely control electronic structure of graphene and thus enable more advanced applications. Here, we will propose some strategies, which enable controlling and tailoring the functionalization process. It will be also shown how tailored functionalization can be applied to optimize function of supercapacitor in graphene /PANI composite and to realize fast, ultrasensitive and broadband 2D detector.

## **Biography:**

Martin Kalbac graduated in inorganic chemistry from Charles University, Prague, Czech Republic, (1998), where he also received his Ph.D. degree in 2002 and has been habilitated in the field of inorganic chemistry (2019). 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, 2D materials, Raman spectroscopy and Spectro electrochemistry, isotope engineering of carbon nanostructures and sensorics.

## **Oral Presentations**

## High Carbon Yielding Polyarylenes *via* Melt Processable Bis-o-diynylarene (BODA)derived Resins for Carbon Carbon Composites

## Ernesto Borrego, Will Johnson, Josh Brown, Charles Pittman, and Dennis Smith\*

Department of Chemistry and the MSU Advanced Composites Institute, Mississippi State University, Mississippi State, MS 39762 USA

#### **Abstract:**

As a special class of enediynes, bis-ortho-diynylarene (BODA) monomers are prepared in three steps from commercial bis-phenols and undergo thermal radical mediated Bergman cyclization and overall step-growth propagation to variable molecular weight reactive resin intermediates. Arylene diradicals formed propagate in stepwise fashion to highly branched processable intermediates that are amenable to current composite fabrication techniques prior to network cure (400-500 °C) and subsequent carbonization (1000-2000 °C) with extraordinarily high carbon yield (>80%). Upon thermal processing via extrusion, infusion, coating, or micro/nano-molding and final

cure, the resulting polyarylene networks are pursued for applications such as thin film dielectrics, carbon fiber matrix composites, carbon-carbon composites, light emitting diodes, and photonic/ electronic sensors. Synthesis, processing, and characterization will be presented with special emphasis on advanced composites for aerospace vehicles and other high temperature applications. Post-carbonization analysis reveals significantly higher density and consolidation in the BODA-derived carbon/carbon (C/C) over existing phenolic-based C/Cs without the need for arduous, multiple infusion and carbonization steps. The modular BODA approach combines and controls: (1) variable melt processability dictated by terminal or spacer group substitution, (2) mild cure kinetics via a non-autocatalytic reaction, (3) high carbon yield (>80%) to provide relatively dense (~1.55 g/ cm3) C/C substrates after a single carbonization at 1000 °C, and (4) remarkable efficiencies that allow fast carbonization ramp rates (10 °C/min) while maintaining high density. Isothermal DSC kinetics, monomer melt stability in air, order/disorder characterization by Raman and WAXS, resin processing under air environments, and cross-section fracture analyses of C/C composites by SEM is discussed.

## **Biography:**

Smith received his BS from Missouri State University and PhD from the University of Florida. He was a Dow Chemical Post-Doctoral Fellow in Germany and Dow Project Leader in the USA. Prior to moving to MSU as Department Head in 2017, he was Professor of Chemistry and MSE at Clemson University then Welch Distinguished Professor at the University of Texas at Dallas. Dr. Smith is Fellow of the ACS and Fellow of IUPAC. He has published 152 refereed journal articles, 28 U.S. patents issued or pending, over 300 conference papers, five book editorships, and more than 200 invited lectures in 23 countries.

## Laser-controlled Carbon Nanotube Assemblies

## Norbert Hampp\*

University of Marburg, Chemical Department, Germany

## Abstract:

Carbon Nanotubes (CNTs) require nanoscaled catalytic particles for their growth from the gas phase. These are prepared by laser processing of stainless steel in controlled sizes as well as in controlled aerial densities. This allows growing CNTs with controlled densities and in particular freely designable areas of vertically aligned CNTs. At increased laser intensities the laser processing is combined with laser machining of the surface. In these areas, cauliflower-like CNTs may be grown which show a very high outer surface. Post-processing of vertically aligned CNTs leads to a meander-like structure of the CNT bundles. A combination of all three laser-controlled growth conditions with further surface laser-structuring processes like laser-induced periodic surface structures (LIPSS) offers a flexible toolbox for spatially and functionally controlled CNT growth.

### **Biography:**

Norbert Hampp completed his first Ph.D. in pharmacy in 1986 and completed his second Ph.D. in Physical Chemistry in 1992. He spent his post-doc time at the Institute of Semiconductor Technology of the FhG. In 1994 he accepted a position at the central research organization of Wacker-Chemicals dedicated to the acquisition of research and technology. Since 1995 he holds a chair as a full professor for physical chemistry at the University of Marburg. He authored more

than 250 research papers and 19 patent families. His research is in the biopolymer field as well as laser-nanostructured surfaces.

### **Fullertubes: From Discovery to Applications**

#### **Steven Stevenson**

Purdue University (Fort Wayne), Chemistry and Biochemistry Department, Fort Wayne, IN, USA

## Abstract:

The recent experimental isolation in 2020 of fullertubes1-3 [e.g. [5,5]-C100-D5d(1)] is generating a large interdisciplinary interest to explore their fundamental research and applications. The fullertube structure possesses a unique molecular architecture from which to leverage new science. This Frankenstein creation of pristine fullertubes consists of two fullerene-based hemispherical endcaps with a single, connecting belt comprised of rolled graphene. Due to its structure, fullertubes offer their own blended properties (e.g., electronic), which are unique from either fullerene alone or nanotubes alone. In this talk, I provide an overview beginning with their experimental discovery and conclude with a brief discussion of possible fullertube applications. 1. J. Am. Chem. Soc. 2020, 142, 36, 15614–15623, https://doi.org/10.1021/jacs.0c08529 2. J. Am. Chem. Soc. 2021, 143, 12, 4593–4599, https://doi.org/10.1021/jacs.0c11357 3. Angew. Chem. 2022, https://doi.org/10.1002/anie.202116727

## **Biography:**

Steven Stevenson received his Ph.D. in Chemistry from Virginia Tech in 1995. Since then, he has worked in diverse sectors, e.g., government, industry, and academic labs. Stevenson is currently a Full Professor in the Department of Chemistry and Biochemistry at Purdue University (Fort Wayne campus). Stevenson's career can be described as a new molecule chaser. Once purified, Stevenson collaborates with other scientists for R&D. His collaborative network of fullertube research includes Japan, China, Canada, USA, Spain, Germany, and others. If interested, feel free to communicate with Stevenson for possible fullertube collaborations.

## Individualization and 'Networking' of Carbon Nanotubes: Interdependent Chemical Modifications in the Quest for Novel Nanomaterils

### Slawomir Boncel\*

Silesian University of Technology University, Poland

#### Abstract:

One of the most challenging problems of transfer of the extraordinary properties of carbon nanotubes (CNTs) from nano- to micro- to eventually macro-scale is control over their surface chemistry. Here, we present – essential for electrical, thermal and mechanical properties – chemical modifications of CNTs enabling both individualization of nanotubes and maintenance of the original C-sp2-skeleton. We extended the scope of possible chemical modifications of CNTs involving recovery of the aromatic sp2-skeleton due to thermally initiated retro-electrocyclization of the '1,3-cyclohexadiene' rings in the bis-CNT-adducts toward the [10] annulene unit. The first scheme was based on (2+1)-cycloaddition reaction of CNTs with in situ generated aromatic nitrenes. As the second route, 1,2-bis-chlorination of CNTs using ICl or I2Cl6 with subsequent Ullmann-type reactions led to products of structures enabling conjugation of p-electrons from the CNT framework with the linkages via O-, NH- or C(Ph)-centers. Also, bis-1,2-hydroxylated CNTs were reacted with chloro-s-tetrazines via nucleophilic substitution. The newly elaborated methods, translated into cross-linking chemistry of CNTs (and other sp2-carbon allotropes), enabled us formation of linkages conjugated with the CNT skeleton while extendable to other nanocarbons. This phenomenon enabled formation of 3D CNT-networks with a decreased number of inter-tube ohmic contacts and a partial replacement of the van der Waals contacts with the covalent conjugated linkages. Those transformations yielded nanomaterials of enhanced electrical and thermal conductivity. As exemplary applications, we have prepared textronic solutions for Holter-like electrocardiography and high-performance heat transfer fluids.

## **Biography:**

**Slawomir Boncel**, PhD DSc Eng, leader of *NanoCarbon Group*, completed MSc Eng degree in chemical technology (2004), PhD in organic chemistry (2009) and habilitation in nanochemistry ('Chemically modified carbon nanotubes and their exemplary applications', 2015) at the Silesian University of Technology in Gliwice, Poland. In 2013 he received a 15-month post-doc scholarship in the Department of Materials Science at the University of Cambridge (UK) financed by Foundation for Polish Science to perform his research on magnetically controlled carbon nanotubes as drug delivery systems. His research interests include synthesis, physicochemistry and applications of carbon nanostructures. He is an author of 50 JCR publications (Hirsch index 14), lecturer in the Department of Organic Chemistry, Bioorganic Chemistry and Biotechnology in his *Alma Mater* and PI in 7 research projects. The projects concern CNT-based composites and hybrid materials with their civil/military applications, *inter alia* magnetic CNT-based drug delivery systems, electroconducting coatings for nanotextronics, elements of *stealth* technology, heat transfer nanofluids and high-performance nanocomposites.

[1] A.W. Kuziel, G. Dzido, R. Turczyn, R.G. Jędrysiak, A. Kolanowska, A. Tracz, W. Zięba, A. Cyganiuk, A.P. Terzyk, S. Boncel, J. Energy Storage 2021, 36, 102396. [2] A.W. Kuziel, K.Z. Milowska, P.-L. Chau, S. Boncel, K.K. Koziol, N. Yahya, M.C. Payne, Adv. Mater. 2020, 2000608. [3] A. Kolanowska, A.P. Herman, R.G. Jędrysiak, S. Boncel, RSC Adv. 2021, 11, 3020-3042.

## **Progresses in Long Acenes**

## André Gourdon<sup>\*1</sup> and Andrej Jancarik<sup>2</sup>

<sup>1</sup>CEMES-CNRS, GNS Group, Toulouse (France)

<sup>2</sup>CRPP-CNRS and Université de Bordeaux, Bordeaux (France)

## Abstract:

Acenes are planar polyaromatic hydrocarbons consisting of linearly fused benzene units and can be considered as the narrowest zig-zag graphene nanoribbons. The small HOMO-LUMO gap and partial open-shell character imprint these compounds with interesting electronic and magnetic properties. They have been predicted for use as molecular wires in single molecule electronics, semi-conductors, for solar-cells applications, organic field-effect transistors, organic light emitting diodes etc. In recent years, we have witnessed enormous progress in the preparation of acenes beyond pentacene and up to dodecacene, however in minute amounts, at low temperature and under high vacuum. In contrast, the synthesis of long acenes in bulk has been described only recently: hexacene in 2012 by T.J. Chow et al. and heptacene by H.F. Bettinger et al., more than 70 years after the first attempted synthesis.

We have developed new improved general methodology for preparation of acenes longer than pentacene: The concept is based on the preparation of "carbon monoxide protected" precursors formed by cycloaddition reaction between carbonyl-masked benzdiene and arynes. The CO bridged aromatic compounds are stable and aromatize quantitatively upon heating under vacuum in the solid state, or during sublimation. We extend our methodology towards the synthesis of pentacene-based starphene, new family of angularly fused acenes and recently by nonacene.

### **Biography:**

André Gourdon is currently Director of Research (emeritus) at CEMES-CNRS, Toulouse (France) in the Nanoscience's Group (https://www.cemes.fr/NanoSciences-Group-GNS-Team?lang=en). His research interests focus on the design, synthesis and structural studies of organic and inorganic molecular devices for nano sciences and molecular electronics.

## **Coal-derived Carbon Products: Lessons Learned and Opportunities**

## Alexander Azenkeng\*, Nicholas N. Stanislowski, James E. Tibbetts, and Jason D. Laumb

Energy & Environmental Research Center, USA.

#### **Abstract:**

Coal is an abundant natural resource with a high carbon density and can be harnessed to make high-value products, such as graphene and synthetic graphite. These carbon-based products have excellent applications in multiple industries, including electronics, manufacturing, and building and infrastructure. Challenges with coal can hinder the optimal derivation of high-value products. Results of such coal-borne impurity impacts on the optical properties of coal-derived graphene quantum dots (GQDs) and coal-derived graphite are presented. It was found that the optical properties of GQDs changed with a coal precursor pre-treatment method. Additionally, synthetic graphite obtained under different graphitization conditions from coal that has undergone different pre-treatments have varying degrees of graphitization. These results provide useful lessons and insights into how to best tailor the properties of coal-derived high- value products to meet the opportunities in the growing lithium-ion battery, electric vehicles, and other markets.

#### **Biography:**

Alexander Azenkeng serves as Associate Director for Critical Materials at the University of North Dakota (UND) Energy & Environmental Research Center (EERC), USA. 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; and coal-derived critical materials such as rare-earth elements, platinum group metals, and high-value carbon materials.

## Colloidal Stability and Spatial Arrangement of Hydrogenated Milled Nanodiamonds in Water

## Jean-Charles Arnault<sup>1\*</sup>, Lorris Saoudi<sup>1</sup>, Hugues Girard<sup>1</sup>, Jocelyne Leroy<sup>1</sup>, Eric Larquet<sup>2</sup>

<sup>1</sup>Université Paris-Saclay, CEA, CNRS, NIMBE, CEDEX, 91 191 Gif-Sur-Yvette, France <sup>2</sup>Condensed Matter Physics Laboratory, UMR CNRS 7643, Ecole Polytechnique, IP-Paris, 91228 Palaiseau, France

## Abstract:

Diamond nanoparticles are produced along two main synthesis pathways: (i) by detonation (DND), giving rise to quasi-monodisperse but defective 5 nm particles or (ii) by milling of synthetic or natural diamond (MND), which preserves the crystalline quality with unique semi-conducting assets of bulk diamond for energy-related applications. Such MND are also suitable to host color centers intensively studied for nanomedicine or quantum applications [1]. Such applications require a fine control of the ND colloidal properties, especially for hydrogen terminated surface. If the route towards stable suspensions of H-DND in water is well identified [2], nowadays, providing colloidal stability over months to hydrogenated MND is still a challenge. The present study aims to investigate the colloidal stability in water of 50 nm H-MND obtained by thermal hydrogenation. We will show that tuning the experimental conditions, we successfully obtain stable suspensions of hydrogenated MND over months. Their colloidal properties, monitored by DLS, zetametry and cryo-TEM, will be correlated to an extended characterization of their surface chemistry and morphology via a combination of FTIR, XPS, Raman, HR-TEM and XRD investigations. In addition, cryo-TEM observations reveal the formation of chain-like structures for H-MND that is not present for oxidized MND. H-MND colloidal stability will be discussed according to the amount of C-H bonds and the residual sp2 carbon. The origin of chain formation will be also addressed. References [1] Nunn et al., Nanoscale, 11 (2019) 11584 [2] Arnault and Girard, Current Opinion in Solid State & Materials Science 21 (2017) 10-16.

## **Biography:**

Jean-Charles Arnault, CEA Research Director, is a recognized specialist of CVD growth and surface properties of diamond epitaxial films and nanodiamonds. From 2010, his research focused on ND surface properties modified by plasma, thermal or chemical treatments. He investigated intrinsic properties of hydrogenated ND towards bio applications, like a remarkable radio sensitization effect on radioresistant human cancer cells. Since 2020, he develops nanodiamonds for photocatalysis. He authored (co-authored) 132 publications, 7 book chapters and gave 47 invited talks. He edited "Nanodiamonds" (Elsevier, 2017) and "Synthesis & Applications of Nanocarbons" (Wiley, 2020). Since 2015, he is an editor of Diamond and Related Materials.

## Effect of Chlorine on Undoped and Heteroatom Doped Carbon Nanomaterials: Their Applications in Electrochemistry

Winny K Maboya<sup>\*1</sup>, Herry K Mmako<sup>1</sup>, Neil J Coville<sup>2</sup>, Sabelo D Mhlanga<sup>3</sup> and Manoko S Maubane-Nkadimeng<sup>2,4</sup>

<sup>1</sup>Department of Chemistry, Faculty of Applied and Computer Sciences, Vaal University of Technology, Private Bag X021, Vanderbijlpark, 1900, South Africa.

<sup>2</sup>DST-NRF Centre of Excellence in Strong Materials and Molecular Sciences Institute, School of Chemistry, University of the Witwatersrand, Johannesburg, WITS, 2050, South Africa.

<sup>3</sup>DST-Mintek Nanotechnology Innovation Centre, Mintek, 200 Malibongwe Drive, Strijdom Park, 2194, South Africa.

<sup>4</sup>Microscopy and Microanalysis Unit, University of the Witwatersrand, Johannesburg, WITS, 2050, South Africa

## Abstract:

The role of chlorine on morphology of undoped and heteroatom doped carbon nanomaterials was evaluated using various catalytic vapor deposition methods over a Fe-Co/CaCO3 catalyst using dichlorobenzene as chlorine source. Carbon nanomaterials of various morphologies were obtained. and their morphologies were found to depend on the presence or amount of chlorine added to the feed. X-ray photoelectron spectroscopy also showed that the type of dominating nitrogen environment in the carbon nanomaterials depended on the amount of chlorine present in the feed. Raman spectroscopy and transmission electron microscopy also demonstrated that chlorine created defects on the outer walls of the nanotubes. Modification of the synthesis method demonstrated formation of open-ended carbon nanomaterials in some cases, whereas in others loading of nanoparticles on the outer walls of the carbon nanomaterials was observed. Application of some of these materials in electrochemistry, proved that some of them can be employed as electrocatalysts in electrochemical reactions like oxygen reduction reaction. Some were applied as electrochemical sensors for selected persistent personal care products and their detection limits were very low and comparable to other carbon nanomaterials found in literature. Figure 1 Transmission electron microscopy images of (a) chlorinated (b) chlorinated sulfur-doped and (c) chlorinated boron-doped carbon nanotubes using dichlorobenzene as chlorine source in all cases.

## **Biography:**

Winny Maboya currently works at the Department of Chemistry, Vaal University of Technology. Winny does research in Electrochemistry, Inorganic Chemistry and Nanotechnology. Their current project is 'Antimicrobial properties of carbon nanotubes decorated with metal oxide nanoparticles'. She was expertise in Material Characterization, Nanomaterials, Nanomaterials Synthesis, Nanoparticle Synthesis, SEM Analysis, XRD Analysis, TEM Image Analysis, FTIR Analysis, Chemical Vapor Deposition, TGA

### Ultrafast Strong-field Emission of Electron in Carbon Nanostructures

#### Doo Jae Park<sup>\*1</sup>, Byeong Hee Son<sup>2</sup>, and Yeong Hwan Ahn<sup>3</sup>

<sup>1</sup>School of Nano-convergence Technonlogy, Hallym University, Chuncheon 24252, Republic of Korea

<sup>2</sup>Cheorwon Plasma Research Institute, Cheorwon-gun 24047, Republic of Korea

<sup>3</sup>Department of Physics and Department of Energy System Research, Ajou University, Suwon 16499, Republic of Korea

#### Abstract:

The electronic control of an ultrafast tunnelling electron emission was demonstrated in the nanogap of a single-walled nanotube (SWNT) and graphene nanostructures, when irradiated by a femtosecond laser pulse. The SWNT apex possesses a nanoscale morphology with a large damage threshold, and thus enabled the achievement of a large emission rate. More importantly, the DC field-emission characteristics varied when the gate bias was changed. This was analysed in terms of the change in the effective barrier height and enhancement factors. Photo-induced electron emission was observed when the gap area was illuminated with a femtosecond laser at a wave-length of 800 nm. As the laser power was increased, a saturated tunnelling current was observed, reaching more than 10 electrons per pulse. Finally, the photo-electron emission yield was tuned with the help of gate-induced variations in the electronic band structures of the SWNTs.

The graphene, which has atomically sharp edges with the large damage threshold, enable us to achieve the strong tunneling regime for the subcycle field emission. The photo-induced signals exhibited an anomalous increase in nonlinear order as a function of incident pulse energy in the presence of static electric field. A dynamical analysis of tunneling electrons based on the semi-classical model, which considers the contribution from the recoil electrons, reproduced our observation successfully. The large field enhancement near the graphene edge enabled us to reach the deep tunneling regime with the extraordinary Keldysh parameter of 0.2 in the near-infrared region.

#### **Biography:**

Ph. D. In Physics, Seoul National University, Republic of Korea (2008)

Postdoctoral Research Fellow, Ajou University, Republic of Korea (2008~2010)

Postdoctoral Research Fellow, Carl-von-Ossietzky University, Germany (2010~2012)

Research Professor, Sungkyunkwan University, Republic of Korea (2012~2015)

Professor, School of Nano-convergence Technology, Hallym University, Republic of Korea (2015~present)

## Spatially Resolved Covalent 2D-patterning of Graphene

## Tao Wei\*, Frank Hauke, Andreas Hirsch

Department of Chemistry and Pharmacy and Joint Institute of Advance Materials and Processes (ZMP), Friedrich-Alexander University of Erlangen-Nürnberg, Germany

## Abstract:

Exploring the tailored physical/chemical properties is the forefront of graphene research, and covalent molecular engineering represents a rather promising solution for this purpose bearing several unique advantages. To this end, we have developed two strategies, including mask-assisted patterning and laser writing, for spatially resolved 2D-functionalization of graphene, providing a variety of well-structured graphene architectures. Furthermore, based on the combination of 2D-patterning techniques and post-functionalization approaches, more promising hierarchically ordered multifunctional graphene architectures were facilely constructed. We further demonstrated that the chemical information of these built 2D-systems can be finely manipulated by establishing complete write/read/erase circles

#### **Biography:**

Tao Wei obtained his Ph.D. from University of Science and Technology of China in 2015. Then

he worked as an Alexander von Humboldt fellow under Prof. Andreas Hirsch at Friedrich-Alexander-University of Erlangen-Nürnberg. In 2021, he initiated his independent research as a Habilitand at the same university. His research interest lies in chemical functionalization of carbon allotropes including fullerene, carbon nanotube, and graphene.

## The Theory of Surface-enhanced Raman Spectroscopy on Organic Semiconductors: Graphene

## John R. Lombardi

Department of Chemistry and Biochemistry

The City College of New York, N.Y

### **Abstract:**

Drawing on a theoretical expression previously derived for general semiconductor substrates, we examine the surface-enhancement of the Raman signal (SERS) when the substrate is chosen to be monolayer graphene. The underlying theory involves vibronic coupling originally proposed by Herzberg and Teller. Vibronic coupling of the allowed molecular transitions with the charge-transfer transitions between the molecule and the substrate have been shown to be responsible for the SERS enhancement in semiconductor substrates. We then examine such an expression for the Raman enhancement in monolayer graphene, and which is dependent on the square of the derivative of the density of states of the graphene. On integration, we find that the discontinuity of the density of states function leads to a singularity in the SERS intensity. Knowledge of the location of this resonance allows us to maximize the Raman intensity by careful alignment of the doping level of the graphene substrate with the charge-transfer transition.

## **Biography:**

BA, CORNELL UNIVERSITY, 1963; PH.D. HARVARD UNIVERSITY, 1970, PROFESSOR, UNIVER-SITY OF ILLINOIS, MIT, CITY COLLEGE OF NEW YORK.

## Synthesis of ZNO on 3D Graphene/Nickel Foam for Photoelectrochemical Water Splitting

#### Rozan Mohamad Yunus\*, Nur Rabiatul Adawiyah Mohd Shah

Nurul Nabila Rosman Fuel Cell Institute, Universiti Kebangsaan Malaysia, 43600 UKM Bangi, Selangor, Malaysia

## Abstract:

Photoelectrochemical (PEC) water splitting is a promising method that involves a direct route to produce green hydrogen (H2). An efficient semiconductor photoelectrode that has a suitable band gap between the valence and conduction band is stable in an aqueous solution and cost-effective. Efficient charge transfer and outstanding light absorption are required to achieve enhanced PEC water splitting performance. However, the wide band gap of current photoelectrode such as zinc oxide (ZnO) limits their ability to transport electron, causing photogenerated electron-hole pair recombination and poor PEC performance. This study aims to design an efficient photoelectrode by incorporating a three-dimensional (3D) graphene with ZnO, where 3D graphene was first syn-

thesized on nickel foam (Nifoam) via chemical vapor deposition method with the flow of argon, H2, and methane gas flow in a quartz tube, followed by the growth of ZnO via a hydrothermal method at 150 °C and 200 °C. FESEM, EDX and Raman confirmed the successful growth of ZnO on 3D graphene/Ni-foam. The flower-like ZnO was observed by FESEM after the hydrothermal method, and the highest photocurrent density was measured at 150 °C (108.2 mAcm2). Therefore, flower-like ZnO flower-like on 3D graphene/Ni-foam can be used as an efficient semiconductor photoelectrode in PEC water splitting.

#### **Biography:**

Rozan Mohamad Yunus obtained her Doctor of Philosophy (PhD) in Material Engineering from Kyushu University, Japan under the supervision of Prof. Hiroki Ago. She is currently a senior lecturer/ research fellow at Fuel Cell Institute of Universiti Kebangsaan Malaysia. Her research interests involve nanotechnology, photo- and electro- catalysis in energy related field. In particular, developing a graphenemetal oxide based photocatalyst and PGM-free electrocatalyst for hydrogen production through water splitting. She has more than 10 years experiences in fundamental of graphene and other nanomaterials.

## Laser-induced Carbonization-setting New Standards for the Application of Bio-based Carbon in Flexible Electronics

Volker Strauss<sup>1, \*</sup>, Huize Wang<sup>1</sup>, Charles Charles Otieno Ogolla<sup>2</sup>, Marco Hepp<sup>2</sup>, Benjamin Butz<sup>2</sup>

<sup>1</sup>Max-Planck-Institut für Kolloid- und Grenzflächenforschung Am Mühlenberg 1, 14476 Potsdam, Germany

<sup>2</sup>Micro- and Nanoanalytics Group, University of Siegen, Paul-Bonatz Str. 9–11, Siegen, 57076, Germany

## **Abstract:**

Fabricating electronic devices from natural, renewable resources has been a common goal in engineering and materials science for many years. In this regard, carbon is of special significance due to its biological compatibility. In the laboratory, carbonized materials and their composites have been proven as promising candidates for a range of future applications in electronics, optoelectronics, or catalytic systems.[1] On the industrial scale, however, their application is inhibited by tedious and expensive preparation processes and a lack of control over the processing and material parameters. Therefore, we are exploring new concepts for the utilization of carbonized materials in electronic applications.

In particular, carbon laser-patterning (CLaP) is emerging as a new tool for the precise and selective synthesis of functional carbon-based materials for flexible on-chip applications.[2] To this end, we design versatile inks made from naturally occurring (molecular) starting materials.[3] Films made from these inks are carbonized with a CO2-laser to obtain functional patterns of conductive porous carbon networks. First, we present mechanistic insights into the process of laser-carbonization. In a series of studies, we introduce methods for the chemical and physical fine-tuning of the laser-patterned carbons (LP-C).[4] Based on this knowledge, we developed high-performance flexible resistive chemical and mechanical sensors. In further studies, we show the general applicabil-

ity of LP-C electrodes in electrochemical applications such as electrocatalysis and charge-storage.

[1] D. Jariwala, V. K. Sangwan, L. J. Lauhon, T. J. Marks, M. C. Hersam, Chem. Soc. Rev. 2013, 42, 2824–2860.

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## **Biography:**

Volker Strauss is a group leader at the Max Planck Institute of Colloids and Interfaces in Potsdam/ Germany.

Volker studied molecular science at the University of Erlangen-Nuremberg and gathered his first practical research experience in organic chemistry at Clemson University. In 2016 he obtained his Ph.D. in photophysics of nano-carbons at the University of Erlangen- Nuremberg. Following this, he moved to the Department of Chemistry at UCLA, where he acquired expertise on synthesis and application of solid-state electronic materials.

His work is dedicated to the investigation of new synthesis routes for functional carbon-based materials and composites. Currently, he focuses on laser-patterning of composite materials from abundant starting materials for room-temperature sensing architectures.

## CO<sub>2</sub> Assisted Synthesis of Novel Copper-based CuxC/Cu<sub>2</sub>O MXene-like Material

## Ahmed Badreldin<sup>1\*</sup>, Ahmed Abdala<sup>1</sup>, and Ahmed Abdel-Wahab<sup>1</sup>

<sup>1</sup>Chemical Engineering Program, Texas A&M University at Qatar, P.P. 23874, Doha, Qatar

## Abstract:

A large subsect of carbon-based nanomaterials are attributed with their excellent mechanical, electrical, chemical, optical, and thermal properties that make them very promising for a wide range of applications such as water treatment, electronics, biomedical, and energy storage and conversion. This has inspired a tremendous effort over the past two decades towards synthesizing and functionalizing different allotropes of these materials including, but not limited to, 1-dimensional (1D) carbon nanotubes, 2D graphene and graphene oxides, 3D activated carbon, and MXenes. The latter group has received increasing attention owing to their unique physical and chemical properties that make them attractive for many applications. Although several TM-based MXenes have been discovered, Cu-based MXenes have only been theorized using density functional theory (DFT) first-principle studies. Through a serendipitous investigation on thermally-assisted reactions between CO2 and copper substrates, we were able to consistently produce large area crystalline Cu-C-O matrices with chemical vapor deposition (CVD) diamond-like surface and graphite-like bulk morphologies, homogenous Cu2O/CuxC crystalline phases, sp2 carbon character, and anomalously unidentified Raman vibration modes. Interestingly, microscopy images upon acid-etching of this material exhibited MXene-like 2D morphologies. Characterization through Raman, HRTEM, FESEM, XPS, AFM, solid-state C-NMR, and XRD showcases the novelty of this material which may lead to future discoveries of CO2- based solid nanocarbon materials towards a variety of energy and environmental applications. In this talk, we plan to present synthesis procedure and characterization results of this material, and to discuss current and future research plan to better understand the nature and intrinsic properties of this potentially novel material group.

## **Biography:**

Ahmed Badreldin is currently a PhD candidate in the Chemical Engineering Department at Texas A&M University. His research focuses on coupling theoretical and experimental basis for material and technology advancement towards electrochemical energy storage and conversion, and CO2 utilization. Ahmed has recently embarked on development of a novel process for CO2 utilization to value-added solid carbon nanomaterials. He has received the Texas A&M University Richard E. Ewing Award for Research Excellence in 2022, and the Early-Stage Research Career Award at the 2 nd International Conference on Sustainable Energy-Water-Environment Nexus in Desert Climate (ICSEWEN21) in 2021.

## **Bifunctional Polymer Binders for Silicon Anode-based Lithium-ion Batteries**

## In Hwan Jung\*

Department of Energy Engineering, Hanyang University, 17 Haengdang-dong Seongdong-gu, Seoul 04763, Republic of Korea

### **Abstract:**

Lithium-ion batteries (LIBs) are one of the most widely used electrical energy storage systems due to their excellent cycle performance and high energy density. However, currently, the higher specific capacity are required for electric vehicles and portable electronics and Si is regarded as one of the most promising anode materials that can replace graphite anode materials for LIBs because of its high theoretical capacity of 3,579 mAh g-1 (Li3.75Si). In case of Si electrode, there is chronic problem of a huge volume change during the alloying and dealloying reactions with lithium, and thus polymeric binders that can make robust binding with Si electrode are necessarily required. Recently, we developed an ambidextrous polymer binder with two functional groups that could form strong bonds with Si and carbon black particles. Due to the improve interaction among Si, carbon black and polymer binder, the Si anode with our binder showed much greater capacity retention over 200 cycles and reversible capacity.

#### **Biography:**

In Hwan Jung earned his Ph. D. (2011) in Department of Chemistry from Korea Advanced Institute of Technology (KAIST). After 3 years of postdoctoral fellow in Department of Chemistry at University of Chicago, he returned to the Korea Research Institute of Chemical Technology as a senior researcher. From 2021 to present, he has been an associated professor in Department of Organic and Nano Engineering at Hanyang University (Republic of Korea). He is interested in development of organic molecules and conjugated polymers for organic photovoltaics (OPVs), organic thermoelectric devices (OTEs), organic photodetectors (OPDs), and Li-ion batteries.

## Importance of Interface: Flavin Mononucleotide Mediated Formation of Highly Electrically Conductive Hierarchical Monoclinic Multiwalled Carbon Nanotube-Polyamide 6 Nanocomposites

## Sang-Yong Ju<sup>1\*</sup>, Minsuk Park<sup>1</sup>, Seulki Yoon<sup>2</sup>, Junmo Park<sup>1</sup>, No-Hyung Park<sup>2</sup>

<sup>1</sup>Department of Chemistry, Yonsei University, Seoul 03722, Republic of Korea

<sup>2</sup>Department of Textile Convergence of Biotechnology and Nanotechnology, Korea Institute of Industrial Technology, Ansan-Si, Gyeonggi-Do 15588, Republic of Korea

## **Abstract:**

Although the multiwalled carbon nanotube (MWNT) is a promising material for use in the production of high electrical conductivity ( $\sigma$ ) polymer nanocomposites, its tendency to aggregate and distribute randomly in a polymer matrix is a problematic issue. In the current study, we developed a highly conductive and monoclinically aligned MWNT-polyamide 6 (PA) nanocomposite containing interfacing flavin moieties. In this system, the flavin mononucleotide (FMN) initially serves as a noncovalent aqueous surfactant for individualizing MWNTs in the form of FMN-wrapped MWNTs (FMNMWNT), and then partially decomposed FMN (dFMN) induces crystallization of the PA on the MWNTs. The results of experiments performed using material subjected to partial dissolution of PA matrix show that the nanocomposite PA-dFMN-MWNT, formed by melt extrusion of PA and dFMN-MWNT, contains a three-dimensional monoclinic MWNT network embedded in an equally monoclinic PA matrix. An increase in monoclinic network promoted by an increase in the content of MWNT increases  $\sigma$  of the nanocomposite up to 100 S/m, the highest value reported for a polymer-MWNT nanocomposite. X-ray diffraction along with transmission electron microscopy reveal that the presence of dFMN induces the formation of monoclinic PA on dFMN-MWNT. The high  $\sigma$ of the PA-dFMN-MWNT nanocomposite is also a consequence of a minimization of defect formation of MWNT by noncovalent functionalization. Hierarchical structural ordering, yet individualization of MWNTs, provides a viable strategy to improve the physical property of nanocomposites

## **Biography:**

Sang-Yong Ju received B.S. degree (1998) from the Hanyang University. After obtaining his M.S. degree (2000) in polymer science at same university, he worked as commissioner researcher at Korea Institute of Science and Technologies (2002). He earned Ph.D. (2008) in Institute of Material Science at University of Connecticut. He worked as a postdoctoral researcher at Cornell University (2011). Then, he joined as assistant professor at Yonsei University (2011) and now associate professor at the same university (present). His research focus is on the synthesis and optical characterization of defined nanomaterials for optoelectronic applications.

## Nanocomposite Derived from Local Ilmenite and Monazite for Solid Oxide Fuel Cell Cathode Material

## Sahrim Ahmad, Muhammad Zaid Ahmad and Chen Ruey Shan

School of Applied Physics, Faculty Sacience and Technology, Universiti Kebangsaan Malaysia 43650 UKM Bangi Selangor

## **Abstract:**

Solid oxide fuel cell (SOFC), which is well-known as a green energy technology, have experienced phenomenal development in recent years. However, the major issue for commercialization of SOFC is to balance the durability and reliability with cost-effective aspects. One of the approaches to solve this problem is to utilize some abundant natural resource for materials cost reduction and thus increasing its sustainability. In Malaysia, ilmenite, an ironbased mineral, and monazite, a mineral that contain oxides of lanthanum, are abundant. Therefore, our main objectives are to develop a nanocomposite of La, Sr, Ti, Fe, (LSTF) for cathode materials application using the local extracted minerals from both ilmenite and monazite. Titanium dioxide and ferric oxide from local ilmenite as well as lanthanum oxide from monazite are extracted with varying degree of purity using extractive metallurgy method. Then, the LSTF powder is prepared using a conventional solid-state reaction method. Finally, the symmetrical SOFC is developed by screen-printing method using LSTF with yttria-stablized zirconia (YSZ) as the electrolyte. While the electrical performance analysis is still ongoing, we predict that the LSTF cathode made from locally extracted materials will give equal if not better performance than the one's made from store-bought materials due to the existence of impurities elements in the local ores that have interesting electrical properties such as cerium and neodymium.

#### **Biography:**

Sahrim Ahmad currently working as a professor in the department of Applied Physics, Faculty of Science and Technology at Universiti Kebangsaan Malaysia. He was expertise in the field of magnetic nanoparticles, polymer blends, composites, biocomposites and nanocomposites.

#### Predicting Thermally Induced Damage in CFRP by Means of Multivariate Data Analysis

## Tanja Vetter<sup>1\*</sup>, Sebastian Eibl<sup>1</sup>, Hans-Joachim-Gudladt<sup>2</sup>

<sup>1</sup>Wehrwissenschaftliches Insistut für Werk- und Betriebsstoffe Erding

<sup>2</sup>Univeristät der Bundeswehr München

## **Abstract:**

Carbon Fiber Reinforced Polymers (CFRP) are applied in light weight applications e.g. in aerospace because of their high strength to weight ratio compared to e.g. metal structures. Due to the polymer matrix, CFRP show limited thermal stability. Therefore, the quantification of thermal damage is indispensable. A non-destructive evaluation method for moderate thermal damage is ATR-FTIR-spectroscopy. Beside surface damage also the degradation into the depth has to be regarded. For this purpose, chemical and mechanical properties were considered inside the CFRP with respect to matrix degradation, loss of fiber-matrix-adhesion such as delaminations and their influence on the residual strength. Based on these findings, ATR-FTIRspectroscopy in combination with chemometric models is used to predict thermal damage in CFRP. It is the aim to reliably predict residual strength and delamination depth by using ATR-FTIRspectroscopy as non-destructive testing method. CFRP of different thickness are irradiated at varying heat fluxes over various time intervals. The inhomogeneously distributed matrix degradation is analysed by means of ATR-FTIR-spectroscopy. Residual interlaminar shear strength (ILSS) is determined and microfocused computed X-Ray tomography is applied for measuring the delamination depth. Principal component analyses illustrate which information of thermal loading is represented in the ATR- FTIR-spectra. Linear discriminant analysis models allow the prediction of the presence or absence of delaminations. Combining spectra taken in different depth of the CFRP allows the development of partial least squares regression models to predict ILSS and delamination depth. Although thermal damage is inhomogenously distributed and models consider varying sample thicknesses and heat fluxes, precise predictions are achieved.

## **Biography:**

Tanja Vetter studied chemistry with the focus on analytical chemistry and finished university with the Master of Science. After working for about two years for Oelcheck with the focus on lubricant analysis, she started to work at the Universität der Bundeswehr München scientific associate and PhD student. Here, the focus on her work is the thermal degradation of Carbon Fibre Reinforced Polymers with the objective to predict thermal damage by using spectroscopic techniques. This was also topic of her dissertation. Since 2021 she works as expert for material protection at Wehrwissenschaftliches Institut für Werk- und Betriebsstoffe in Erding.

## Carbon Nanofiber-assisted Construction of 1D Functionalized Nanocomposites for Electrocatalysis and Energy Storage

#### Feili Lai<sup>1,2\*</sup>

<sup>1</sup>Department of Chemistry, KU Leuven, Belgium

<sup>2</sup>Department of Molecular Spectroscopy, Max Planck Institute for Polymer Research, Germany

## Abstract Not available!!

## Highly Efficient Blue Organic Materials with Long OLED Device Lifetime and Perovskite Emitters

#### Jongwook Park\*

Integrated Engineering, Department of Chemical Engineering, Kyung Hee University, Republic of Korea

#### **Abstract:**

To develop materials that emit deep blue light with high efficiency, molecules were systematically designed and studied using the following three suggestions. (1) The key factor of deep-blue light is to select a core chromophore that controls intrinsic properties such as absorption and emission properties, thermal properties, and quantum efficiency. (2) Bulky aromatic rings were introduced as side groups to prevent broad and bathochromic emissions. (3) Aromatic amine groups were also tested as side groups to maintain the wide band gap. Ten compounds introducing various side groups were designed and synthesized. OLED device shows a high current efficiency of over 7 cd A-1. The compounds yield electroluminescence (EL) spectra showing peaks with narrow full width at half maximum values of 37-40 nm and hence indicative of high color purity. Moreover, one compound shows a very high external quantum efficiency of 9.25% and a very long lifetime, with an LT50 of 30,000 h. Perovskites is a very promising material that is being extensively studied at the bulk and nanosize scales because it has outstanding optical properties, including high

quantum efficiency and narrow emission spectra. The EL spectra of the WPeQD-OLEDs showed EL maximum peaks at 460, 527, and 640 nm; the CIE color coordinates of the emitted light were (0.33, 0.40). The EL results confirmed that the maximum luminance was 49,000 cd m-2 and the maximum luminance efficiency and power efficiency were 4.48 cd A-1 and 2.16 lm W-1.

### **Biography:**

Jongwook Park is Professor at Department of Chemical Engineering of Kyung Hee University in Korea. He received his Ph.D. from Korea Advanced Institute of Science and Technology. He is the author of 364 papers and holds 72 patents in the field of organic semiconducting materials. He was chairman of 12 large-scale projects of Korean industry in relation with electronic materials. He received the Prime Minister and President Awards from Korean government in 2012 and 2020. He was elected SPIE Fellow in 2018 in the United States as well as Kyung Hee University Fellow in 2019.

## **On-surface Carbon Chemistry Probed by Electron Spectroscopies**

## E. Salomon\*, N. Kalashnyk, S. Clair, F. Dumur and T. Angot

In the blooming field of on-surface synthesis, molecular building blocks are designed to self-assemble and covalently couple directly on a well-defined surface, thus allowing the exploration of unusual reaction pathways and the production of specific compounds in mild conditions [1, 2]. Here we report on the creation of functionalized organic nanoarchitectures on the Ag surfaces [3].

On the one hand, C–H bond activation and homo-coupling of the precursors is achieved upon thermal activation. Anisotropic substrate acts as an efficient template fostering the alignment of the precursors, leading to the formation nanoribbons. The length of those ribbons can be sequentially increased by controlling the annealing temperature, from dimers to a maximum length of about 50 nm, limited by epitaxial stress. More isotropic surface favors Knoevenagel condensation and lead to the formation of more complex architectures.

The different structures are characterized by room-temperature scanning tunneling microscopy. Distinct signatures of the covalent coupling are measured with high-resolution electron energy loss spectroscopy, photoelectron spectroscopy and supported by density functional theory calculations.

## **Poster Presentations**

## Larger Diameter Selection of Carbon Nanotube by Two Phase Extraction using Amphiphilic Polymeric Surfactant

## Seokhyeon Son\*, Hyunjun Park, Woodong Jang and Sang-Yong Ju

Department of Chemistry, Yonsei University, 50 Yonsei-ro, Seodaemun-Gu, Seoul 03722, Korea

## Abstract:

Single-walled carbon nanotubes (SWNTs) have unique properties that depend on their chirality, called a pair of integers (n, m). Due to the heterogeneity of SWNTs, it is important to separate

the chirality. Among the various SWNT separation methods, the aqueous two-phase extraction method based on poly(ethylene oxide)/dextran has a simple experimental procedure and low cost. However, fine tuning of hydrophilicity by using two surfactants inevitably changes the binding affinity and obscures the binding affinity difference with other SWNT chiralities. In this regards, one amphiphilic surfactant might be beneficial to sorting of SWNT. In this poster, we report that amphiphilic poly(2-ethyloxazoline)-benzyl ether derivative not only disperse SWNT efficiently in both water and p-xylene but also can be utilized a single surfactant partitioning SWNT from water to p-xylene in diameter (dt) selective manner. For this purpose, poly(2-ethyl oxazoline)-alkylated second-generation benzyl ether (POBE BzE) was used as a universal surfactant for both aqueous and organic phases. Importantly, the dt-selective extraction of the polymer/SWNT adduct from water to p-xylene was investigated by varying amounts of either phase transfer catalyst or sodium chloride. Quantitatively determine dt-selective extraction by obtaining absorption spectroscopy-based partition constants K (K = ctop/cbottom where ctop and cbottom represent concentrations of SWNT in top and bottom layers). The large dt selectivity mechanism was proposed by the interaction of SWNT-interacting moiety with respect to surrounding media.

## **Biography:**

Seokhyeon Son is currently a master's student at Yonsei University in Korea. He graduated Daegu university, Daegu, Korea (2021). His research topic of interest is "study of carbon nanotube separation". In free time, Seokhyeon enjoys cultural life, such as going to exhibitions and museums.

## Vibronic Features in Single Chirality Enriched Single-walled Carbon Nanotubes Wrapped by Flavin Surfactant

## Seongjoo Hwang\* and Sang-Yong Ju

Department of Chemistry, Yonsei University, 50 Yonsei-ro, Seodaemun-Gu, Seoul 03722, Korea

## **Abstract:**

Comprehending the optoelectronic features of single-walled carbon nanotubes (SWNTs) with distinct electronic band structures is more fully elucidated by accounting for excited electron and vibration. The optical spectrum of a single chirality SWNT gained by dispersion of N-dodecyl isoalloxazine (FC12) as a surfactant and subsequent adding of chloroform to the dispersion was investigated in this work. The absorption spectra of the sorted (8,6) tube shows prominent first (e11) and second (e22) transitions at 1.028 eV and 1.680 eV, respectively. Furthermore, those bands, which were followed by broad bands, separated e11 and e22 from the high energy sides by ~190 meV. Those bands are ascribed to electron-phonon interactions arising from Raman modes G and G' bands. We also noticed a minor side band of e11 and e22 on the lower energy side whose origin is currently unknown. Those electron-phonon bands are easily distinguishable from the optical transitions in the photoluminescence excitation (PLE) map. The AFM picture of SWNTs evenly surrounded by FC12 in a helical shape supports the spectroscopic features of SWNTs generated from FC12.

## **Biography:**

Seong Joo Hwang is currently a MD-PhD student in Chemistry at Yonsei University in Korea. He received his B.S. in Chemistry from Yonsei University in Korea. His research topic of interest is "op-toelectronic study on single chirality of single walled carbon nanotube". His hobbies include seeing

musicals and plays, and he enjoys having a BBQ outside every weekend.

## Sulfide Interlayered Co-(NiFe) Oxynitride Towards Efficient Oxygen Evolution Reaction in Neutral pH Environments

## Ahmed Badreldin<sup>1\*</sup> and Ahmed Abdel-Wahab<sup>1</sup>

<sup>1</sup>Chemical Engineering Program, Texas A&M University at Qatar, P.P. 23874, Doha, Qatar

## **Abstract:**

Development of water impurity-resilient electrocatalysts serves to support existing commercial electrolyzers that face predominant downtimes from upstream water quality upsets due to severe catalyst performance-dependent relation with water guality. Impure water systems have detrimental effects on the stability, kinetics, and activity of the already kinetically challenging four-electron transfer anodic oxygen evolution reaction (OER) electrocatalysts under different pH conditions. This predicament becomes compounded under neutral and near-neutral pH seawater electrolysis due to the requirement of an initial overpotential-heavy water dissociation step and undesired chlorine evolution reaction (CER). However, neutral pH operation during electrolysis of impure water systems has significant implications on elimination of Mg/Ca precipitants that block catalytically active sites and foul membrane dividers. In this work, we developed a homogenous surface charge delocalized Co-(NiFe) oxynitride active layer atop a NiSx interlayer grown on porous nickel foam substrate. The developed material serves to enhance water dissociation kinetics towards OER and CER suppression during electrolysis, consequently enhancing typically limited neutral-pH performance and stability. An array of characterization techniques including, but not limited to, HRTEM, XAS, XPS, XRD, and electrochemical analyses were employed to depict the intrinsic properties of the developed OER catalysts and their electrocatalytic performance. The optimum Co-(NiFe)N@NiSx@NF required low overpotentials of 350 and 430 mV in alkaline and neutral pH synthetic seawater electrolytes, respectively, to reach a high current density of 100 mA cm-2. Further, in situ gas chromatography analysis yielded 94.5 and 88.6% OER Faradaic efficiencies under alkaline and neutral pH synthetic seawater for the same NiSx interlayered sample.

#### **Biography:**

Ahmed Badreldin is currently a PhD candidate in the Chemical Engineering Department at Texas A&M University. His research focuses on coupling theoretical and experimental basis for material and technology advancement towards electrochemical energy storage and conversion, and CO2 utilization. Ahmed has recently embarked on development of a novel process for CO2 utilization to value-added solid carbon nanomaterials. He has received the Texas A&M University Richard E. Ewing Award for Research Excellence in 2022, and the Early-Stage Research Career Award at the 2<sup>nd</sup> International Conference on Sustainable Energy-Water-Environment Nexus in Desert Climate (ICSEWEN21) in 2021.

## Characterization of Different Types of Carbons for Energy Storage Applications

M. Matrakova<sup>1</sup>, A. Aleksandrova<sup>1\*</sup>, B. Mladenova<sup>1</sup>, S. Veleva<sup>1</sup>, L. Soserov<sup>1</sup>, S. Uzunova<sup>2</sup>, A. Stoyanova<sup>1</sup>

<sup>1</sup>Institute of Electrochemistry and Energy Systems"Acad. Evgeni Budevski", Bulgarian Academy of Sciences, Sofia, Bulgaria

<sup>2</sup>University of Chemical Technology and Metallurgy, Sofia, Bulgaria

## **Abstract:**

Modern industry, technology and everyday life are constantly in need of reliable energy sources, portable in many applications, cheap and, last but not least, less polluting for the environment. Many research have been focusing on the usage of different types of carbons as electrode material for electrochemical energy storage. Various characteristics like purity, surface area, porosity, particle size, conductivity, etc. are of critical importance for the electrochemical application of carbon materials. Production of low-cost carbon materials is essential for future development of batteries and supercapacitors.

The aim of the present study is to characterize "green" carbon material obtained from rice husks (RHC), synthetic organic carbon xerogel (CXG) and activated carbon xerogel (ACXG) as potential electrode materials or additives for supercapacitors or batteries.

The specific treatment conditions have strong impact on the phase composition, microstructure, porosity, surface reactivity, conductivity etc. of the selected carbon materials and thus reflect in their specific applications.

The rice husks are a widely available and low-cost raw material and are successfully used for production of bio-fuels or products for waste water treatment and cleaning. The porous low-ash-content carbonaceous material RHC sample was prepared by pyrolysis of rice husks and extraction of SiO2. First, rice husks were washed with hot water several times to remove mechanical admixtures. The washed and dried raw material were carbonized at 450 °C and then activated with water vapor at 700 °C. Finally, the solid product was treated with HF acid to remove the SiO2 and the obtained carbonaceous material sample was washed and dried [1].

The preparing processes of organic carbon gels are comparatively quick, simple and cheap and give potentiality to control the purity and porosity of the materials. The organic xerogel samples were synthesized by a microwave-assisted polycondensation of resorcinol and formaldehyde using deionized water as solvent [2]. The process of carbonization takes place in an inert atmosphere (100 ml/min N2), heating up to1000°C. The ACHG sample was produced by process of activation that consists of heating (50°C / min to 1000°C) in a reactive atmosphere (200 ml / min CO2).

The samples characteristics phase composition, specific surface and porosity, microstructure and morphology of the carbonaceous materials was investigated by X-ray diffraction analysis, surface area measurements (BET method) and scanning electron microscopy.

Acknowledgement: The project "Twinning cooperation for boosting excellence in electrochemical energy storage on the platform of supercapacitors (BIScapcs)" is funded by the Ministry of Education and Science of the Republic of Bulgaria under the National Program "European Scientific Networks" (Agreement D01-286 / 07.10.2020)

## Investigation of Different Types of Carbons as Additives in Electrode Materials for Energy Storage Applications

M.Matrakova<sup>1\*</sup>, A.Aleksandrova<sup>1</sup>, S.Veleva<sup>1</sup>, L.Soserov<sup>1</sup>, N.Rey-Raap<sup>2</sup>, A.Arenillas<sup>2</sup>, A. Stoy-

#### anova<sup>1</sup>

<sup>1</sup>Institute of Electrochemistry and Energy Systems"Acad. Evgeni Budevski", Bulgarian Academy of Sciences, Sofia, Bulgaria

<sup>2</sup>Instituto de Ciencia y Tecnología del Carbono, INCAR-CSIC, Oviedo, Spain

## Abstract:

The aim of the present study is to investigate the applicability of low-ash-content porous carbonaceous "green" material obtained from rice husks (RHC) or of carbon xerogel (CXG) as additives to the negative electrodes of lead batteries (LBs). For comparison, a commercially available product, carbon black PBX®51 (Cabot Corp., USA), widely used in the lead battery technology, was also used in our study. The use of carbon additives in the negative active mass (NAM) suppresses their progressive sulfation during high rate partial state of charge (HRPSoC) cycling (specific for HEV) [1-3].

The RHC sample was prepared by pyrolysis of rice husks and extraction of SiO2 [4]. The CXG sample was synthesized by polycondensation of resorcinol and formaldehyde using deionized water as solvent [5]. The control material carbon black PBX51was prepared employing a method known as decomposition of hydrocarbons feedstock at high temperature (1000-1500°C) [6, 7]. The different types of studied carbons, their specific surface area and loading concentrations in the negative electrodes of test lead cells are summarized in the table below.

Carbon type Specific surface area, m2g-1 Loading, %

Rice husks carbon (RHC) 610 0.50

Ccarbon xerogel (CXG) 1050 0.25

Carbon black PBX51 1400 0.50

Small-sized laboratory lead test cells comprising one negative and two positive plates per cell were assembled for capacity and cycle life tests. The obtained results show that carbon materials used as additives in NAM have beneficial effect on the discharge capacity of lead cells and improve the cycleability of the cells under HRPSoC conditions compared to the Blank cell (w/o carbon additive). These results demonstrate that the tested carbon materials are promising for use as negative electrode additives for energy storage applications.

## **Biography:**

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[2]. D.P. Boden D.V. Loosemore, M.A. Spense, T.D. Wojcinski, J. Power Sources, 195 (2010) 4470.

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## Metformin Degradation using $TiO_2/CuO$ Heterojunction Supported on Sand Granules in a Fluidized Bed Photoreactor (FBF)

## **Ricardo Solano Pizarro**

University of Cartagena, Colombia

## Abstract Not Available!!!

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

Laura Kalder<sup>1\*</sup>, Eneli Härk<sup>2</sup>, Riinu Härmas<sup>1</sup>, Jaan Aruväli<sup>3</sup>, Enn Lust<sup>1</sup>

<sup>1</sup>Institute of Chemistry, University of Tartu, Estonia

<sup>2</sup>Helmholtz-Zentrum Berlin, Germany

<sup>3</sup>Institute of Ecology and Earth Sciences, University of Tartu, Estonia

## Abstract:

Hard carbon materials have been found suitable for many specific technical applications due to the high variability and specific configurations of disordered sp2 structures and porosity. The precise and reliable estimation of the structure of hard carbons could aid in developing more efficient applications in areas such as electrochemical cells, filters, pharmaceutical agents, etc. Small-angle and wide angle scattering methods enable to study the structural units with length scale from 0.03 to 450 nm describing the size and order of graphene sheets as well as the porous structure of carbon material. Thus, we present the complementary utilization of wide-angle X-ray scattering (WAXS) and smallangle neutron scattering (SANS) methods to determine the synthesis temperatures' influence on the structure of hard carbons. Detailed characterisation of hydrothermally synthesized glycose derived hard carbons with various pyrolysis temperatures were carried out using WAXS Ruland and Smarsly algorithm1 and SANS model-free graphic analysis with combined Schiller, Mering, Perret, and Ruland approaches 2,3. This study revealed quantitative relations between the nanostructure of disorganized carbons and the pyrolysis temperature. The results indicated the threshold of extensive graphitization of glycose derived hard carbons, that could promote the further research on developing optimal conditions for approach in electrochemical cells.

## **Biography:**

I am a first year PhD student in University of Tartu and the focus of my studies is the physical characterization of the nanostructured carbon materials, applied inside sodium-ion batteries using small-angle and wide-angle scattering methods detailed data analysis. During masters studies I investigated the structure of partially graphitized carbons synthesized from D-glycose via hydrothermal carbonization to determine the influence of the pyrolysis temperature. I aim to seek the relations between the structure of the carbon material and electrochemical performance of the cell. (1) Ruland, W.; Smarsly, B. X-Ray Scattering of Non-Graphitic Carbon: An Improved Method of Evaluation. J. Appl. Crystallogr. 2002, 35 (5), 624–633. https://doi.org/10.1107/S0021889802011007. (2) Schiller, C.; Mering, J.; Cornuault, P.; Du Chaffaut, F. Defauts structuraux dans les carbones graphitables effets des traitements thermiques—partie II. Carbon 1967, 5 (5), 507–516. https://doi.org/10.1016/0008-6223(67)90027-9. (3) Perret, R.; Ruland, W. X-Ray Small-Angle Scattering

of Non-Graphitizable Carbons. J. Appl. Crystallogr. 1968, 1 (5), 308–313. https://doi.org/10.1107/ S0021889868005558.

## Laser Direct Writing of BaTiO<sub>3</sub> Thin Films to Applications in Nonlinear-optical Devices

## José Clabel Huamán<sup>1\*</sup>, Euclydes Marega Junior<sup>1</sup>, Cleber Renato Mendoça<sup>1</sup>

<sup>1</sup> São Carlos Institute of Physics, University of São Paulo, P.O. Box 369,13560-970, São Carlos, SP, Brazil

## Abstract:

Ferroelectric thin films with luminescent properties applied as photonic devices require high linear and non-linear electro-optical coefficients and the bandwidth that gives high performance for the near-visible infrared response. Barium titanate (BaTiO3) films doped with Er atoms with concentrations of 3 mol % (BT:Er) were grown on Pt/Si(100) substrates by spin coating. The crystallinity and morphology of the BT:Er films were characterized by the X-ray diffraction analysis and SEM, respectively. The ferroelectric and fluorescence properties of the BT: Er films were measured at room temperature. Polycrystalline BT:Er films with the tetragonal phase were grown, in which the Er concentration was kept at less than 3 mol %. The remnant polarization value of the ~230-nm-thick BT:Er films with Er concentration of 3 mol % was approximately 0.86  $\mu$ C/cm2 . The fluorescence properties were evaluated by performing the upconversion of the luminescence of the BT:Er thin films using the Confocal Fluorescence Microscopy (CFM). Green and red up-conversion emissions at 520, 550, and 670 nm were observed from the BT:Er films with 790, 800, and 980 nm excitations. The fluorescence results suggest a clear dependence of excitation wavelength on the emission intensity. A ~3-fold enhancement in emission has been demonstrated under Er3+ (800 nm) excitation, which can be attributed to an effective energy transfer between the Er3+ ions.

**Acknowledgment:** We acknowledge to the São Paulo Research Foundation, project number 2021/11484-5, São Paulo, Brazil.

## **Biography:**

He is working as a researcher at the Institute of Physics of São Carlos – University of São Paulo, Brazil. He received his Ph.D. in Physics from the Federal University of São Carlos in 2015. He has remained a post-doctoral fellow at the Brazilian Agricultural Research Corporation and Institute of Physics of São Carlos – University of São Paulo. His main research experience is in Condensed-Matter Physics and Materials Science. His interdisciplinary research interests include investigating multiferroic composites and Ferro-/piezoelectric and luminescent materials for structural and functional applications. He has published more than 24 research articles in high-impact international journals.

## A Study on the Electrochemical Performance of Silicon / Graphene compounds as Efficient Negative Electrode for Lithium Batteries Prototype

## Atef Y. Shenouda\* and Mustafa S. Sanad

Central Metallurgical Research and Development Institute (CMRDI), Tebbin, P.O. Box 87 Helwan, Egypt.

## Abstract:

Different percentages of nanoparticles graphene were added to Si powder as follows: 10, 20, 30 and 40 % graphene powder with Si wt./wt. ratios. The mixed powders were sonicated for 60 min. in acetone solvent. The crystal structure of Si powder pattern has cubic phase. EIS measurements reveal that pure Si electrode has high Rct, 1825 Win comparison with Si/graphene one. We conclude that graphene serves as a conductive pathway and decreases the charge transfer resistance of Si up to certain concentration, which is 30% giving Rct, 18 W resulting an enhanced conductivity. Furthermore, increasing the graphene concentration up to 40% with 60% Si increasing the Rct to be 279 W.

CV measurement for cell composed of pure Si/ Li shows a broad cathodic peak at 0.85V for the formation of solid electrolyte interface (SEI) layer with Si particles. There is another cathodic peak at 0.19V for the lithiation process of Si to form lithium silicide. There is an anodic oxidation peak at 0.56 V vs. Li+. This peak is due to the oxidation of LixSi into Si and Li ion. The specific discharge capacity of 70% Si-30% G cell delivered about 900 mAhg-1 up to 100 cycles.

### **Biography:**

Atef Youssef Shenouda is the former head of the Electrometallurgy Department, Central Metallurgical Research and Development Institute (CMRDI). He was born in Cairo in 1962. He got his B. Sc. in Chemistry (Hons.), Faculty of Science, Ain-Shams University, Cairo in 1983, M. Sc. and Ph.D in Electrochemistry, Faculty of Science, Cairo University, respectively. Research interesting: Lithium batteries, semiconductor materials used for photovoltaic solar cells, Electro Extraction, winning and refining of metals and Electrodeposition of alloys. His results have been published in several international refereed journals.

## Effect of Carbon Additives in a Cathode Electrode for Sulfide-based All Solid-state Batteries

## Ji-Sang Yu\*, Woo Suk Cho, Seung Ho Choi

Advanced Batteries Research Center, Korea Electronics Technology Institute, 25 Saenari-ro, Bundang-gu, Seongnam, Gyeonggi, 13509 Republic of Korea

## **Abstract:**

Among advanced rechargeable batteries, sulfide-based all-solid-state batteries are attracting attention from academia and industry due to their high energy density and superior safety. Argyrodite-type Li6PS5Cl especially shows a high Li-ion conductivity comparable to that of commercial Li-ion batteries, but an electrochemical decomposition on surface of Li6PS5Cl during charge process at over 3.5 V has been reported. Especially, structural degradation between carbon additive and Li6PS5Cl leads to a detrimental effect on Li-ion transport channel, resulting in poor cycle retention and increasing battery resistance. Therefore, a choice of appropriate carbon additive is crucial to minimize undesirable electrochemical side reactions upon repeated cycling. Herein, in order to identify an effect of carbon additives in cathode, we fabricate cathode electrodes with various carbon additives (carbon black, micro-sized carbon fiber, and vertical-grown carbon fiber) and evaluate their electrochemical properties, such as cycle retention, rate performance, and ion/ electron conductivity. Furthermore, we also investigate the correlation between physical properties of carbon additives and battery performances.

## **Biography:**

Ji-Sang Yu is a leader of advanced batteries research center at Korea Electronics Technology Institute (KETI). He received his B.S. degree of Materials Science and Engineering in 1993 from Korea University and Ph.D. degree of Materials Science and Engineering in 2000 from Korea Advanced Institute of Science and Technology. His research interest lies in next-generation rechargeable batteries, especially all-solid-state batteries.

## Biomass-derived Carbon Transition Metal Oxide Composites for Photodegradation

## Kaiying Wang\*

Department of Microsystems, University of South-Eastern Norway, Horten 3184, Norway

## Abstract:

In this work, methyl Orange (MO) dye in aqueous solution was selected to be the model organic pollutant in wastewater to evaluate the photocatalytic activity of the synthesized biomass-derived carbon modified TiO2, SiO2, FeSO4 nanostructure samples. Their photocatalytic activities under different conditions were measured by the photodegradation rates of MO solution under UV irradiation with wavelength between 250-320 nm.

The synthesis method in this work to prepare analyzed photodegradation activity of the samples were cost-effective and does not require high and expensive techniques such as high pressure or temperature, allowing for a wider choice of substrates and indicating a greater chance of scaling-up in the industry.

## **Biography:**

Kaiying Wang received Ph.D. in condensed matter physics from the Institute of Physics, Chinese Academy of Sciences. He had been a postdoc at the University of New Orleans, USA. He joined the University of South-Eastern Norway (USN) in 2007 as an associate professor and was promoted to professor in 2010. His research interests focus on microfabrication and nanotechnology, electrochemistry, photochemistry, and nanodevices for environment and energy applications.

## TUESDAY, OCTOBER 11, 2022 IN-PERSON

## **Plenary Presentation**

## Mesoporous Silica Materials and Their Applications in Bone Diseases

## María Vallet-Regi\*, Daniel Lozano, Montserrat Colilla and Miguel Manzano

Chemistry in Pharmaceutical Sciences, School of Pharmacy, Universidad Complutense de Madrid, Research Institute Hospital 12 de Octubre (i + 12), Pz/Ramón y Cajal s/n, Madrid 28040, Spain. Networking Research Centre on Bioengineering, Biomaterials and Nanomedicine (CIBER-BBN), Madrid 28029, Spain

## Abstract:

The outstanding textural properties of mesoporous silica materials quickly inspired their translation to the nanoscale dimension leading to mesoporous silica nanoparticles (MSNs).

The different aspects of introducing pharmaceutical agents into the pores of these nanocarriers, together with their possible biodistribution and clearance routes, would be described.

The development of smart nanocarriers that are able to release a high local concentration of the therapeutic cargo on-demand after the application of certain stimuli would be reviewed here, to-gether with their ability to deliver the therapeutic cargo to precise locations in the body.

The huge progress in the design and development of MSNs for biomedical applications, including the potential treatment of different diseases together with the required work that still needs to be done to achieve the clinical translation of these materials is the content of this conference.

## **Biography:**

María Vallet-Regi is a pioneer in the field of mesoporous silica materials with application in controlled drug release. She is the manager of the Intelligent Biomaterials Research Group (GIBI), CIBER-BBN, at Complutense University of Madrid, where currently she is developing different strategies to cure bonerelated diseases such as cancer, osteoporosis or infections in implants. She was the first woman to receive the gold medal from the European Federation of Materials Science Societies (FEMS) and the George Winter Award from the European Biomaterials Society (ESB).

## **Oral Presentation**

## Lock-In Thermography for the Analysis of Graphene

Christoph Geers<sup>1\*</sup>, Giulia Mirabello<sup>2</sup>, Mathias Bonmarin, Marco Lattuada<sup>2</sup>

<sup>1</sup>NanoLockin GmbH, Route de la Fonderie 2,1700 Fribourg, Switzerland

<sup>2</sup>University of Fribourg – Department of Chemistry, Fribourg, Switzerland

<sup>3</sup>Zürich University of Applied Sciences – Institute of Computational Physics, Winterthur, Switzerland

## Abstract:

A large variety of methods exists to analyze mostly inorganic engineered nanoparticles (NPs) in dispersions, as thin films or embedded (e.g. in nanocomposites). However, many standard analyses (e.g. chemical analysis) fail when it comes to carbon-based nanomaterials and the analysis often requires complicated sample preparation (e.g. microtome cutting) or labelling.

Methods used to detect and quantify carbon-based nanomaterials or analyze their size, size distribution, and colloidal state in analytically complex environments (e.g. cell culture media, serum) like dark-field hyperspectral imaging, electron microscopy or dynamic light scattering require complex and time-consuming sample preparation, are lacking spatial information and only analyze a small portion of the sample. Additionally, the quantification of carbon nanomaterials is even more challenging and methods for their quantification are simply missing.

Carbon nanomaterials have the ability to produce heat upon external stimulation by absorbing and scattering light [1], [2].

In this talk I will present a new technique based on lock-in-thermography (LIT) to measure and quantify the heat produced by carbon nanomaterials upon light stimulation. This heat can be recorded with an infrared camera and is processed by a specially developed LIT algorithm to yield 2D-images for analyzing carbon nanomaterials. The advantage of this set-up is the fast and accurate analysis of carbon nanomaterials in a variety of matrices, without requiring complicated sample preparation. Additionally, the method can be used for semi-quantitative analysis [3], [4].

## **Biography:**

After his bachelor's degree in biotechnology in Emden and a subsequent master's degree in biomedical engineering in Sigmaringen, Christoph Geers went to Fribourg, Switzerland, to do his doctorate in materials science at the Adolphe Merkle Institute in 2016.

In 2018 Mr. Geers Co-Founded the company NanoLockin, where he remains Managing Director to this day.

## High Pressure for Tuning Properties of Carbon Materials for Energy Applications

V. Pischedda<sup>1\*</sup>, S. Le Floch<sup>1</sup>, T. Gaudisson<sup>1</sup>, M. Dubois<sup>2</sup>, S. Radescu<sup>3</sup>, S. Pailhes<sup>1</sup>, V. Nesvizhevsky<sup>4</sup>

<sup>1</sup>Institut Lumière Matière, Université Lyon1, Villeurbanne, France

<sup>2</sup>ICCF, Université Clermont Auvergne, Aubière, France

<sup>3</sup>Departamento de Física, Universidad de La Laguna, Tenerife, Spain

<sup>4</sup>Institut Laue-Langevin (ILL), Grenoble, France

## Abstract:

Due to its flexibility in forming sp, sp<sup>2</sup>, and sp<sup>3</sup> bonds, carbon can adopt a wide range of structures with dramatically different mechanical and physical properties. Applying high pressure is a powerful method to modify chemical bonding so as to tune a material's properties. The application of external static pressure of several GPa to various allotropic forms of carbon such as carbon nanotubes, graphite and nano-diamonds can irreversibly modify their structure, morphology, density and/or the guest-host interaction in intercalated compounds offering new opportunities in the design of materials for energy uses. In this talk, I will present some recent research projects where pressure was used to i) modify CF bonding and the electro-chemical properties which have an interest as cathodes in Li/Na primary batteries ii) to diminish porosity to improve the electrical properties of carbon nanotube micro-wires, iii) to sinter nanodiamonds for the first ever efficient reflector for slow neutrons.

## **Biography:**

Vittoria Pischedda is Associate Professor at the Institut Lumiere Matiere, Université Claude Bernard Lyon in France. She holds a PhD in Crystallography, obtained at the University of Turin in Italy. Her research is focused on the physical-chemistry and thermodynamic stability of nanomaterials and carbon-based materials at extreme conditions of pressure and temperature in view to elaborate new materials with physical and mechanical properties interesting for energy applications. She is an active member of the high pressure scientific and technology network in France.

#### **Structural Properties of Ice in Confinement**

## Małgorzata Śliwińska-Bartkowiak<sup>1,2\*</sup>, Monika Jażdżewska<sup>1</sup>, Anatolii Beskrovnyi<sup>1</sup>, Keith E.Gubbins<sup>3</sup>

<sup>1</sup>Adam Mickiewicz University, Poznan, Poland

<sup>2</sup>NanoBioMedical Centre Adam Mickiewicz University, Poznan, Poland

<sup>3</sup>Department of Chemical & Biomolecular Engineering, North Carolina State University, USA

### Abstract

Water confined in nanoscale exhibits unique structural properties compared to the bulk phase. The effects of confinement of water in carbon nanopores were investigated in this study using differential scanning calorimetry (DSC), dielectric spectroscopy (DS), and neutron diffraction (ND) methods. The ice was confined in slit-shaped micropores of activated carbon fibers (ACF) and cy-lindrical-shaped mesoporous system (ordered carbon mesoporous structure - CMK-3) of different inner diameters. Melting behavior of the confined ice was studied using DSC and DS methods, while ND technique was used to determine the structure of confined ice. ND measurements for D2O in different carbon nanopores were taken in a temperature range of 300 to 100 K. The results of the DS and ND studies show the existence of hexagonal ice, Ih, and cubic ice, Ic at temperatures below the pores melting points. We have found that the content of confined hexagonal and cubic ice phases depend on the type of porous materials used. Our results show that the confined ice in the carbon nanopores revealed the features of stacking disordered ice Isd, formed by disordered hexagonal and cubic ice layers, as a combination of intertwined hexagonal and cubic stacking sequences. This form of ice recognized as having the space group P3m1 has been recently reported in the literature .

## **Biography:**

Currently the authors interest is focused on nano-porous materials - solid materials having pores of nanometer dimension. Nano-porous materials play a prominent role in chemical processing, particularly in separation and as catalysts and catalyst supports. They can also form the basis of future technologies, involving energy storage, as nano-reactors, as sensors, fabrication of small devices of molecular dimensions, etc. Using mainly dielectric, XRD and neutrons diffraction and scanning microscopy methods they are working on freezing and melting phenomena of host nano-phases in these materials , with particular emphasis on the effects of phase behavior, thermodynamics, surface properties and structure.

## **Exotic Behavior of Liquids Confined in Nanocarbons**

### Jana K. Vejpravova\*

Charles University, Faculty of Mathematics and Physics, Czech Republic

## **Abstract:**

Liquids are strongly affected by confinement, e.g., in nanocarbons [1], as the space-filling of the molecules is very different from the bulk. For example, water inside carbon nanotubes reveals enhanced diffusivity and flow rate [2], and it can freeze solid even at high temperatures that would typically set it to boiling [3]. Recently, we challenged capturing the water molecules below an atomically thin graphene membrane structured into a net of regular wrinkles. We employed cryogenic Raman spectroscopy to monitor the phase changes of the confined water as a function of the temperature. Experimental findings were supported with classical and path integral molecular dynamics simulations suggesting that surface premelting of the ice starts at ~200 K and the melting process is complete at ~240 K, which is far below the melting temperature of bulk water ice. The "supercooling" behavior of water entrapped under the graphene contrasts with the high-temperature "freezing" of water captured inside carbon nanotubes.

#### **Biography:**

Jana K. Vejpravova is a full professor at the Department of Condensed Matter Physics, Charles University (Prague). Her current research interests cover the experimental physics of nanocarbons, two-dimensional materials, and magnetic nanoparticles, with a focus on advanced spectroscopic methods in extreme environments. She published about 160 papers in impacted journals and three book chapters. Her research was already supported by ~ 15 national and EU projects as PI and received multiple recognitions, including Scopus/Elsevier Award (2010), Otto Wichterle Award (2014), ERC Starting grant (2016), and F. Behounek Award (2019). More information at vejpravova.eu

## Small Angle X-ray Scattering as a Tool to Characterize Carbon Structure

## Heinz Amenitsch\*

Graz University of Technology, Austria

## **Abstract:**

Simultaneous Small and Wide-Angle X-ray Scattering (SWAXS) has been proven to be a valuable tool for characterization of nanostructures in the size range from 0.1 nm till 100 nm in all states

of matter generally, and in particular for carbon materials. One of its key benefits based as X-ray technique is the versatility with respect to the control of physical or chemical parameters such as temperature, chemical potential or environment, humidity, pressure etc., which is limited or not so straightforward with other structure determining methods e.g. electron microscopy. Further the availability of very intense synchrotron radiation facilitates the cinematographic observation of structure forming or varying in situ/in operando providing new insights in the underlying processes.

In this presentation - besides a short introduction and outline of the general experimental possibilities at the Austrian SAXS beamline at the synchrotron radiation facility ELETTRA - an overview of the recent opportunities of the SWAXS technique in the field of carbon based materials is given, which is highlighted in the following examples: (i) carbon in energy applications [1],[2], (ii) the synthesis of quantum nanodots [3], and (iii) gas adsorption in carbon materials [4].

### **Biography:**

Heinz Amenitsch, currently working as a Associate professor Graz University of Technology. He focussed on Small-angle X-ray scattering, Chemical engineering, Crystallography, Scattering and Nanotechnology. His Small-angle X-ray scattering study combines topics in areas such as in situ, Phase, Membrane, Synchrotron and Analytical chemistry. His research integrates issues of thin film, Porosity, Mineralogy and Mesoporous material in his study of Chemical engineering.

## **Density Functional Theory in Cartesian Grid**

Amlan Kusum Roy IISER, India

Abstract Not Available!!!

## Raman Scattering of Neutron Irradiated Nuclear Graphite

#### Mohamed-Ramzi AMMAR

CNRS ICMN UMR7374, Université d'Orléans, F-45071 Orléans, France

#### Abstract:

Nuclear grade graphite has been widely used as a neutron moderator, reflector and fuel matrix in various types of nuclear reactors since the late 1940s. Its characteristics made it a material particularly suitable for the nuclear application. Consequently, graphite represents the greatest volume of radioactive waste at the end of the reactor's life. To date, about 250,000 tonnes have been accumulated worldwide. This is typically the case of the French UNGG or the British MAGNOX nuclear reactors developed independently in the same period. The long-term storage or disposal of the nuclear graphite waste requires a special management strategy and the challenges for the fundamental management options are reflecting the chemical, physical and structural properties of the material itself, its retrieval from the core and the associated inventory of long lived radio-isotopes such as chlorine (36Cl) or carbon (14C) that result from neutron activation processes. Therefore, prior to select any management option for the neutron-irradiated graphite, a comprehensive understanding of the structural properties of raw and structurally modified graphite is needed, so

as to provide efficient and effective solutions. Raman spectroscopy appears to be an appropriate technique to probe the structural modifications of nuclear graphite. The present paper will discuss the Raman response through the various types of defects that may appear in the nuclear graphite after being exposed to neutron bombardments and upon ion-beam irradiation. For this latter, a special device was developed allowing in situ monitoring of nuclear graphite behavior under light ions beam supplied by a cyclotron.

## **Biography:**

Mohamed-Ramzi AMMAR was graduated from Maine University (Le Mans-France) in drug delivery systems and Habilitation in supervising research from Orléans University-France. Dr. M.R. AMMAR is an associate professor in the institute of Orléans ICMN « Interface, confinement, Materials and Nanostructures » affiliated to CNRS. The main research is devoted to the study of the optical properties, particularly by Raman spectroscopy, of nanostructured 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.

## **Ultrafast Supercapacitor for AC Line Filtering**

## Miao Zhang\* and Jiayin Yuan

Department of Materials and Environmental Chemistry, Stockholm University, Stockholm, Sweden

### **Abstract:**

Electrochemical capacitors (ECs), also termed supercapacitors, have been in a striking position in the spectrum of energy-related devices since they reached the market in 1978, Ultrafast electrochemical capacitors with alternating current line filtering function have attracted growing attention owing to their potential to replace the state-of-the-art bulky aluminum electrolyte capacitors. In spite of rapid advance recently involving nanomaterials as electrode building units, it remains largely unexplored how to structurally and chemically engineer electrodes of satisfactory performance from renewable resources. Herein, wood as a renewable resource was used to fabricate highly conductive, robust, porous thin carbon membranes as free-standing electrodes for ultrafast electrochemical capacitors. Transformation of wood slice to carbon membrane proceeds via wet-chemical treatment of wood slices and subsequent morphology-maintaining carbonization by spark plasma sintering. This carbon membrane-based electrochemical capacitor exhibits excellent frequency response with efficient 120 Hz filtering (phase angle = -83.50). Compared to the latest electrodes for line filtering application that are fabricated from carbon nanotubes, graphene, and MXene.

### **Biography:**

Miao Zhang received his B.S. degree from Jilin University, China in 2012, and finished his Ph.D. at Tsinghua University, China, in 2016. After two years' postdoctoral research on energy storage at Tsinghua University, he joined the Department of Materials and Environmental Chemistry, Stockholm University for further postdoctoral research. His research interests span over 2D materials, polyelectrolyte, conductive polymer and their applications in energy and environmental fields, with special focus on the synthesis, modification, and assembly of ionic 2D materials. Currently, he is a Principal Investigator (PI) at Stockholm University

## **Crumpled Carbon Nanotubes as Advanced Electrode for Supercapacitor**

## Shuang Zong <sup>a,b</sup>, Aibing Chen<sup>a</sup>, Xinying Liu<sup>b\*</sup>

<sup>a</sup>College of Chemical and Pharmaceutical Engineering, Hebei University of Science and Technology, 70 Yuhua Road, Shijiazhuang, China.

<sup>b</sup>Institute for the Development of Energy for African Sustainability (IDEAS), University of South Africa (UNISA), Florida Science Campus, Private Bag X6, Johannesburg 1710, South Africa.

## Abstract:

The morphology and electronic structure of carbon materials are the key factors affecting their electrocatalytic property. Unique morphology nanostructure in carbon materials have the advantages of high specific surface area, more exposed active sites, and faster mass transfer for supercapacitors. Heteroatomic doping can construct defects, adjust the electronic structure, and improve the electrical conductivity of carbon materials. Here, a rapid hard-template method is adopted to synthesize N-doped crumpled carbon nanotubes (NCTs), in which 3-aminophenol resin (3AF) as carbon precursor can in situ introduce nitrogen species. Systematic experimental studies reveal that the surface morphology can be well adjusted by changing the amount of 3AF and reaction temperature, realizing transformation of different crumpled degree and different shell thickness. Experimental results confirmed that the wrinkled degree and shell thickness have significant impact on the electrochemical performance. The optimized NCTs as electrode material shows a high capacitance, outstanding cycling stability, and good rate performance, indicating the great potential for supercapacitor.

## **Biography:**

Xinying Liu is a full professor and head of catalysis research group at the Institute for development of Energy for African sustainability, a research institute at the University of South Africa. His research interests cover synthetic gas conversion for fuel and chemical production, CO<sub>2</sub> utilization and application of carbon materials for catalysis and energy storage.

## PdNPs/Carbon dots/Silica Hybrid Nanostructure: Development of an Electrochemical Sensor

## Thiago C Canevari\* and Joao H. A. Ferreira LabNaHm

Multifunctional hybrid nanomaterials laboratory. Engineering School, Mackenzie Presbyterian University, São Paulo, SP, Brazil

## Abstract:

Hybrid nanostructures can be defined as the formation of chemical interaction between nanomaterials or nanomaterials bonded to another material, which will result in the formation of nanostructures with different physicochemical properties compared to isolated materials. Based on this, the formation of hybrid nanostructures in that carbon dots was used as a catalyst have been obtained and the hybrid nanostructures have been applicated in the development of sensors electrochemical. The hybrid nanostructures formed by PdNPs/Carbon dots/Silica were prepared in a single step, without external catalysts, by mixing TEOS with PdNPs/Cdots, where the Cdots have been previously prepared by electrochemical means using n-propanol as carbon source. Palladium nanoparticles (PdNPs) containing Cdots (PdNPs-Cdots) were prepared from the palladium chloride complex Na2[PdCl4]. The printed carbon electrode, CSE, was used as a working electrode, which had its surface modified by adding 60 uL of an aqueous solution of the PdNPs/Carbon dots/SiO2 nanostructure. The CSE/PdNPs/Carbon dots/SiO2 electrode showed an excellent electrocatalytic response for the simultaneous determination of dopamine and serotonin, in the presence of AA, as shown in figure 1, in which the electrocatalytic current increased, I, proportionally in function of the increase concentration, for both species. Measurements were performed differential pulse voltammetry in PBS, pH 7.0, in the presence of ascorbic acid, with the concentration fixed at 1 x 10-4 mol/l and concentrations of dopamine and serotonin ranging from 5 x 10 - 7 to 7 x 10 -6 mol/L. The detection limits obtained were 114 nmol L-1 of dopamine and 152 nmol L-1 of serotonin.

## **Biography:**

Graduated in Chemistry, Bachelor's degree with Technological option from the State University of Londrina, Master's in Inorganic Chemistry, and Doctorate in Materials Chemistry from the State University of Campinas. He has two postdoctoral internships at the University of São Paulo of area of nanotechnology. Leader of the research group, consolidated by CNPq, called Multifunctional Hybrid Nanomaterials (NaHM). He works mainly on the following topics: electrocatalysis, (Bio) electrochemical sensors, multifunctional hybrid nanomaterials, filtering nanomembranes, and solgel process. He is currently a professor in the chemistry course and in the postgraduate program in Materials and Nanotechnology Engineering at Universidade Presbiteriana Mackenzie.

## Amorphous Carbon Layer by Atomic Layer Deposition for Phase Change Memory Electrode

## Seung-min Chung<sup>1\*</sup>, Tae Hyun Kim<sup>1</sup>, Myoungsub Kim<sup>2</sup>, Seungwon Park<sup>1</sup>, Seunggyu Na<sup>1</sup>, and Hyungjun Kim<sup>1</sup>

<sup>1</sup>School of Electrical and Electronics Engineering, Yonsei University, 50 Yonsei Ro, Seodaemun-gu, Republic of Korea

<sup>2</sup>SK Hynix, 2091, Gyeongchung-gaero, Bubal-eup, Icheon-si, Gyeonggi-do, Republic of Korea

## Abstract:

The need for high-performance memory semiconductors that can process large amounts of data quickly increases with the development of the fourth industry, such as big data and artificial intelligence. Recently, phase change memory (PCM) is the most regnant new memory for leading the future semiconductor industry. Furthermore, Intel's research on 3dimensions cross-point (3D X-point) memory is also being conducted using memory cells and selectors where word lines and bit lines intersect in 3D to create a highly integrated PCM. However, the most critical factor for these PCM devices' high efficiency and integration is reducing the current device operation. Recently, studies have been actively conducted to increase the joule heating efficiency by increasing the specific resistance of the electrode. Carbon, which exhibits various resistivities [1], [2] depending on the state of atomic bonding, is an attractive material as a PCM electrode. So far, PVD (Physical Vapor Deposition) and CVD (Chemical Vapor Deposition) processes have been used to deposit carbon thin films. However, it is not easy to deposit a uniform carbon thin film on a three-dimensional structure with the conventional method and control carbon's physical properties. Therefore, a carbon process using ALD (Atomic Layer Deposition) was developed in this study; the carbon

thin film properties were analyzed according to the process conditions (reactant type, temperature, pressure, time), and the corresponding mechanism was studied.

## **Biography:**

Seung-min Chung is currently working as a professor at Yonsei University. His research interest mainly includes in the areas of Material engineering with material science and chemistry. A variety of analytical skills and understanding of semiconductor. Have insight that can be strategic choices and focus on material of DRAM or LOGIC.

## Activated Carbons as Electrode Material for Use in Supercapacitors

Antonia Stoyanova<sup>1\*</sup>, Ana Arinalis<sup>2</sup>, N. Ray<sup>2</sup>, B. Karamanova<sup>1</sup>, S. Veleva<sup>1</sup>, L. Soserov<sup>1</sup>, B. Mladenova<sup>1</sup>, T. Stankulov<sup>1</sup>

<sup>1</sup>Institute of Electrochemistry and Energy System "Academician Evgeni Budevski " – Bulgarian Academy of Sciences, Bulgaria

<sup>2</sup>The Carbon Science and Technology Institute (INCAR),

### Abstract:

Lately, Supercapacitors rapidly have attracted a growing attention as an energy storage device due to their unique properties, such as a long cycle life, and high power density. However, there are still some challenges and obstacles in these systems such as relatively inadequate energy density and high manufacturing cost. Basically, the performances of the supercapacitors are determined by the structural and electrochemical electrode properties. Activated carbon is one of the most versatile materials for this application due to the desirable pore sizes and their higher specific surface area as compared to the other carbonaceous material.

The present study reveals the capacity characteristics of different activated carbons - carbon xerogels synthesized by different techniques and under different conditions as well as YP-50F (commercial product, Kuraray Europe GmbH), in symmetric and hybrid supercapacitors using aqueous and organic electrolytes. The structure, morphology and porous texture properties of electrodes materials are analyzed by means of various physiochemical methods and their electrochemical performances are determined by cyclic voltammetry, galvanostatic charge/discharge as well as long-term tests.

The effect of the carbon microstructure and functional groups related to it, as well as the influence of the electrolyte type on the obtained supercapacitor performances, are discussed in detail. The capacitance characteristics of electrodes based on activated carbon composite combined with metal oxides/hydroxides are also considered. The obtained data can serve as a basis for the development of more efficient electrode materials in energy storage systems.

## **Biography:**

Antonia Stoyanova, currently working as an associate professor in the Department of Nanoscaled Materials at Institute of Electrochemistry and Energy Systems, Bulgarian Academy of Sciences. She was expertise in the fields of Electrochemistry, Electrochemical Energy systems, Nanomaterials, Materials Characterization, Nano material synthesis.

## Structure Design of Carbon Nanomaterials for Their Enhanced Performance in Electrochemical Energy Storage and Conversion

## Pai Lu\*

Department of Microsystems, University of South-Eastern Norway, Campus Vestfold, Raveien 215, 3184 Borre, Norway

## Abstract:

Carbon materials in their nanoscale formats (e.g., fullerene, carbon nanotube, graphene, nanoporous carbon) have been playing critical roles in the energy relevant fields, encompassing energy storage (batteries, supercapacitor) and energy conversion (power to gas, e.g., green H2 production). Structure design of carbon nanomaterials has been regarded as an effective route to adjust their functionalities, and exert the optimal effectiveness. In this talk, effective structure design principles of carbon nanomaterials will be demonstrated by summarizing our recent experimental research outcomes. (1) To enhance the areal capacity for overcoming the insufficient energy density, a unique template directed assembly route of fullerene decorated carbon nanotubes (FC-CNTs) has been developed to adjust the packing density and porous structure of CNT films. Benefiting from the compactly pack CNTs yet porous structure of the electrode films, a world-leading high-energy supercapacitor performance has been achieved. (2) To improve the specific capacity of battery electrode materials and meanwhile stabilize their cycling performance, mesoporous carbon buffer scaffolds and thin carbon coatings have been designed. (3) To extend the span life of electrodes of water electrolyzers, carbon conformal nano-coatings have been designed, which stabilize the nanoparticulate electrocatalysts, but do not shield the Co-based catalytic sites.

## **Biography:**

Pai Lu works as a Research Scientist (Permanent Position, Principle Investigator) at University of South-Eastern Norway. His main research interests encompass Functional Materials applied for (1) Electrochemical energy storage (Li-, Na-batteries, Supercapacitor) and (2) Electrochemical energy conversion (Green H2 production pathway). He has co-authored ~50 scientific publication (Google Scholar: https://scholar.google.com/citations?hl=en&user=Rril8H8AAAAJ). He has hosted 9 research projects as project manager (1 international collaboration project, 6 within the academic research program at National and Area level, 2 within the industrial R&D program) both in China and Norway. Currently, he is managing 1 International Collaboration Research Project (EEA Grant) and 1 Regional Research Project/Norway at University of South-Eastern Norway.

## Influence of Carbon Porosity on the Sulfur Utilization in Lithium-sulfur Battery cells with Sulfidic Electrolyte

#### Magdalena Fiedler

Fraunhofer Institute for Material and Beam Technology, Germany

## Abstract Not Available!!!
### Carbon Capture and Utilization towards a Future Sustainable Europe

# Sandra Adelung, Ralph-Uwe Dietrich<sup>\*</sup>, Felix Habermeyer, Simon Maier, Moritz Raab, Yoga Rahmat, Francisco Rossel, Julia Weyand

German Aerospace Center (DLR e.V.), Institute of Engineering Thermodynamics, Pfaffenwaldring 38-40, 70569 Stuttgart, Germany

### Abstract:

EU's Fit-for-55 package requires all sectors to contribute to the collective pledge of greenhouse gas (GHG) emissions reduction in all sectors by at least 55 % by 2030, compared to 1990 levels. On top of that, demand for energy security and independence increases the necessity to transfer the entire society towards sustainability and carbon neutrality. While future carbon neutrality and carbon usage sound contrary, its not on the sustainability pathway by using "green" carbon (from biomass or air) or by dual use of waste carbon streams instead of releasing them into the atmosphere.

If the transport sector, especially aviation, shipping and heavy load, will continue to rely on liquid fuels, carbon-based fuels might be unavoidable for the foreseeable time. With countless options of sustainable fuels, feedstocks and production routes, its difficult to determine preferences of one over the others. We present a methodology to assess these options fair and transparent simultaneously technically, economically as well as environmentally for comparison and selection.

Because aviation is one of the fastest growing sectors in terms of CO2 emissions, the regulatory initiative ReFuelEU Aviation was introduced to mitigate the impact of aviation on the environment. Significantly reduced GHG emissions and lower abatement costs require technological innovations of Power-to-liquids, Biomass-to-liquids and Power enhanced Biomass-to-liquids processes. A detailed discussion of sustainable aviation fuels prospects will be presented.

The methodology of techno-economic and environmental assessment will be applied to other transport applications and industry decarbonization efforts as well to address all sectors contribution towards Fit-for-55.

### **Biography:**

Ralph-Uwe Dietrich has led a research group on techno economic and ecological assessment at the DLR since 2015. There he applies his knowledge of chemical engineering process design and simulation to the assessment of new production routes for chemicals and fuels. Before that, he received 10 years of experience and a PhD in high- temperature fuel cells research. Dr. Dietrich worked for 15 years in project development and management at different process and automation enterprises (SME and Fortune 500).

### Water Interactions with Polar C<sub>1</sub>N<sub>1</sub> Nanopores

Mateusz Odziomek <sup>1\*</sup> Waldemar Keil<sup>2</sup>, Karlo Nolkemper<sup>2</sup>, Julian Heske<sup>2</sup>, Janina Kossmann<sup>1</sup>, Hossam Elgabarty<sup>2</sup>, Claudia Schmidt<sup>2</sup>, Thomas Kühne<sup>2</sup>, Nieves López-Salas<sup>1</sup>.

<sup>1</sup>Colloid Chemistry Department, Max Planck Institute of Colloids and Interfaces, Am Mühlenberg, Potsdam, Germany

<sup>2</sup>Dynamics of Condensed Matter and Center for Sustainable Systems Design, Chair of Theoretical

Chemistry, University of Paderborn, Warburger, Paderborn, Germany

### **Abstract:**

The interaction between water molecules and surfaces of nanoporous carbonaceous materials are of paramount importance for energy storage and energy conversion applications. Water confined in narrow nanopores experiences stronger interactions with walls of a host than with other water molecules. This has significant implication on the properties of the liquid and thus on its redox potential, electrical double layer or wettability. Solid state NMR is a powerful tool to study the local environment and dynamics of water molecules in a porous host. Although such studies exist on carbon materials, they are very limited for nitrogen-rich carbonaceous materials.

In this contribution, we studied the interaction of water with highly porous C1N¬1 materials and compared them to pure carbons having similar pore structure. The studies unraveled that liquid water does not enter narrow nanopores of polar C1N1 while it does in hydrophobic carbon. This behavior has a dramatic effect on energy storage properties, wherein pure carbon show much higher capacitance than C1N1 material, despite their similar porosity. The results were further rationalized by DFT calculations, which showed lower adsorption energy of water molecules in polar C¬1N¬1 nanopores than in non-functionalized carbon. This study further confirms the complexity of interaction of nanoporous materials with electrolytes and necessity for their in-depth studies.

### **Biography:**

Mateusz Odziomek obtained his Ph.D. in chemistry in 2018 from Ecole Normale Superieure in Lyon and University of Science and Technology AGH in Krakow. He worked on the development of porous nanoparticle-based functional materials through colloidal assembly. Then he continued his work in Paris as maitre de conference associe, under the supervision of Prof. Clement Sanchez at College de France and Sorbonne Universite. Since 2021, he has been working as a Post-doc and since 2022 as Humboldt Fellow at Max Planck Institute in Potsdam with prof. Markus Antonietti on rational design and new low-temperature synthetic concepts of porous carbon materials.

### Nanosized Photothermal-responsive Carbon Dots for Light-triggered Drug Release

### Salvatore Petralia<sup>1\*</sup>, Grazia Maria Letizia Consoli<sup>2</sup>, Ludovica Maugeri<sup>1</sup> and Giuseppe Forte<sup>1</sup>

<sup>1</sup>Department of Drug Science and Health, University of Catania, Italy

<sup>2</sup>CNR-Institute of Biomolecular Chemistry, 95126 Catania, Italy

### Abstract:

Luminescent and photothermic carbon-based polymer dots are one of the most important achievements in the fast-growing field of nanotechnology. The combination of multi-responsive polymer-shell based on Poly(N-isopropylacrylamide) with luminescent and photothermal carbon-core has led to promising applications in various fields such as optics, electronics, and medicine. These nanomaterials are largely employed as promising photothermal agents in emerging nanotechnologies such as photoinduced-enzymatic reaction, photothermal antibacterial effect, photothermal and photodynamic therapies (PTT and PDT), gene-therapy and photothermal triggered drug and gene delivery. In our laboratories, we have developed innovative synthetic procedures based on photochemical and chemical reactions for the preparation of luminescent and photothermal nanostructured materials based on core-shell nanocomposites, carbonized polymers nanodots and boron nitride carbon-doped quantum dots. The nanostructured materials, whose design was supported by Molecular Dynamic simulation investigations, exhibited high photothermal conversion efficiency and no toxicity to eukaryotic cells. Experiments confirmed also an excellent thermally induced drug release activity to be used for photothermally controlled drug release.

### **Biography:**

Salvatore Petralia, received the PhD in Chemistry from University of Catania (Italy), in 2003. In 2020 he joined University of Catania as Researcher of Chemistry. From 2004-2020 he was Technology Development sect. Manager at STMicroelectronics, covering several R&D positions and leading multidisciplinary teams focused on the development of nanostructured materials and chemical processes for biosensing applications. The research activity over the years has covered multidisciplinary aspects of chemistry, photochemistry, nanostructured materials, biosensing and bioMEMS silicon technology. In this field he is co-author of 120 peer reviewed scientific publications, 1 chapter of book and co-inventor of 8 patent applications.

### Single-molecule Enzymology Using Carbon Nanocircuits

Gregory A. Weiss<sup>1,2,3\*</sup>, Kristin N. Gabriel<sup>2</sup>, Mackenzie W. Turvey<sup>4</sup>, Wonbae Lee<sup>4</sup>, Jeffrey J. Taulbee<sup>4</sup>, Calvin J. Lau<sup>4</sup>, Sudipta Majumdar<sup>1</sup>, and Philip G. Collins<sup>4\*</sup>

<sup>1</sup>Department of Chemistry, University of California Irvine; Irvine, CA, USA.

<sup>2</sup>Department of Molecular Biology & Biochemistry, University of California Irvine; Irvine, CA, USA.

<sup>3</sup>Department of Pharmaceutical Sciences, University of California Irvine; Irvine, CA, USA.

<sup>4</sup>Department of Physics and Astronomy, University of California Irvine; Irvine, CA, USA.

### Abstract:

The Weiss laboratory uses carbon nanotubes to invent new tools for dissecting biology. Specifically, the lab directly wires individual proteins into carbon nanotube-based electronic circuits, and "listens" to their motions, which happen when the proteins interact with binding partners and substrates. With collaborator Prof. Phil Collins, we have spot-welded individual proteins into these electronic circuits, termed "nanophones," to record the sounds made by proteins in motion. The tethered single molecule can be examined at high-speeds with microsecond resolution for long durations up to weeks in real-time during protein unfolding, folding, binding, and enzymatic catalysis. The approach has been used to dissect the inner-workings of enzymes, including several DNA polymerases and protein kinase A.

Recently, we have used these nanocircuits to dissect the PCR enzyme, Taq DNA polymerase. This enzyme functions at elevated temperatures with fast conformational dynamics, which challenge conventional single molecule studies. In our experiments, single-walled carbon nanotube transistors allowed monitoring of the motions of Taq enzymatically processing substrates at a range of temperatures up to 85 °C. The whole-enzyme closures for catalytic events could be distinguished from more rapid, 20-µs closures the enzyme's active site testing substrate complementarity and orientation. On average, one transient closure was observed for every nucleotide binding event; even complementary substrate pairs averaged five transient closures between each catalytic in-

corporation at 72 °C. The rate and duration of the transient closures and the catalytic events had almost no temperature dependence. Thus, Taq's temperature sensitivity is due to its rate-determining open state.

### **Biography:**

Gregory Weiss, a tenured Professor at UCI, earned a BS from UC Berkeley and PhD from Harvard. Awarded an NIH postdoctoral fellowship, he pursued post-doctoral studies with Dr. Jim Wells at Genentech. His laboratory at UCI (founded in 2000) focuses on the interface between chemistry and biology, including studies of enzymes, molecular recognition, and bioelectronics. He has been awarded UCI's Outstanding Professor in Physical Sciences, Beckman Foundation Young Investigator, AAAS Fellow, and an Ig Nobel Prize. Co-founder of biotech companies (including PhageTech and Debut Biotechnology), he was named UCI's Entrepreneurial Leader of the Year and a Faculty Innovation Fellow.

### Carbon-based Materials for Reading and Writing in the Central Nervous System

Serge Picaud<sup>1\*</sup>, Julie Zhang<sup>1</sup>, Diep Nguyen<sup>1</sup>, Claudia-Antonella Wilfinger<sup>2</sup>, Lionel Rousseau<sup>2</sup>, Xavi Illa<sup>3,4</sup>, Jose de la Cruz<sup>5</sup>, Jose A Garrido<sup>5,6</sup>

<sup>1</sup>Paris Vision Institute, Sorbonne Université, INSERM, CNRS, France

<sup>2</sup>ESIEE Paris, France

<sup>3</sup>Instituto de Microelectrónica de Barcelona, IMB-CNM (CSIC), Spain

<sup>4</sup>Centro de Investigación Biomédica en Red en Bioingeniería, Biomateriales y Nanomedicina (CIBER-BBN), Spain

<sup>5</sup>Catalan Institute of Nanoscience and Nanotechnology, Spain

<sup>6</sup>ICREA, Spain

### Abstract:

A major aim in the field of Neurosciences is to read (measure) and write (stimulate) the neuronal activity in order to diagnose, treat neurological diseases or even restore lost information. The functionality of these Read/Write technologies depends highly on the electrode properties for interfacing with the neuronal tissue. The high conductivity and the expected high biocompatibility of carbon-based materials such as graphene and doped-diamond have raised great interest for building up the future generation of such medical devices.

Our aim is to investigate how these materials could improve recording at the retinal and cortical levels while investigating the material biocompatibility for long term implantation of prostheses for visual restoration.

To assess the material biocompatibility, inactive polyimide substrates layered with graphene and diamond on were introduced in the subretinal space of blind rats. Both diamond and graphene did not trigger any significant immune reactions or neuronal cell loss demonstrating thereby their high biocompatibility. In the reading mode, we showed that graphene electrodes can measure electroretinogram on the eye surface of rodents to monitor retinal neuronal activities while whole diamond implants were used to record visually evoked potentials at the cortical surface. Then, in

the stimulation mode, we have shown the possibility to stimulate retinal neurons with graphene electrodes in isolated tissues or in vivo conditions.

These studies demonstrate the feasibility to both read and write neuronal activity using carbon-based materials. Their observed biocompatibility further supports their relevance for the creation of implanted devices for monitoring or stimulating neurons such as visual prostheses.

### **Biography:**

Serge Picaud (SP) has contributed to the development of retinal prostheses and optogenetic therapy for restoring vision at the retinal level. These strategies are currently investigated in ongoing positive clinical trials on patients affected by age-related macular degeneration and retinitis pigmentosa, respectively. Serge Picaud is chairing the Paris Vision Institute. This work was supported by the European Union's Horizon 2020 research and innovation programme under grant agreement No. 785219 (Graphene Flagship Core 2) No. 881603 (Graphene flagship Core3) and the ERC starting grant 2017 (NEURODIAM).

### Zeolite@Carbon Monolithic Adsorbent with Efficient CO<sub>2</sub> Capture Performances

### Matjaž Mazaj\* and Sebastijan Kovačič

National Institute of Chemistry, Hajdrihova 19, 1000 Ljubljana, Slovenia

### **Abstract:**

The demands for technological use of CO2 are in last decades increasing and its efficient harvesting from post-combustion systems, still represents a challenge. Zeolites and porous carbon materials represent the most promising adsorbents for post-combustion CO2 capture applications. In the light of searching an optimal adsorbent with the requirements for efficient post-combustion CO2 capture we developed new approach to design zeolite@carbon monolithic composite with high CO2 capture performances even in the presence of water. Innovative method included the immobilization of zeolite Beta nanoparticles within polyHIPE (high internal phase emulsions) matrix and its subsequent controlled carbonization resulting in the production of highly porous zeolite Beta@ carbon monoliths with N-doped carbon walls. Zeolite Beta@carbon monolith are almost completely accessible within the carbon matrix due to its highly opened macroporous texture. CO2 adsorption capacity of the composite increases for 50 % whereas IAST selectivity against N2 increases for 250% if compared to the pristine material. Such pronounced improvement can be assigned to the ultramicroporosity of the carbon walls which together with high zeolite micropore accessibility synergistically contribute to the high affinity toward CO2 adsorption. Hydrophobic nature of the carbon matrix also contributes to the lower affinity toward water making its adsorption on the developed composite less competitive with CO2. Moreover, carbonized matrix exhibits notable electric conductivity of 3 S/m enabling high thermoelectric response by employing the voltages up to 6 V. Therefore the newly designed zeolite@carbon material can be easily regenerated by electric swing adsorption process.

### **Biography:**

Matjaž Mazaj is a Senior Associate Researcher in the Laboratory for Inorganic Chemistry and Technology at the National Institute of Chemistry in Ljubljana. He finished his PhD in Chemistry in 2008 at the University of Ljubljana. From 2008 to 2009 he was a visiting researcher at the University of Versailles, France. His research interests are design and structural characteritation of nanoporous materials (MOFs, zeolites) by different diffraction, microscopy and sorption techniques.

### **Carbon Materials in Lithium Sulfur Batteries**

G. Luque<sup>1</sup>, V. Bracamonte<sup>2</sup>, A. Calderón<sup>2</sup>, S. Raviolo<sup>2</sup>, F. García Soriano<sup>2</sup>, G. Lener<sup>1</sup>, M. Rojas<sup>2</sup>, P. Vélez<sup>1</sup>, Martin E. Zoloff Michoff<sup>1</sup>, Flavia E. Lobo Maza<sup>3</sup>, J. Luque Di Salvo1, G. De Luca<sup>4</sup>, D. Barraco<sup>2</sup>, E. Leiva<sup>1</sup>

<sup>1</sup>INFIQC, Departamento de Química Teórica y Computacional, Facultad de Ciencias Químicas, Universidad Nacional de Córdoba, CONICET, Ciudad Universitaria, X5000 Córdoba, Argentina

<sup>2</sup>IFEG, Facultad de Matemática Astronomía, Física y Computación, Universidad Nacional de Córdoba, CONICET, Ciudad Universitaria, X5000 Córdoba, Argentina

<sup>3</sup>CREAS, CONICET and CIFTA, Facultad de Ciencias Exactas y Naturales, Universidad Nacional de Catamarca, Catamarca, Argentina

<sup>4</sup>Institute on Membrane Technology, National Research Council of Italy, Calabria, Italy

### Abstract:

Lithium-sulfur batteries (Li-S) are among the most promising electrochemical energy storage devices of the near future. The main reason is due to the low price, abundant availability, environmental friendliness of sulfur, as cathode material and its high theoretical capacity in comparison to lithium-ion technologies. Nevertheless, Li-S batteries face many challenges that have to be overcome in order to replace li-ion batteries. A Li-S battery typically consists of a sulfur cathode and a metallic lithium anode with a porous separator and a non-aqueous electrolyte in between. During discharge, lithium ions are formed at the anode and migrate to the cathode side, whilst the electrons move from the anode to the cathode through the external circuit. Sulfur is reduced to lithium sulfide [1], and the opposite takes place during charging.

One of the main problems of this type of batteries is the insulating nature of sulfur, being mandatory to embed it into a conductive material. In this sense carbon materials, has many advantages such as low cost, wide window potential, versatility, etc. They can also mitigate the volume expansion that take place during discharge. Another problem of Li-S batteries lay on the high solubility of long chain polysulfides that form during cell function and shuttle between anode and cathode. This can be overcome by using functionalized carbon materials in/on the cathode, or modifying the separator as polysulfides barrier [2].

In the present work, we present experimental and computational studies performed in our lab with the objective of overcoming the different problems that Li-S batteries present, by means of using different carbon based materials.

### **Biography:**

Guillermina Luque currently working in the department of Theoretical and Computational Chemistry at National University of Cordoba, Argentina | UNC. Her research interest includes Theoretical and experimental studies of graphene and its application as electrochemical (bio) sensors, as electrodes in lithium batteries and for hydrogen storage. [1] L. Borchardt, M. Oschatz, S. Kaskel; Chem.Eur.J.2016,22,7324-7351.

[2] Chen, L., Yu, H., Li, W., Dirican, M., Liu, Y., & Zhang, X; J. Mater. Chem. A, 2020,8, 10709-10735.

# ${\rm TiO}_{_2}$ Photocatalyst Loaded onto Activated Carbon Support from Wood Waste for Visible Light Photocatalysis

### Luminita Andronic\* and Cristina Cazan

Transilvania University of Brasov, Product Design, Mechatronics and Environment Department, Romania

### **Abstract:**

Titanium oxide/active carbon nanocomposites are components of advanced green technologies for pollutants removal from synthetic and real wastewater containing contaminants of emerging concern (CECs). The CECs solution containing amoxicillin, ampicillin, ibuprofen and imidacloprid was prepared using ultrapure water or municipal wastewater after secondary treatment. This research aims to evaluate the photocatalytic activity of the titanium dioxide/active carbon nanoparticles derived from wood waste as an eco-friendly photocatalytic material. Activated carbon with a surface area of 450 m2/g was obtained by carbonizing wood wastes and activating them at 850°C in an oxygen-free atmosphere. The titanium oxide spherical particles were successfully grown on the surface of active carbon, with ratios of active carbon 1, 5, and 10 wt %, via the hydrothermal method. Immobilized photocatalyst thin layers of composite material AC/TiO2 were obtained by cold spraying a dispersion on the microscopic glass substrate. X-ray diffraction (XRD), scanning electron microscopy coupled with energy dispersive X-ray (SEM-EDX), optical band gap measurements, and particle size characterized the as-prepared powders and thin films. In addition, the materials' pore structure was investigated by N2 adsorption-desorption analysis. The photocatalytic activity of thin films was evaluated for CECs degradation and mineralization under simulated solar irradiation. The stability and recyclability of thin films were good after four cycles of the photodegradation process, which proved that this technology could be used in industrial applications.

### **Biography:**

Luminita Andronic obtained her PhD title in 2010 in Materials Science, she continuously conducted her research activity at the Transilvania University of Brasov. The scientific recognition has been proven through publishing more than 60 contributions to International Conferences with posters and oral presentation, over 65 publications in peerreviewed journals and conference proceedings, 40 publications indexed in ISI Thomson Journals, 2 books in recognized publishing houses (CNC-SIS) and 4 chapters in books publish in international publishing houses. The scientific research carried out so far led to the coordination of the two projects as director and 1 project as scientific responsible, member in over 15 national and international projects.

### Metal Chloride Activation Revisited: A Sol-gel Process to Functional Carbons

# Tim-Patrick Fellinger<sup>\*1, 2</sup>, Jonas Pampel<sup>1</sup>, Asad Mehmood<sup>1</sup>, Davide Menga<sup>2</sup>, Burak Koyutuerk<sup>2</sup>

<sup>1</sup>Bundesanstalt für Materialforschung und -prüfung (BAM), Berlin, Germany;

<sup>2</sup>Chair of Technical Electrochemistry (TEC), Department of Chemistry and Catalysis Research Center, Technische Universität München, Garching, Germany.

### Abstract:

Porous carbon materials are known for their applicability in important areas such as sorption, catalysis and electrochemistry (e.g. fuel cell catalysts, supercapacitor or battery electrodes). It was shown that nitrogen doped carbons (NDCs) act as an inexpensive and highly active non-metal catalyst in the oxygen reduction reaction (ORR), with the potential to reach performances of practical need one day. A key strategy towards improvement for this aim comprises the generation of advantageous porosity, which typically means high surface area and mass transport pores as well as the control over the chemistry of catalytically active sites. My group is developing novel sol-gel type strategies that are using molten salts or molten acids as unconventional reaction medium for the porogenesis in doped carbons, thereby revisiting classic activation techniques.[1,2] Carbon materials with extra high surface area of  $\sim$ 2800 m2 g-1 and pore volumes, up to four times as high as in commercial activated carbons, are obtained.[3] It turns out that the meso- and macrostructure is generated by means of phase separation rather than leaching reactions. However, chemical reactions between the carbon precursor and the melt are also involved. The salt cations Mg2+ and Zn2+ act as template ions, which results in metal coordination sites, embedded into the carbon structure.[4,5] The imprinted structure may be utilized as catalytically active site by performing ion-exchange reactions. The novel preparation strategy towards highly active electrocatalysts will be presented for Mg and Zn and further discussed for lighter elements.

### **Biography:**

Tim Fellinger obtained his PhD in 2011 at University of Potsdam supervised by Markus Antonietti. After a postdoc stint at Ichiro Yamanaka's lab (Tokyo Institute of Technology) he started his independent research on Carbon-based Electrode Materials (MPI Colloids and Interfaces). His scientific vision to tailor carbon-based materials to transfer biochemical principles to energy applications, earned him the Ernst-Haage Prize in 2018. 2017- 2020 his group was hosted by Hubert Gasteiger (TUM), which shifted the focus to more applied topics. Since 2020 he is heading the Lab for Energy Materials at the German Federal Institute for Materials Research and Testing (BAM).

## Adsorption of Anionic Dye by Chitosan-date Palm Seed-derived Activated Carbon Composites

### Hani Hussain Sait<sup>1</sup>, Ahmed Hussain<sup>1</sup>, Mohamed Bassyouni<sup>2,3</sup>, Imtiaz Ali<sup>2</sup>, Ramesh Kanthasamy<sup>2</sup>, Bamidele Victor Ayodele<sup>4</sup> and Yasser Elhenawy<sup>5</sup>

<sup>1</sup>Department of Mechanical Engineering, Faculty of Engineering Rabigh, King Abdulaziz University, Rabigh 21911, Saudi Arabia

<sup>2</sup>Department of Chemical and Materials Engineering, Faculty of Engineering Rabigh, King Abdulaziz University, Rabigh 21911, Saudi Arabia

<sup>3</sup>Department of Chemical Engineering, Faculty of Engineering, Port Said University, Port Fouad City 42526, Egypt

<sup>4</sup>Institute of Energy Policy and Research, Universiti Tenaga Nasional, Jalan Ikram-Uniten, Kajang 43000, Selangor, Malaysia

<sup>5</sup> Department of Mechanical and Power Engineering, Faculty of Engineering, Port Said University, Port Fouad City 42526, Egypt

### Abstract:

Adsorbent materials from renewable resources like biomass, biopolymers (chitosan), or composites are being used to remove contaminants from wastewater and effluents. The aim of this research is to develop and test chitosan-activated carbon (CA) composites as anionic blue dye adsorbents. The pyrolysis of hybrid date palm seeds was carried out in a fixed-bed pyrolizer that was custom built for the task. The effect of pyrolysis temperature (400–1000 oC) on the different physico-chemical properties of date seed biochar formed by the pyrolysis process was investigated. Date seeds pyrolysis at 1000°C showed the highest carbon contents. In terms of adsorbent concentration, mixing duration, pH, and dye initial concentration, a series of batch tests were conducted. Brunauer–Emmett–Teller (BET), Scanning Electron Microscope (SEM), Zeta Potential analysis, and Fourier-transform infrared spectroscopy were used to characterize the CA composites. Chitosan-activated carbon composites was successfully able to remove up to 99 % of anionic dye from wastewater. Equilibrium data fitting is best to the Langmuir isothermal model with R2= 0. 99.

# Peroxidase Mimicking of $Fe_3C/Nitrogen-doped$ Carbon and the Application in Colorimetric Sensors

### Sadaf Saeedi Garakani\*, Jiayin Yuan

Department of Materials and Environmental Chemistry, Stockholm University, Sweden

### Abstract:

Over the recent years, functional nanomaterials with peroxidase mimicking properties, unique structure, and morphologies have attracted great interest, owing to high catalytic performance, low cost, easy preparation and separation, and desirable stability. Small iron carbide nanoparticles demonstrate promising catalysts like nanozymes; however, their activity suffers from aggregation. Nitrogen-doped carbon matrix with a large pore volume and high surface area can support the better distribution of the nanoparticles, as well as improve the electronic conductivity and chemical stability. Approaching this goal, we coated a mixture of PILs and iron (III) chloride on the surface of the treated wood and carbonized it in optimized condition, which provided iron carbide nanoparticles encapsulated in nitrogen-doped porous carbon membrane (denoted as Fe3C/N-C). Expectedly, Fe3C/N-C exhibited an excellent peroxidase-mimicking activity toward the oxidation of 3,3',5,5'-tetramethylbenzidine (TMB) generating a colored solution in the presence of hydrogen peroxide. This unique catalyst is utilized as an efficient sensing platform to selectively determine ascorbic acid (AA, commonly known as vitamin C). Indeed, the blue color formed by catalyzed oxidation of TMB by H2O2 is extinguished in the presence of vitamin C according to its antioxidant property. This artificial enzyme, which mimics peroxide effect with perfect catalytic efficiency, demonstrates a quick, facile, and sensitive colorimetric method, with high tolerance to high temperature, cost-effectiveness, and excellent stability in even extreme H2O2 concentration.

### **Biography:**

I received a B.Sc and M.Sc in Chemical engineering from University of Tehran, Iran in 2016 and 2019, respectively. During my studies, I completed an internship with Dilmurat Abliz in Clausthal

University of Technology, Germany. Currently, I am a Ph.D. candidate in the Department of Materials and Environmental Chemistry at Stockholm University under the guidance of Prof. Jiayin Yuan. During my Ph.D., I am focusing on poly (ionic liquids) derived functional porous carbon membranes and accurately controlling their porosities, heteroatom doping effects, and morphologies.

## Chemical and Molecular-level Insight into On-surface Reactions of Organic Molecular Tectons

### Francesco Allegretti\*

Physics Department, Technical University of Munich, D-85748 Garching, Germany

### Abstract:

In this presentation I will describe some prototypical examples of low-dimensional organic architectures that we have achieved on model metal surfaces by combining self-assembly of molecular tectons with on-surface chemical reactions. This is shown to yield molecular products as well as covalent and organometallic networks that are not straightforwardly accessible by solution chemistry, notably due to the crucial role of the substrate surface, which not only acts as a confining template but also may catalyze specific reactions. Surface science in ultra-high vacuum (UHV) provides a rich toolbox of experimental methods which enable to get insight into the molecular products and bonding schemes down to the atomic or sub-molecular scale and also provide structural, electronic and chemical information. Here, I will treat a number of examples from our case studies on coinage metal surfaces, the (111) surfaces of Ag, Cu and Au single crystals, illustrating the occurrence of C-H bond activation. Ullman coupling reactions, organometallic and carboxyl-amide coupling, depending on the specific tailoring of the individual molecular tectons. I will show that by combining X-ray spectroscopies with scanning probe microscopy, it is possible to elucidate chemical changes as well as topography and structural aspects with unprecedented sensitivity. Future goals to extend these studies beyond UHV and to improve the long-range order of the prepared surface-supported assemblies will be discussed.

### **Biography:**

Francesco Allegretti received his PhD from the University of Modena and Reggio Emilia (Italy) in 2003. Thereafter he held research posts at the University of Warwick (United Kingdom) and the Karl-Franzens University of Graz (Austria). In 2010 he joined the Physics Department at the Technical University of Munich, where he obtained the German Habilitation and the venia legendi in 2016. His current research focus is on the study of the structural, electronic and chemical properties of functional hybrid interfaces based on organic nanostructures and 2D materials, particularly by combining synchrotron radiation spectroscopy and scanning probe techniques.

### Boron-doped Diamond Cathodes for Electrochemically Assisted Ozonation Processes.

### Elisabetta Petrucci

Università di Roma, Italy

### Abstract not Available!!

# B WEDNESDAY, OCTOBER 12, 2022

### Probing Single Molecule Magnets with Graphene Quantum Dots

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### Abstract:

Single molecule magnets (SMMs) are clusters of magnetic ions or single ions embedded in a ligand shell and they can be modeled as single-spin quantum systems. Their spectra have an energy barrier to magnetization reversal yielding magnetic biostability at low temperature and widely spaced spin states, making them very attractive for high-density data storage, molecular spintronics and quantum computing. SMMs are typically studied in bulk samples, but most applications require molecules deposited on surfaces, therefore it is important to understand whether the interaction with the surfaces may substantially alter the SMM properties.

Here we use epitaxial graphene on SiC patterned into quantum dots to probe the properties of SMMs. The graphene quantum dots serve as highly sensitive photodetectors for in-situ electron paramagnetic resonance (EPR) spectroscopy of the SMMs.[1-3] The interaction between the SMMs and the graphene also affects the transport properties of the quantum dots, opening the possibility to implement an electrical readout of the magnetic state of the molecule. Previous work demonstrated spin valve effects in hybrid devices made of carbon nanotube or graphene quantum dots decorated with a few TbPc2 SMMs, at temperatures below 0.6 K and by tuning the gate voltage of the quantum dot away from the Coulomb blockade regime [4]. We present electrical detection of magnetization switching using graphene quantum dots decorated with Mn12. These devices are not gated and the spin valve effect persists at temperatures as high as 60K, allowing studies of SMM switching dynamics in a wide temperature range.

### **Biography:**

Paola Barbara is a physics professor at Georgetown University in Washington, DC, USA. Her research interests include quantum transport and superconductivity, as well as novel nanoscale devices based on atomically thin materials, ranging from chemical sensors to detectors and sources of electromagnetic radiation. She received her M. S. degree (Laurea in Fisica) at the University of Salerno, Italy, and her Ph. D. in Physics at the Technical University of Denmark, in Lyngby, Denmark. Prior to joining the faculty at Georgetown University in 2000, she worked at the Center for Superconductivity Research (now Quantum Materials Center) at the University of Maryland.

# In situ Investigation of the Crystalline Phase Composition During (De)Deuteration of NaAlD<sub>4</sub> Confined in Mesoporous Carbon Black

Rasmus Palm<sup>1,2\*</sup>, Kenneth Tuul<sup>2</sup>, Frank Elson<sup>1</sup>, Elisabetta Nocerino<sup>1</sup>, Ola K. Forslund<sup>1</sup>, Thomas C. Hansen<sup>3</sup>, Jaan Aruväli<sup>4</sup>, Martin Månsson<sup>1</sup>

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<sup>4</sup>Institute of Ecology and Earth Sciences, University of Tartu, Ravila 14a, 50411, Tartu, Estonia

### Abstract:

Solid-state hydrogen storage methods are potentially safe and efficient alternatives to contemporary hydrogen storage methods. NaAlH4-based composites are viable candidates as solid-state hydrogen storage material. Nevertheless, the confinement of NaAlH4 exhibits inherent problems regarding cyclability, efficiency, and temperatures and hydrogen pressures required for full utilization.

The effect of the mesoporous carbon black on the confinement of NaAlH4 is presented and analysed based on temperature programmed decomposition and in-house X-ray diffraction measurements in case of different carbon/alanate mass ratios. The crystalline phase composition of the deuterated 60 wt% NaAlD4/mesoporous carbon black composite is determined in situ with neutron powder diffraction during four (de)deuteration cycles. Based on the in-situ diffraction measurements, the main limiting factors for efficient cyclability and the hydrogen release capability of effectively confined hydride are presented.

### **Biography:**

Rasmus Palm defended his PhD 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, PhD Palm attained experience in electrochemistry, gas adsorption methods and hydride-based hydrogen storage materials. Since 2020 PhD Palm has been working as a postdoctoral researcher at the Royal Institute of Technology, Sweden. The current research focus is on the application of in situ neutron scattering methods to study hydrogen storage and carbon materials.

# Mode Coupling, Bi-stability, and Spectral Broadening in Buckled Carbon Nanotube Mechanical Resonators

Yuval E. Yaish\*, Sharon Rechnitz, Tal Tabachnik, Michael Shlafman, and Shlomo Shlafman

Andrew and Erna Viterbi Faculty of Electrical Engineering, Technion, Israel

### Abstract:

Bi-stable mechanical resonators play a significant role in various applications, such as sensors, memory elements, quantum computing and mechanical parametric amplification. While carbon nanotube (CNT) based resonators have been widely investigated as promising NEMS devices, a bi-stable CNT resonator has never been demonstrated. In this talk we present a new class of CNT resonators in which the nanotube is buckled upward. We show that a small upward buckling yields record electrical frequency tunability, whereas larger buckling can achieve Euler-Bernoulli (EB) bi-stability, the smallest mechanical resonator with two stable configurations to date. Furthermore, we present a three-dimensional theoretical analysis revealing significant nonlinear coupling between the in-plane and out-of-plane static and dynamic modes of motion, and a unique three-dimensional EB snap-through transition. We utilize this coupling to provide a conclusive explanation for the low-quality factor in CNT resonators at room temperature, key in understanding dissipation mechanisms at the nano scale.

### **Biography:**

Yaish is faculty at the ECE and the Zisapel Nano-Electronics Center at the Technion – Israel Institute of Technology. He earned his B.Sc. and M.Sc. in Physics from Tel-Aviv university and received his Ph.D. in Experimental Physics in Condensed Matter from the Technion. Dr. Yaish did his postdoc in Physics at Cornell University, and since then his research is focused on electrical, thermal, and mechanical properties of 1- and 2-dimensional nano scale materials such as Silicon Nanowires, Carbon Nanotubes, Graphene, and 2-dimensional van der Waals materials.

# Tailoring Multifunctional and Lightweight Hierarchical Hybrid Graphene Nanoplatelet and Glass Fiber Composites

## Nello D. Sansone, Zahir Razzaz, Meysam Salari, Anthony V. Tuccitto, Rafaela Aguiar, Patrick C. Lee\*

Multifunctional Composites Manufacturing Laboratory (MCML), Department of Mechanical and Industrial Engineering, University of Toronto, Canada

### **Abstract:**

In this work, hybrid polypropylene (PP)-based composites reinforced with graphene nanoplatelets (GnP) and glass fiber (GF) were fabricated by injection molding, to elucidate how the hybrid approach can produce synergistic effects capable of achieving properties and functionalities not possible in biphasic composites. Synergism between the reinforcements translated to improved mechanical performance, which was attributed to the chemically and/or electrostatically assembled hierarchical structure which facilitates load transfer at the interface, while simultaneously tailoring the crystalline microstructure of the matrix by inducing transcrystallization and  $\beta$ -crystal formation. It was demonstrated that there exists an optimal concentration of 0.5 wt.% GnP, producing the greatest mechanical properties and synergistic effect, corresponding to the highest degree of crystallinity (~6% greater than Neat PP) and peak formation of -crystals within the PP matrix. The greatest synergistic effect was found to be ~52% and ~39% for the specific tensile strength and flexural strength, respectively. The same optimal concentration of GnPs was found to produce the highest synergistic effect for thermal conductivity of ~68%, due to the volume exclusion effect induced by the GFs combined with the higher crystallinity of the microstructure, promoting the formation of thermally conductive pathways. Ultimately, the mechanisms contributing to the synergistic effect presented in this work can be used to maximize the performance of hybrid composite systems, giving them the potential to be tailored for a variety of high-performance industrial applications, to meet the rising demands for ultra-strong, thermally conductive, and lightweight materials.

### **Biography:**

Lee is an Associate Professor in the Department of Mechanical and Industrial Engineering at the University of Toronto. His research areas focus on processing and characterization, and processing-structure-property relationships of hybrid nanocomposites and foams. He has 72 journal papers, over 100 refereed conference abstracts/papers, 3 book chapters, and 20 filed/issued patent applications. Among his honors, Dr. Lee received the G.H. Duggan Medal from Canadian Society for Mechanical Engineering in 2020, the AKCSE Early Achievement Award in 2019, the US National Science Foundation Early Faculty Career Development Award (NSF CAREER) in 2018, the Polymer Processing Society Morand Lambla award in 2018.

# The Role of Molybdenum Disulfide for Solar Cell Applications: Properties, Mechanism and Application

Norasikin Ahmad Ludin<sup>1\*</sup>, Abu Dzar Al-Ghiffari<sup>1</sup>, Rozan Mohamad Yunus<sup>2</sup>, Matthew L. Davies<sup>3</sup>, Mohd Sukor Suait<sup>1</sup>

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### Abstract:

Molybdenum disulfide (MoS2) has received much interest due to its revolutionary development and advantageous properties; particularly in its configurable bandgap that can transit from indirect to direct as the phase changes from the bulk form into the monolayer. MoS2 has found use in a range of solar cell technology as a hole transport layer (HTL) to facilitate charge separation and a blocking layer (EBL) to suppress the occurrence of recombination at the materials interface (silicon solar cells), a back contact at the interface between CdTe and Au, resulting in the reduction of charge carrier recombination thus improving hole extraction/collection at the back contact (CdTe solar cells), a hole extraction layer (HEL) in organic solar cells, a counter electrode (CE) by replacing classical platinum (Pt) in dye-sensitized solar cells (DSSC) and as a HTL instead of conventional materials such as PTAA, spiro-OMeTAD, and PEDOT:PSS in perovskite solar cells. The integration of MoS2 with other materials within a specific solar cell's architecture can negatively impact device performance. Therefore, this study identifies gaps and issues of using MoS2 in multiple types of solar cells in detail, alongside its highest performance use in every application.

### **Biography:**

Norasikin Ahmad Ludin hold a PhD in Chemistry from University of Wales, United Kingdom in 2012. Currently, she is the Associate Professor of Renewable Energy (RE) at Solar Energy Research

Institute, Universiti Kebangsaan Malaysia. She has experienced and involved in the field of RE for more than 20 years. Her research interest is solar photovoltaic technologies (solar cells materials and devices) and impact analysis of the systems such as economic, environment and policy. She has published and presented more than 100 papers in high impact journals and conferences. She is also a member of Royal Society of Chemistry, United Kingdom.

### Clean Energy and Decarbonization Research at Oak Ridge National Laboratory

#### Xin Sun

Associate Laboratory Director, Energy Science and Technology Directorate, Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA,

### Abstract:

Oak Ridge National Laboratory (ORNL) is the largest US Department of Energy Office of Science Laboratory. Located in Oak Ridge, Tennessee, ORNL delivers scientific discoveries and technical breakthroughs that accelerate the development and deployment of solution for clean energy, decarbonization and global security. The Energy Science and Technology Directorate (ESTD) at ORNL leads transformational science and technology in enabling integrated, flexible, secure, and autonomous energy systems of the decarbonized energy infrastructure of the future. We are accelerating decarbonization in the US with a three-pronged approach on integrated energy systems: 1.) Achieve deeper energy savings through enhanced energy efficiency efforts across all spectrums of the energy service sectors, i.e., buildings, industry, and transportation; 2.) Accelerate net-carbon neutrality by capturing and converting CO2 into valuable materials, fuels, and feedstocks for downstream utilizations; and 3.) Enable bi-directional electron flows between the grid and end users with at-scale energy storage and transactive controls to enable a sustainable, resilient, and secure energy infrastructure.

Buildings and transportation sectors combined consume 70% of raw energy in the US. In the transportation area. ORNL's research covers combustion, electrification, and hybridized propulsion, vehicle and mobility systems research, and vehicle communications, systems integration, and decision science. ORNL's building technologies research focuses on accelerating the development and integration of advanced building equipment, novel dynamic envelope materials, as well as control systems to enable affordable, efficient, and resilient buildings. ORNL's manufacturing science research focuses on the development and implementation of next-generation advanced manufacturing technologies through research and scale-up of new processes and technical capabilities enabling new materials, systems and products. Our research portfolio covers four primary focus areas: composite science and technology, energy and industrial decarbonization, precision manufacturing and machining, and secure and digital manufacturing. ORNL's energy infrastructures research focuses on reducing the cost and improving the efficiencies of at-scale energy storage systems and the improvement of the reliability and sustainability of the electric grid in the areas of controls, and advanced power electronics. Exemplary ORNL RD&D advancements in all the areas above will be presented and future opportunities and challenges in the integrated energy systems approach will be discussed.

### Carbon-incorporated Titanate Nanotubes as Catalyst Support for PEM Fuel Cells

### Julia Hoppe\*, Olaf Kottas, Dominik Eitel, Uta Helbig

Nuremberg Institute of Technology, Department of Materials Engineering, Germany

### Abstract:

Polymer exchange membrane fuel cells (PEM-FC) gain rising attention and are an important element in the energy and mobility sector in the course of the impending energy revolution. One limiting factor of current PEM fuel cells is the degradation of the carbon support in the catalyst layer due to hydrogen starvation at the electrode or start/stop cycles. Based on titanate nanotubes synthesized via alkaline route, we developed a novel catalyst support material. The nanotubes are fabricated in a two-step process using nanoscale TiO2 powder as precursor. First, carbon is incorporated into titanium oxide powder by heat treating the material in acetylene/nitrogen gas flow. The resulting powder is subsequently transformed into carbon containing titanate nanotubes in hot alkaline solution. SEM investigation, X-ray diffraction and gas sorption analysis revealed the successful fabrication of nanotubes. X-ray diffraction showed the typical pattern for titanate nanotubes, but no additional phases were detected. The material shows a specific surface area of 300 m2 /g up to 400 m2 /g. Thermogravimetry paired with infrared-spectroscopy proved the presence of carbon in the product. The carbon content increases with increasing temperature of the heat treatment of the precursor and is between 5 wt.-% and 11 wt.-%. Electrical properties were determined using impedance spectroscopy to investigate the correlation between carbon content and electronic conductivity. The conductivity of the nanotube material is strongly dependent on the carbon content. Conductivity values up to ~10-2 S/cm could be achieved.

### **Biography:**

Julia Hoppe is a PhD student at Nuremberg Institute of Technology. She studied Materials Technology at the Nuremberg Institute of Technology and joined the group of Prof. Dr. Uta Helbig obtaining her B.Eng. in the field of conservation science on corrosion of a historic silver medal. For her master studies she did research on corrosion of showcase glasses as effect of air pollutants and obtained her M.Sc. in 2018. Her current research is based on the formation process and structure of carbon containing titanate nanotubes.

### Developing Highly Stable Solid-state Organic Lithium Metal Batteries Powered by Carbon Current Collector Single Ion Polymer Electrolyte

Yunfan Shao<sup>1</sup>, Fannie Alloin<sup>1</sup>, L. Picard<sup>3</sup>, V. Gouget<sup>3</sup>, Dominic Bresser<sup>2</sup>, Cristina Iojoiu<sup>\*1</sup>

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### <sup>2</sup>CEA, LITEN, Grenoble, France

<sup>3</sup>Helmholtz Institute Ulm (HIU), Helmholtzstrasse 11, Ulm 89081, Germany.

### Abstract:

Lithium ion battery (LIB) plays dominant role among all the energy storage technologiesdue to its high energy and power density. To meet the dramatically increasing demand for the LIB which

needs more safe, sustainable, and low cost, a novel battery with organic active materials (OAM), single ion polymer electrolyte (SIPE) and carbon current collector (CCC) was came up. By using OAM and CCC, the pricy metal in the battery such as Cu, Ni and Co can be substituted by earth abundant elements C, N and O to reduce cost and ensure the sustainability[1]. In addition the SIPE allows to reinforce the safety by its solidstate nature and ability to suppress the lithium dendrite formation by its cationic transport number (t + ) close to 1 [2]. In this presentation very new results on all solid-state lithium metal batteries (LMB) with organic cathode, CCC and SIPE will be presented. Various SIPEs are designed and synthesized to achieve high cationic conductivity and wide electrochemical window. The cathode with perylene based polyimide active material was impregnated on CCC and assembled with SIPE and lithium metal and tested in coin cells. These new systems exhibit very high-performances with a low overpotential, high capacity (whole the cathode capacity is accessed) and a long-term stability. The excellent results make these long lasting, sustainable and safe organic LMB very promising for the future energy storage. [1] L. Picard et al, ACS Appl. Mater. Interfaces 2016, 8, 22762. [2] C. lojoiu et al.Energy & Environmental Science 2018,11, 3298-3309.

### **Biography:**

Cristina IOJOIU is senior researcher at National Scientific Research Center in the laboratory of Electrochemistry and Physico – chemistry of Materials and Interfaces, France. She has worked for 18 years in the synthesis, characterization and degradation of electrolytes for electrochemical devices (fuel cells and batteries) based on polymers and ionic liquids. She is heading the team "Material Interface and Electrochemistry" from LEPMI. She is leader of many national and international projects on polymer electrolytes for energy storage and conversion. She published more than 90 peer-reviewed papers and 5 book chapters and is co-inventor of 15 patents dealing with electrochemical energy sources.

### Pathway Toward Fabrication of Efficient and Stable Perovskite Solar Modules

### Narges Yaghoobi Nia<sup>1,2\*</sup>, Mahmoud Zendehdel<sup>1</sup>, Aldo Di Carlo<sup>1,2</sup>

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<sup>2</sup>CNR-ISM Istituto di Struttura della Materia, via del Fosso del Cavaliere, Rome, Italy

### **Abstract:**

Perovskite solar cells (PSCs), as the most well-known emerging thin-film photovoltaics (PVs), attracted large scientific and technological interest due to their unique properties (e.g., high efficiency, cost-effective printable fabrication and band-gap tuning) that allow different applications. Nevertheless, PSC degradation, stability against light and thermal stresses, high quality film and optimal thickness especially for large scale deposition on module size are important aspects that still need to be properly address. In our activities, several approaches to reach efficient stable perovskite solar module have been developed. In 2017, 350 h light stable perovskite solar module fabricated reaching an efficiency on 10.1 cm2 active area (AA) 1 . Later, by identifying a specific doping strategy of the P3HT polymer, a 13.3% efficient large area module (43cm2 AA) was fabricated2 . In 2019, an efficiency above 20% on small area and 17% on large area module (43cm2 AA) maintaining above 90% of the initial efficiency after 800h thermal stress was demonstrated by exploiting polaron arrangement polymeric HTM3 . This result was recently improved with the fabrication of a 45.6cm2 AA module with an efficiency of 18.45%4 . In addition, by using a universal approach for layer-by-layer deposition of 3D/2D perovskite films with zero waste permitted to fabricate 18.8% perovskite solar module, thermal stability at 85 °C of T90=1000h5 . In the present work, extending the reported strategy by using novel stable 2D perovskite passivation layers, we report on the fabrication of high efficiency, stable perovskite solar module reaching and efficiency of 20.2% and more than 3000 hours thermal and light stability. 1. Yaghoobi Nia, N., Zendehdel, M., Cinà, L., Matteocci, F. & Di Carlo, A. J. Mater. Chem. A 6, 659–671 (2018). 2. Yaghoobi Nia, N. et al. Small 15, 1904399 (2019). 3. Yaghoobi Nia, N. et al. Nano Energy 69, 104441 (2020). 4. Zhang, H. et al. Nat. Commun. 13, 89 (2022). 5. Zendehdel, M., et al. Sol. RRL (2021). doi:10.1002/solr.202100637.

### **Biography:**

Narges Yaghoobi Nia Ph.D. in Electronics Engineering and M.Sc. of Physical Chemistry. She was awarded a MARIE CURIE Fellowship as a part of the EU-funded project (Destiny FP7/2007–2013). She is currently Assistant professor of Department of electronic engineering, University of Rome Tor Vergata. She has several years' experience in the fields of emerging thin film PVs (especially perovskite solar cells/modules and tandem). She was a member of Espresso, ENEA, PRIN, Perseo project and collaborator for ASI project. She is currently member of VIPERLAB project and Principal investigator P4SPACE project, MARIE CURIE Global fellowship 2022 (Sapienza University aerospace school and EPFL).

### Applications of Functional Activated Carbon Impregnated with Elementary Iodine

### Katsuyoshi Tatenuma<sup>1\*</sup>, Fabio Spaziani<sup>1,2</sup>, Yoshiaki Kinase<sup>1,3</sup>

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### Abstract:

lodine has well-known antibacterial and antiviral properties, making it the active ingredient of disinfectants such as Povidone-iodine, lodine-tincture, etc. We developed an activated carbon impregnated with molecular iodine (I2), named IodAC, incorporating the abovementioned antiseptic feature, showing low water solubility and low volatility of iodine, low corrosiveness to metals, and other functional properties.

Antibacterial test (on Escherichia coli) and antiviral test (on an avian influenza virus strain) were conducted, demonstrating the effectiveness of IodAC against the pathogens. IodAC was also compared to slaked lime, which is used for the disinfection of outdoor spaces and livestock areas. The data confirmed again the performance of IodAC against viruses and bacteria, but also evidenced a more stable and long-lasting disinfecting power compared to slaked lime (since IodAC does not undergo a gradual decrease in disinfecting power, which instead occurs in slaked lime due to the reaction with atmospheric carbon dioxide).

The overall results show that lodAC is a promising material, having the potential to be employed

for several purposes, including granules to spread for sanitation of livestock spaces and public sites, use for water disinfection, zoonotic diseases countermeasures (e.g., as an animal feed additive for avian influenza control), post-harvest food storage. Its characteristics also prospect the testing in the medical field, such as therapies for blood or intestine (HIV, sepsis, irritable syndrome, ulcerative colitis therapy), or production of medical supplies (antibacterial bandages, gauze, cotton, etc.).

### **Biography:**

Tatenuma's favorite R&D fields are chemical analysis, nuclear medicine, and related materials. Recently he is focusing on the development of innovative disinfectant and material for environmental purification based on iodine. Dr. Spaziani's activity is focused on environmental chemistry research at ENEA (Italian National Agency for New Technologies, Energy and Sustainable Economic Development) in Roma (Italy), and on the development of innovative materials for environmental and nuclear-fusion energy applications by joining the research group of Kaken Inc. in Japan.

### Fabrication of 2D materials based Nanoarchitectures via Innovative CVD Processes

### Marc González Cuxart, Technical University Munich, Germany

Physics Department E20, Technical University of Munich, Germany.

Instituto Madrileño de Estudios Avanzados en Nanociencia (IMDEA-Nanociencia), Spain.

#### Abstract:

The abilities to combine complementary two dimensional (2D) materials and to introduce modifications at the nanoscale open compelling

routes to engineer the material's properties and grant novel functionalities [1,2]. Here, we present two innovative CVD processes that enable (i) the growth of an atomically thin 2D elemental material beyond graphene for the first time, also in combination with

another 2D material, and (ii) the fabrication of 2D arrays of impurities structurally embedded in graphene. Specifically, the use of diborane as precursor gas yields large single-crystalline borophene domains (i.e., an atomically thin layer made of elemental boron) on distinct metal supports. Subsequent addition of

borazine as precursor in the process allows to synthesize hexagonal boron nitride (hBN) conjointly with borophene, which can selectively form lateral or vertical heterostructures. When combined laterally, borophene and hBN form uniform covalent lateral interfaces, while vander Waals stacks in which borophene is protected from immediate oxidation are produced whencombined vertically [3]. On the other hand, the use of a single molecular precursor (borane tetrahydrofuran) providing boron and carbon enables the fabrication of 2D arrays of boron substitutional species in graphene. These are formed due to segregation of the boron atoms, which is guided by the naturally occurring moiré superstructures in Ir(111)-supported graphene [4].

Our findings are based on a comprehensive surface-science approach that combines atomic-scale and surface averaged characterization techniques (i.e., scanning tunneling microscopy and spectroscopy STM/STS, low energy electron diffraction LEED and x ray photoemission spectroscopies XPS/ ARPES), together with first-principles calculations that provide insight into the material's structure, chemical and electronic properties, and interfacial interactions.

### **Biography:**

[1] Sierra, J. F. et al. Van der Waals heterostructures for spintronics and opto-spintronics. Nat Nanotechnol. 2021, 61 (8), 1748.

[2] Ullah, S. et al. Advances and Trends in Chemically Doped Graphene. Adv. Mater. Interf. 2020, 7 (24), 2000999.

[3] Cuxart, M.G. et al. Borophene Made Easy. Sci. Adv. 2021, 7 (45), 1-8.

[4] Cuxart, M.G. et al. Spatial Segregation of Substitutional B Atoms in Graphene Patterned by the Moiré

Supperlattice on Ir(111). Under peer-review process as of July 2022.

## Optical Band Gap of Carbon Modified TiO<sub>2</sub>

## Dominik Eitel1\*, Julia Hoppe1, Johanna Graml1, Uta Helbig1

<sup>1</sup>Nuremberg Institute of Technology, Department of Materials Engineering, Germany

### Abstract:

Photocatalytic water splitting with inorganic semiconductors like TiO2 recently aroused interest as a path towards sustainable hydrogen generation. The eligibility of titanium dioxide as photocatalyst relies on the generation of free charge carriers through absorbed photons as well as a sufficiently long lifetime of excited states. The photon wavelength suitable for the photogeneration of free charge carriers depends on the band gap. For anatase as well as rutile the type of band gap transition and band gap energies are extensively discussed in the literature. The high band gap energies (3.2 eV for anatase, 3.05 eV for rutile) result in a low photocatalytic activity as only the UV region of the spectrum can be utilized. As a result, band gap narrowing with doping materials is an important research topic. Both experimental and theoretical publications reported carbon as a promising dopant material for band gap tailoring. We developed a carbothermal process for the incorporation of carbon in the TiO2 structure [1]. X-ray diffraction and thermogravimetric analysis proved that the resulting material is carbon containing anatase. Diffuse reflectance spectroscopy in combination with the theory of Kubelka and Munk was used as a tool for band gap determination. Contrary to our expectations, a shift towards higher energies as well as absorption before the actual band gap was discovered, leading to the assumption of the occurrence of a Burstein-Moss effect. [1] U. Helbig, K. Herbst, J. Roudenko, J. Helbig, B. Barton, and U. Kolb, J. Mater. Res., vol. 33, no. 09, pp. 1288-1300, 2018, doi: 10.1557/jmr.2018.49.

### **Biography:**

Dominik Eitel is a PhD student at Nuremberg Institute of Technology. He studied Materials Technology at the Nuremberg Institute of Technology and obtained his B.Eng. in the field of heat and corrosion resistant surface coating for SiC/SiC in 2019. For his master studies he joined the group of Prof. Dr. Uta Helbig, researching about carbon-doped titanate nanotubes for proton exchange membrane fuel cell applications, where he obtained his M.Sc. in 2021. His current research is based on the formation and stabilization of defects in carbon doped TiO2 nanomaterials.

### THURSDAY, OCTOBER 13, 2022 Virtual Presentations

## Plenary Session 1

Multifunctional Synergy Strategies for Materials Design, Processing and Applications

Shi Xue Dou

University of Wollongong, Australia

Abstract not available!!

### **Chemically Modified Graphene for Real-world Applications**

Sang Ouk Kim KAIST. South Korea

Abstract not available!!

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

### **Bunsho Ohtani**

Professor Emeritus, Hokkaido University/Nonprofitable Organization touche NPO, 1-6-414, North 4, West 14, Sapporo 060-0004, Japan

### Abstract:

How can we design functional solid materials, such as catalysts and photocatalysts? What is the decisive structural parameters controlling their activities, performance or properties? What is obtained as structural properties by popular conventional analytical methods, such as X-ray diffraction (XRD) or nitrogen-adsorption measurement, is limited to bulk crystalline structure and specific surface area, i.e., no structural characterization on amorphous phases, if present, and surface structure has been made so far. This is because there have been no macroscopic analytical methods to give surface structural information including possibly present amorphous phases. Recently, we have developed reversed double-beam photoacoustic spectroscopy (RDB-PAS) which enables measure energy-resolved 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 guantitatively evaluated as degree of coincidence of ERDT/CBB patterns. An approach of material design based on the ERDT/CBB-pattern analyses especially for carbon-nitride samples is introduced [3]. [1] Chem.

Commun., 2016, 52, 12096–12099. [2] Electrochim. Acta, 2018, 264, 83–90. [3] Catal. Today, 2019, 321–322, 2–8.

### **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 form the societies related to chemistry, photochemistry, electrochemistry and catalysis chemistry.

## **Keynote Session 1**

### Atomic Layer Deposition of Noble Metals with Low Concentration Ozone

### Alfred ling Yoong Tok\*

School of Materials Science & Engineering, Nanyang Technological University, Singapore.

### Abstract:

Noble metal thin films have several potential applications in electronics, protective coating, and catalyst industries. The atomic layer deposition (ALD) of noble metal films are currently achieved using either oxygen or hydrogen as precursors or annealing agents, requiring high temperatures leading to increased risks of explosion and fire. ALD methods not using oxygen or hydrogen as precursors or annealing agents have so far resulted in noble metal oxides instead of pure metal films. An ALD process has been developed for noble metal thin films preparation utilizing low concentration ozone (1.22 g/m3) as a reactant, without the need for any oxygen or hydrogen. This process has been successfully demonstrated for the fabrication of Rhodium (Rh) and Palladium (Pd) thin films. Both metal films exhibited extremely uniform surface with the root mean square (RMS) surface roughness below 0.2 nm. The 20 nm thick metal films had very low resistivity of  $12\mu\Omega$ cm for rhodium and 63  $\mu\Omega$  cm for palladium, showing the deposited metal films had a high purity. The reaction mechanism of palladium ALD from Pd(hfac)2 and low concentration ozone was also studied by density functional theory (DFT). The simulation results show that Pd(hfac)2 dissociative chemisorbed on Si (100) surfaces. Subsequently, ozone reacted with Pd(hfac)\* by cleaving its C-C bond to produce gaseous oxygen and adsorbed CF3-OC and CF3-CO-CHO with a relatively low activation barrier. Hence, the reaction was kinetically favourable. The adsorbed complex carbide was then depleted by the excess ozone. The calculated results reveal that pure palladium can be prepared by Pd(hfac)2 and ozone in low concentration without oxygen or hydrogen. All the results indicate that this low concentration ozone based ALD process could yield high quality noble metal films in low temperature and safer way.

### **Biography:**

Alfred Tok has been a faculty member in the School of Materials Science and Engineering (MSE) since 2003. He studied Mechanical Engineering at the Queensland University of Technology, Australia, and graduated with First Class Honours in 1995. He was also conferred the Dean's Award

for Excellence for being the top graduate. After graduation, he worked as a mechanical engineer at ST Aerospace Engineering. In 1997, he was awarded 2 scholarships at Nanyang Technological University to pursue his PhD in Mechanical Engineering. He obtained his MBA (Dean's List) in 2009 from the Nanyang Business School. His research areas focus on the processing and applications of inorganic materials in the areas of smart materials, biosensors and renewable / sustainable energy. He also consults extensively for companies from various industries.

### **Oral Session 1**

# The Effect of Carbon Atoms to the Ferroelectricity in ZnO:C Nanocolumnar: Experimental and Density-functional Studies

### Yudi Darma

Institut Teknologi Bandung, Indonesia

Abstract not available!!

### Effect of Interfacial Chemistry on the Nanotribology of Graphite

### J.M. Kim, Arnaud Caron<sup>\*</sup>

KOREATECH - Korea University of Technology and Education, Cheonan, 31253 Rep. of Korea

### Abstract:

Graphite and its derived materials have been used extensively as a solid lubricant or as additives in oilbased lubricants. The lubricating effect of graphite owes to the weak interactions between its basal planes. Graphite is commonly accepted as chemically inert since its sp2-bonded basal planes do not exhibit any dangling bonds. In this work, we apply atomic force microscopy to study the friction and wear of highly oriented pyrolytic graphite (HOPG) upon reciprocal sliding of nanometer-scaled asperity of different chemistries: SiOx, Pt, and diamond. We find that friction and wear between these various couples strongly depend on the chemistry of the AFM-tips. In the case of SiOx and Pt asperities friction and wear are highest at the surface steps of HOPG. In these cases, chemo-mechanical interactions lead to flakes removal from the HOPG surface steps while the interior of terraces remains unaffected up to large normal force values. In contrast, the friction and wear of HOPG and diamond are significantly larger. We thus demonstrate that despite its assumed inertness the tribology of graphite is strongly affected by the chemistry of its counter body.

### **Biography:**

Arnaud Caron is a materials scientist with expertise in the multi-scale mechanical behavior of materials, surfaces and micro-components. Since 2015 Arnaud Caron is Assistant Professor in the School of Energy, Materials and Chemical Engineering at KoreaTech – Korea University of Technology and Education, Republic of Korea. Arnaud Caron obtained his engineering degree in Materials Science in 2004 from the University of Saarland, Germany and was awarded the Schiebold Medal. In 2009, he earned his doctoral degree in Materials Science from the University of Saarland, Germany. Arnaud Caron worked at the Institute of Micro- and Nanomaterials of the University of Ulm, Germany, the WPI-AIMR at the Tohoku University, Japan and the Leibniz – Institute for New Materials, Germany.

# Superb Flexibility and Stretchability of Highly Conductive Large-area Graphene Grown Directly on PDMS substrate at 100 °C

### Yire Han, Jang-Su Jung, and Soon-Gil Yoon\*

Department of Materials Science and Engineering, Chungnam National University, Daeduk Science Town, 34134, Daejeon, Republic of Korea

### Abstract:

The direct synthesis of inherently defect-free, large-area graphene on flexible substrates is a key technology for soft electronic devices. In the present work, in situ plasma-assisted thermal chemical vapor deposition (PATCVD) is implemented in order to synthesize 4-inch-diameter high-quality graphene directly on 10-nm-thick Ti-buffered substrates at 100 °C. The in situ synthesized mono-layer graphene displays outstanding stretching properties coupled with low sheet resistance. Further improved mechanical and electronic performances are achieved by the in situ multi-stacking of graphene. The 4-layered graphene multi-stack is shown to display an ultralow resistance of ~ 6 W per square, which is consistently maintained during the harsh repeat stretching tests and is assisted by self-p-doping under ambient conditions. Graphene-field effect transistors fabricated on polydimethylsiloxane (PDMS) substrates reveal an unprecedented hole mobility of ~ 21,000 cm2V-1s-1 at a gate voltage of -4V, irrespective of the channel length, which is consistently maintained during the repeat stretching test of 5,000 cycles at 140% parallel strain.

### **Biography**

Soon-Gil Yoon received his Ph.D. from the Korea Advanced Institute of Science and Technology, Korea in 1988. He is a distinguished professor in Materials Science and Engineering, Chungnam National University, Korea since 1990. He published about 405 peer-reviewed papers since 1990. His representative papers are Nano Letters (2010), Advanced Materials (2011, 2012), Nano Energy (eight papers) for piezoelectric energy harvesting using organic/inorganic perovskite thin films, Advanced Science and Nano Today (2021) for high flexibility and high stretchability of the transfer-free, high-quality, large-area monolayer graphene grown at 100 oC. His current research interests are Antibacterial activity, Transfer-free Graphene, Piezoelectric energy harvesting using organic/inorganic halide perovskite.

Keywords: Transfer-free graphene; high flexibility; high stretchability; large area graphene growth at 100  $^{\circ}\text{C}$ 

### Pair Distribution Function (PDF) Analysis of Multiwalled Carbon Nanotubes

### Bagautdin Bagautdinov\* and Koji Ohara

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### Abstract:

Structural features of multiwalled carbon nanotubes (MWCNTs) have been analyzed quantitatively by high-energy X-ray diffraction (HE-XRD) with atomic pair distribution function (PDF) technique. Comparative study of local structures for strolled type carbon nanotubes fabricated by arc dis-

charge method and nested ones produced by chemical vapor deposition is performed. It has been found that the nanotubes own an atomic arrangement defined on the nanometer length scale in terms of a unit cell and symmetry. The structural information at different length-scales was used to probe the interlayer spacing distribution within the nanotubes.

For strolled type nanotubes the radial dependence of interlayer spacing were observed. They exhibit multipart local (sub-nanometer) and intermediate range (nano-length-scale) structures. The radial interlayer differences present tendency for alteration to uniform spacing of layer in the course of heating-cooling cycles. These spatial changes illustrate modification of Fermat type stroll with uneven interlayer distances in pristine nanotubes to more stable equidistant interlayer Archimedean spiral type in the treated ones [1].

Contrary, the PDF structures of the nested MWCNTs can be described in terms of the unique graphite model with  $\approx$ 3.4 Å inter-wall spacing and they present superior short-range 3D correlation amongst neighboring walls.

The nanolength-scale PDF structures of MWCNTs possessing extremely small correlation lengths of interlayers are vital to gain insight into their structure-property relationships.

[1] B. Bagautdinov, K. Ohara, A.A. Babaev. Carbon, 191, 75-83 (2022).

### **Biography:**

Bagautdin Bagautdinov received his PhD in the Institute of Solid State Physics of the Russian Academy of Sciences (Chernogolovka) and then conducted research in McMaster University (Canada), University of Bayreuth (Germany) and Hyogo University (Japan). From 2001 was affiliated to crystallography division of Protein3000 project in RIKEN/SPring-8 (Japan) and from 2008 up to now employed in JASRI/Spring-8, Diffraction and Scattering Division. His current research interest devoted to pair distribution function (PDF) analysis for structure-function imaging.

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

### Joong Tark Han<sup>\*1,2</sup>

<sup>1</sup>Nano Hybrid Technology Research Center, Electrical Materials Research Division, Korea Electrotechnology Research Institute, South Korea

<sup>2</sup> Department of Electro-Functionality Materials, University of Science and Technology, South Korea

### Abstract:

Graphene oxide (GO), produced by oxidation of graphite powder, is intensively utilized in electrodes, templates for hybrid materials, interfacial modifiers, three-dimensional structures, etc., with its performance as an electrode material being determined by its chemistry and structure. In particular, the topological defects present in the basal plane of reduced GO (rGO) can significantly affect its electrical and electrochemical properties. Importantly, the structural properties of GO and rGO nanosheets critically depend on the oxidation degree of GrO and exfoliation conditions. However, the chemical structure of GO nanosheets is hard to precisely define due to being dependent on the specific oxidation conditions used. In addition, The GO nanosheets are commonly synthesized by the exfoliation of graphite oxide (GrO), which can be produced by permanganate (MnO4)- or chlorate (CIO3)- based oxidation using a huge amount of a strong acid. However, this is recognized as a hurdle in the mass production of GO from graphite due to massive acid wastes and high processing costs. In the case of H2SO4-based oxidation, some studies have been trying to recycle the used acid to reduce the processing cost of graphite and to overcome environmental issues. In chlorate-based oxidation, fuming nitric acid is typically used to fabricate high-quality graphene, because fuming nitric acid and ClO3 can produce less defective graphene oxide nanosheets. However, the fuming nitric acid cannot be reused as it releases toxic gases, which poses a threat to researchers' health and the environment. Hence, there is a need to develop a method to oxidize graphite for high quality graphene via chlorate-based oxidation.

### **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 Nano-Hybrid Technology Research center at Korea Electrotechnology Research Institute (KERI). His research interests are in exploring nanostructures and electronic structures of electrical nano-materials such as nanocarbon materials (carbon nanotube, graphene, etc.), nano-metal, metal oxide nanoparticles, for future smart electric devices.

### Carbon Chemistry using Alkali Metals and Electrochemical Reduction

### Toshihiro Shimada\*

Hokkaido University, Japan

### Abstract:

We are studying the chemical and electronic interaction of carbon with melted alkali metals and synthesis of carbon materials using alkali metals and/or strongly reducing conditions. The reaction environment is under inert gas and we sometimes use sealed niobium tubes. I will introduce some of the findings as follows:

1. It is possible to synthesize ultrathin glassy carbon films by spin-coating followed by calcination of sp3-based (HC)x polymer synthesized from polymerization using Na-K alloy.[1]

2. Diamond is etched above 600oC in melted lithium. (100) surfaces are selectively etched. Na shows slight etching, while K did not show etching at 800 oC. NV- center seems to lose electrons when heated with melted K. This can be explained by band bending, which is clearly showed by electronic structure calculations.[2]

3. Electrochemical reduction can be used in zigzag edge of graphite.[3]

### **Biography:**

Toshihiro Shimada currently working as a professor at the Hokkaido University Faculty of Engineering Solid State Chemistry Laboratory in April 2010. He was previously an associate professor at The University of Tokyo, School of Science, Department of Chemistry, where he was engaged in research in areas such as organic semiconductors, organic thin films, and high-energy carbon science. He is currently interested in subjects such as substances for which it is difficult to control reactions for synthesis, such as diamonds and carbon nanotubes, and the development of catalysts that are usable in high-temperature and high-energy environments.

### The Effective Dispersion Method for Carbon Nanotube/Protein Composite Yarn

### Yongyoon Cho<sup>1\*</sup> and N. Okamoto<sup>1</sup>, S. Yamamoto<sup>1</sup>, B. Hiroaki<sup>1</sup>, M. Nakamura<sup>1</sup>

<sup>1</sup>Nara Institute of Science and Technology (NAIST), Japan

### Abstract:

Carbon nanotube (CNT) has been emerging as a promising thermoelectric material due to the light weight, flexibility, superior electrical and mechanical properties. On the other hand, its high thermal conductivity needs to be suppressed for the higher thermoelectric efficiency. Among various CNT composites with inorganic and organic materials in the previous studies. CNT composite with cageshaped protein shell (C-Dps) has also been reported with significantly reduced thermal conductivity. However, CNT/C-Dps composite has been only fabricated as a film-type sample rather than yarn-type which is more suitable for wearable device and beneficial to obtain the temperature difference. Furthermore, circumstantial sensitivity of protein and Van der Waals interaction of CNT have disturbed the spinning process of CNT yarn. Therefore, in this study, we aimed to develop the dispersion method for efficient CNT/C-Dps composite yarn. By using ionic liquid (IL) and amphiphilic surfactant with dialysis process, we achieved high retrieval rate of CNT and good coverage of C-Dps on CNT bundles. Figure 1 represents different dispersion methods used in this research. Method A is a conventional way to disperse CNT and C-Dps, as CNT/C-Dps film was formed. In method B and C, IL is firstly applied to disperse CNT, while dilution and dialysis are processed for the IL removal, respectively. In method D, IL as well as polymeric surfactant are introduced, followed by centrifugation and dialysis. CNT yarns are fabricated with dispersed CNT/C-Dps composites by wet-spinning process. In the presentation, the change in thermoelectric performances and their origins will be discussed.

### **Biography:**

Yongyoon Cho received his B.E and M.E in chemical engineering from Kyoto University, Japan and PhD in School of Photovoltaic and Renewable Energy Engineering from UNSW, Australia. From 2011 to 2016, he was an engineer in Samsung Electro-mechanics. In 2020, he was a JSPS research fellow in the Graduate School of Engineering, Kyoto University, Japan. Afterward, he joined the Material Science in Nara Institute of Science and Technology, Japan in 2021. His research interests include synthesis and characterization of nanomaterial composites using both organic and inorganic materials for photovoltaic and thermoelectric applications.

### **Conductive Carbon Materials for Lithium-sulfur Battery**

### Almagul Mentbayeva<sup>a,b\*</sup>, Fail Sultanov<sup>a</sup>, Sandugash Kalybekkyzy<sup>a,b</sup>, Zhumabay Bakenov<sup>a,b</sup>

<sup>a</sup>Department of Chemical and Materials Engineering, Nazarbayev University, Kabanbay Batyr Ave. 53, Nur-Sultan, Kazakhstan

<sup>b</sup>National Laboratory Astana, Nazarbayev University, Kabanbay Batyr Ave. 53, Nur-Sultan, Kazakhstan

### Abstract:

Lithium-sulfur batteries (LSB) are recognized as the next generation energy storage systems due

to their high theoretical capacity of 1675 mAh g-1 and energy density of 2600 Wh kg-1. However, such disadvantages as low sulfur electrical conductivity, polysulfides shuttle effect and volume expansion are limiting their practical application.

Herein, we report on the light weight carbon nanofibers fabricated by a simple electrospinning method and used as a 3D structured current collector for a sulfur cathode. Along with a light weight, this 3D current collector allowed us to accommodate a higher amount of sulfur composite, which led to a remarkable increase of the electrode capacity from 200 to 500 mAh per 1 g of the electrode including the mass of the current collector.

Also, the advantages of carbonized electrospun, using bio-waste-derived graphene-like porous carbons (GPCs) as a carbon matrix for sulfur immobilization are discussed. GPCs were obtained by carbonization of pre-washed, dried and milled rice husk wastes. The sulfur was immobilized on the formed carbon matrix by melt-diffusion and mechanochemical methods. As a result, the sulfur content in the matrix was 68-70 wt%.

The electrochemical performance was studied by CV, which demonstrated the good reversibility of sulfur reduction and lithium polysulfides oxidation. The initial discharge capacity of the cell was 906 mA h g-1 at 0.1 C. Further research will be focused on the preparation of composite GPCs with various modifiers (MXene, metal oxides) to create the additional sites for chemical adsorption of polysulfides and reduce the shuttle effect.

### **Biography:**

Almagul Mentbayeva is Assistant Professor at the Department of Chemical and Materials Engineering, School of Engineering and Digital Sciences, Nazarbayev University. She received a Ph.D. degree in chemical engineering from Al-Farabi Kazakh National University in 2012. Her Ph.D. thesis was on thin film polyelectrolyte multilayers for catalytical and biomedical application. Then she was working for one year in R&D department of Sika Technology AG developing superplasticizers for chemical admixtures in Switzerland. In 2014 she joined Nazarbayev University. Her research interests focus on advanced materials for energy storage and conversion, self-assembly of macromolecules at surfaces, responsive polymer multilayers.

## **Keynote Session 2**

### **Resonance Raman Spectroscopy in Twisted Bilayer graphene**

Marcos A Pimenta<sup>\*1,</sup> M. V. O. Moutinho<sup>2</sup>, G. S. N. Eliel<sup>3</sup>, A. Righi<sup>1</sup>, R. N. Gontijo<sup>1</sup>, M. Paillet<sup>4</sup>, T. Michel<sup>4</sup>, Po-Wen Chiu<sup>5</sup> and P. Venezuela<sup>5</sup>

<sup>1</sup>Departamento de Fisica, Universidade Federal de Minas Gerais, Belo Horizonte, MG, Brazil <sup>2</sup>NUMPEX-COMP, Campus Duque de Caxias, Universidade Federal do Rio de Janeiro, RJ, Brazil <sup>3</sup>Instituto de Fisica, Universidade Federal da Bahia, Salvador, BA, Brazil <sup>4</sup>Laboratoire Charles Coulomb, CNRS, University of Montpellier, Montpellier 34095, France <sup>5</sup>National Tsing Hua University, Hsinchu 30013, Taiwan <sup>6</sup>Instituto de Fisica, Universidade Federal Fluminense, Niteroi, Rio de Janeiro, Brazil

### Abstract:

Raman spectroscopy is a fundamental tool to study twisted bilayer graphene (TBG) systems since the Raman response is hugely enhanced when the photons are in resonance with transition between vHs and new peaks appear in the Raman spectra due to phonons within the interior of the Brillouin zone of graphene that are activated by the Moire superlattice. These new peaks can be activated by the intralayer and the interlayer electron-phonon processes [1]. In order to study how each one of these processes enhances the intensities of the peaks coming from the acoustic and optical phonon branches of graphene, multiple excitation Raman measurements were performed in many different TBG samples with twisting angles between 4o and 16o and using several different laser excitation energies in the near-infrared (NIR) and visible ranges (1.39 eV to 2.71 eV). Distinct enhancements of the different phonons of graphene were observed for the intralayer and interlayer processes and results are nicely explained by theoretical calculations of the double resonance (DR) Raman intensity in graphene by imposing the momentum conservation rules for the intralayer and the interlayer electron-phonon processes [2]. Our results show that the enhancement of the Raman response in all cases is affected by quantum interference and obey symmetry requirements for the DR Raman process in graphene.

### **Biography:**

Marcos Pimenta works with two of the biggest modern developments in nanoscience: graphene, thin 2-dimensional sheets, and nanotubes, carbon atoms arranged into a minuscule cylinder. Both of these pure carbon substances are extremely hard, excellent conductors of heat, and scientists and engineers often use them to produce electronic devices and new materials. In 1989 he became professor at the Department of Physics of Federal University of Minas Gerais (UFMG) in Belo Horizonte, Brazil. In 1992, he created the Raman Spectroscopy Laboratory at UFMG. He has served in high-level positions for several Brazilian nanoscience organizations and is currently director of the Brazilian Institute for Science and Technology (INCT) of Carbon Nanomaterials. He has won national and international awards, including the 2009 Somiya Award for International al Collaboration from the International Union of Materials Research Societies, for collaborative works with scientists in the United States, Mexico and Japan. In 2010, he received the command of the Brazilian Order of Scientific Merit.

[1] Resonance Raman enhancement by the intralayerand interlayer electron-phonon processes in twisted bilayer graphene, M. V. O. Moutinho, G. S. N. Eliel, A. Righi, R. N. Gontijo, M. Paillet, T. Michel, Po-Wen Chiu, P. Venezuela, and M. A. Pimenta, Scientific Reports, 11, 1, 17206 (2021)

[2] Intralayer and interlayer electron-phonon interactions in twisted graphene heterostructures, G. S. N. Eliel, M. V. O. Moutinho, A. C. Gadelha, A. Righi, L. C. Campos, H. B. Ribeiro, Po-Wen Chiu, K. Watanabe, T. Taniguchi, P. Puech, M. Paillet, T. Michel, P. Venezuela, and M. A. Pimenta, Nature Communications 9, 1221 (2018)

## **Oral Session 2**

Carbon Nano-onions: Fundamental Insights into Their Potassium Intercalation, Functionalization and Statistical Characterization

Eugenia Pérez-Ojeda<sup>1\*</sup>, Edison Castro<sup>2</sup>, Claudia Kröckel<sup>3</sup>, Matteo Andrea Lucherelli<sup>4</sup>, Ursula Ludacka<sup>5</sup>, Jani Kotakoski<sup>5</sup>, Katharina Werbach<sup>5</sup>, Herwig Peterlik<sup>5</sup>, Manuel Melle-Franco<sup>6</sup>, Julio C. Chacón-Torres<sup>7</sup>, Frank Hauke<sup>3</sup>, Luis Echegoyen<sup>2</sup>, Andreas Hirsch<sup>1,3</sup>, and Gonzalo Abellán<sup>4</sup>

<sup>1</sup>Department of Chemistry and Pharmacy, Chair of Organic Chemistry II, Friedrich-Alexander University of Erlangen-Nürnberg, Germany.

<sup>2</sup>Department of Chemistry, University of Texas at El Paso, USA.

<sup>3</sup>Joint Institute of Advanced Materials and Processes (ZMP), Friedrich-Alexander University of Erlangen-Nürnberg, Germany.

<sup>4</sup>Instituto de Ciencia Molecular, Universidad de Valencia, Spain.

<sup>5</sup>Faculty of Physics, University of Vienna, Austria.

<sup>6</sup>CICECO-Aveiro Institute of Materials, University of Aveiro, Portugal.

<sup>7</sup>School of Physical Sciences and Nanotechnology, Yachay Tech University, Ecuador.

### Abstract:

Carbon nano-onions (CNOs) exhibit outstanding properties such as large surface area to volume ratio, low densities and a graphitic multilayer morphology which makes them excellent candidates for many applications. Different synthetic procedures for CNO functionalization have been investigated [1]; however, the benchmark reductive route using intercalation compounds [2] which is probably one of the most efficient strategies for other carbon allotropes such as graphene and CNTs, has not been explored.

Herein we report the synthesis of covalently functionalized CNO via reductive route using intercalation compounds, in particular KC8.[4] For the first time, an in situ Raman study of the controlled intercalation process with potassium has been carried out, revealing a Fano resonance formation. The intercalation was further confirmed by transmission electron microscopy (TEM) electron energy loss spectroscopy and X-ray diffraction. We have used the negatively charged K doped-CNOs for their covalent functionalization in model nucleophilic substitution reactions. The functionalized CNOs were exhaustively characterized by statistical Raman spectroscopy (SRS), thermogravimetric analysis coupled with gas chromatography and mass spectrometry (TGA/GC/MS), dynamic light scattering (DLS), UV-vis and FTIR-ATR spectroscopy. Differently from classic organic materials, the characterization of CNOs requires a cross-correlated analysis with several techniques to prove the functionalization, special significance have on this regard the statistical approach employing SRS.

Scheme 1: Synthesis of K- intercalated CNOs

### **Biography:**

Pérez-Ojeda is junior group leader at Friedrich Alexander Universität Erlangen-Nürnberg (FAU), Germany. Her research being "Caging Carbon: Intercallation of Nanoonions and Supramolecu-

lar encapsulation of synthetic carbon allotropes". She graduated in Chemistry in 2008 at Complutense University of Madrid (Spain). After a Master degree in Polymer Science at the Spanish Research Council (CSIC), she obtained her PhD in 2014 with "Sobresaliente cum Laude" at Complutense-CSIC, which was granted three awards. Later, she joined FAU with a Marie-Curie fellowship. In 2019, she received the Emerging Talent Initiative and Renate-Wittern-Sterzel-Preise. Since 2020, she is PI at the DFG collaborative research center SFB-953-A9.

### Production of Metal/Metal Oxide Decorated Carbon Nanotubes-based Inks for Application as Printable Gas Sensors on Industrial Work Clothes.

### Rubia Young Sun Zampiva<sup>1</sup>, Marco Rossi<sup>1</sup>

<sup>1</sup>Department of Basic and Applied Sciences for Engineering (SBAI) - Sapienza University of Rome, Italy

### Abstract:

Portable and stationary gas detection systems find applications in all industrial fields. In general, industrial processes require the use and processing of large quantities of hazardous substances, such as toxic and flammable gases. Therefore, occasional gas leaking is inevitable, which can put at risk the plant, the workers and the population living nearby. Accidents in confined places occur essentially due to the lack of personal protective equipment (PPE) such as gas sensors that allow workers to avoid exposure to the risk in time. Currently used gas sensing devices are rather bulky and expensive, not sufficiently precise and with a tendency to saturate. Based on that, it is evident the importance of developing suitable technological solutions to integrate efficient sensors into easy-to-use miniaturized devices. In this context, carbon nanotubes (CNTs) can represent an effective solution thanks to their high surface area, electrical and mechanical properties, and their ability to detect gas molecules even at very low concentrations when combined with metal/metal oxide particles. In this work, CNTs were decorated with different nanoparticles (MD-CNTs) and water based printable inks were produced to directly print small, flexible, and lightweight sensor devices on work clothes. The main goal is the development of highly sensitive gas sensors for industrial application as PPE. Emphasis was placed on the production of MD-CNTs and their printing parameters, on their chemical and structural characterization and on the relationship between the different compositions of the structures and the signal detected in the presence of specific gases.

### **Biography:**

Rubia Zampiva has been working for the last 2 years as a researcher at Sapienza University of Rome – Italy, in the department of Basic and Applied Sciences for Engineering (SBAI). She is a chemist with a master's and a PhD degree in materials engineering from Federal University of Rio Grande do Sul - Brazil and University of California Davis – USA (sandwich PhD). She has experience on ceramic nanomaterials, CVD and wet chemical synthesis, optical systems and she is currently working on gas sensors based on nanomaterials.

## Fullerene/Nanocellulose Hybrid Materials: 2D-assemblies and (Photo) Electrochemical Properties

Livia Giotta<sup>1\*</sup>, Shadi Sawalha<sup>2</sup>, Francesco Milano<sup>3</sup>, Maria R. Guascito<sup>1</sup>, Paola Semeraro1,

### Simona Bettini<sup>1</sup>, Tatiana Da Ros<sup>4</sup>, Maurizio Prato<sup>4,5</sup>, Alessandra Operamolla<sup>6</sup> Ludovico Valli<sup>1</sup>

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<sup>2</sup>Department of Chemical Engineering, An-Najah National University, P.O. Box 7, Nablus, Palestine

<sup>3</sup>Istituto di Scienze delle Produzioni Alimentari (ISPA), Consiglio Nazionale delle Ricerche (CNR), S.P. Lecce-Monteroni, I-73100, Lecce, Italy

<sup>4</sup>Center of Excellence for Nanostructured Materials (CENMAT) and INSTM, Unit of Trieste, Dipartimento di Scienze Chimiche e Farmaceutiche, Università di Trieste, via Giorgieri 1, 34127 Trieste, Italy

<sup>5</sup>Center for Cooperative Research in Biomaterials (CIC biomaGUNE), Basque Research and Technology Alliance (BRTA), Paseo de Miramón 182, 20014 Donostia San Sebastián, Spain

<sup>6</sup>Dipartimento di Chimica e Chimica Industriale, Università di Pisa, Via Giuseppe Moruzzi 13, 56124 Pisa, Italy

### Abstract:

Due to outstanding electron acceptor properties, fullerenes are suitable candidates for several applications in the field of electronics and optoelectronics. Their organization in 2D-ordered films has been extensively investigated, aiming at the development of advanced functional materials. However, wet processing may be detrimental for the 2D organization of C60-based materials, owing to the high hydrophobic character of the fullerene cages that tend to crystallize into large aggregates, compromising the electrochemical behavior and the photo-response of the active layers. On the other side, nanocelluloses have shown high potentialities as dispersing agents for carbon nano-allotropes, such as fullerenes, nanotubes and graphene. Moreover, being polyelectrolytes, sulphated cellulose nanocrystals (CNCs) are amenable to sequential film growth by layer-by-layer technique, suggesting their suitability for the assembly of 2D architectures in association with cationic fullerene derivatives. We have assessed the ability of anionic CNCs to assist the two-dimensional organization of cationic fulleropyrrolidines (FPs) at the air/water interface, leading to hybrid FP/CNC floating films, successfully transferred onto electrode surfaces by Langmuir-Schäfer (LS) technique. Interestingly, the electrochemical characterization of FP/CNC LS films revealed that nanocellulose strongly improves the electrical properties of organized fullerene layers, by increasing their conductivity and favoring the hydrogen evolution reaction. Moreover, the well-established C60 photoactivity proved to be enhanced by CNCs, as demonstrated by the higher intensity of both cathodic and anodic photocurrents. This outstanding impact of CNCs on fullerene properties paves the way to the development of more performing C60-based electrochemical devices, able to better exploit the unique properties of carbon nanostructures.

### **Biography:**

Livia Giotta, chemist (M.Sc. 1999), Ph.D. in chemical sciences (2004), researcher and lecturer in physical chemistry at the University of Salento, Department of Biological and Environmental Sciences and Technologies. During her career she has been dealing with different research fields, boosting her skills in various physico-chemical techniques to assemble 2D and 3D (bio)nanomaterials and to investigate their bulk and surface properties, as well as processes occurring at the interface between materials surface and aqueous media. In recent years she has been working on bio-based active layers for applications in sensing and photovoltaics and on all-organic 2D materials for photo-electrocatalysis.

### **Electronic and Transport Properties of Suspended Porphine-GNRs and SWNTs**

### Aldilene Saraiva-Souza<sup>1\*</sup>, Vincent Michaud-Rioux<sup>1</sup>, Chen Hu<sup>2</sup>, and Hong Guo<sup>1,2</sup>

<sup>1</sup>Nanoacademic, 666 Rue Sherbrooke O Suite 802, Montréal, QC, Canada, H3A 1E7

<sup>2</sup>Center for the Physics of Materials and Department of Physics, McGill University, Montreal, Quebec H3A 2T8, Canada.

### Abstract:

The ability to control and manipulate the charge and spin transport properties in nanostructures has been hotly pursued by chemists, physicists, and materials engineers. In fact, the ability to reversibly turn "on/off" the electronic current through a nanoscale device is one of the most important and challenging tasks in the field of nanotechnology. Carbon-based materials with strong spin-orbit interactions are especially attractive in this sense as they can be tailored to generate spin/valley-polarized currents. Furthermore, promising results were found in this area when molecular properties were combined with spintronic properties of low-dimensional carbon structures. In this talk, I shall discuss how destructive quantum interference can be used to control spin-polarized quantum transmission at the molecular level, using a porphine molecule attached via different  $\beta$ - and meso- connections to the zigzag graphene nanoribbons (zGRN). We found that this molecular device has inherent spin-polarization along the edges and the hybridization between porphine and 6zGNR disturbs the bipartite graphene lattice, leading to spin-frustration. Moreover, we will discuss the electronic properties of a topological effect on single-walled carbon nanotubes (SWNTs) structures. In previous work, the general-purpose KS-DFT solver RESCU was used to study the electronic structure of such heteronanotubes, hinting they could be used as a platform for realizing topological low-dissipation CNT-based nanoelectronics. We will show via quantum transport calculations realized with NanoDCAL+, which employs the nonequilibrium Keldysh Green's function (NEGF) formalism in combination with DFT, whether this holds true now taking contacts into account in a suspended geometry.

### **Biography:**

C. Hu, V. Michaud-Rioux, W. Yao, H. Guo. Theoretical Design of Topological Heteronanotubes. Nano Lett. 19 (2019), pp. 4146–4150. A. Saraiva-Souza, M. Smeu, J. G.da Silva Filho, E. C. Girão, and Hong Guo. Spin-Negative Differential Resistance in Zigzag Graphene Nanoribbons with Side-Attached Porphine Molecule. : J. Phys. Chem. C 122 (2018), pp. 15911–15921.

### Structure and Properties of Periodic Porous Architectures Prepared by 3D Printing

Alain Celzard<sup>1\*</sup>, Alexander Zharov<sup>1</sup>, Pauline Blyweert<sup>1</sup>, Dzimtry Bychanok<sup>2</sup>, Jan Macutkevic<sup>3</sup>, Polina Kuzhir<sup>4</sup>, Vanessa Fierro<sup>1</sup>

<sup>1</sup>Institut Jean Lamour, UMR 7198 CNRS and Université de Lorraine, Épinal, France

<sup>2</sup>Institute for Nuclear Problems, Belarusian State University, Minsk, Belarus

<sup>3</sup>Faculty of Physics, Radiophysics Department, Vilnius University, Vilnius, Lithuania

<sup>4</sup>Institute of Photonics, Department of Physics and mathematics, University of Eastern Finland, Joensuu, Finland

### Abstract:

The issue of 3D printing of resins to convert them into glassy carbon will be discussed, using different techniques depending on the nature of the precursor resins. The result is periodic 3D architectures (Fig. 1) or arrays of hollow spheres (Fig. 2) whose physical properties are studied. These architectures, associated with different electrical conductivities, depending on the nature of the carbon produced and its heat-treatment temperature, make it possible to obtain authentic photonic crystals in the microwave range. Perfect resonant or broadband absorptions can thus be obtained, depending on the desired application. Figure 1: Periodic 3D carbon architectures produced by SLA (left and center) or FDM (right), based on Gibson-Ashby (left and right) or Kelvin (center) cells. Figure 2: Hollow carbon spheres: of the same diameter (0.8 - 1 mm) and different conductivities (from  $3.5 \times 10-6$  to  $15 \times 103$  S/m) on the one hand (left), and of different diameters (5, 4, 3, 2, 1 and 0.8 mm) but the same conductivity (125 S/m) on the other hand (right) The presentation will end with a few avenues of improvement for these carbonaceous structures, whether it is to optimize the formulation of the precursor resins, to increase the carbon yield and the mechanical properties, or to better target the resulting electromagnetic properties.

### **Biography:**

Alain Celzard develops a global approach to the study of materials for energy, environmental and electromagnetic applications: synthesis, characterization, properties, modeling and integration. He also conducts fundamental research on complex, disordered and/or porous heterogeneous systems, including their optimization for various applications. This work has allowed him to coauthor about 400 publications and book chapters and 9 patents, and has earned him the title of junior member of the Institut Universitaire de France, as well as 3 national prizes including 2 first prizes, and 2 international prizes. He is now director of a joint laboratory with a major producer of activated carbons and biochars.

### Carbon, a Key Piece to Positioning Hydrogen in the Energy Transition

### Vanessa Fierro\* and Alain Celzard

Université de Lorraine, CNRS, IJL, 88000 Epinal, France

### Abstract:

Hydrogen is an energy carrier that provides new solutions, complementary to the control of energy consumption and the development of renewable sources, such as electricity storage, energy network management or greener mobility. Hydrogen, rarely present in gaseous form, must be produced, stored and transported, and finally transformed into electricity to power an engine or any other electrical use using a hydrogen fuel cell. In all these steps, carbon plays an essential role since it can be used as (i) electrode material in low temperature electrolyzers to produce hydrogen; (ii) adsorbent for storage by adsorption under cryogenic conditions; (iii) adsorbent for hydrogen gen fuel cells. In this talk, a particular emphasis will be put on carbon for hydrogen storage and compression.

### **Biography:**

Vanessa FIERRO is a CNRS Research Professor and a member of one of the technical groups of

the Research Fund for Coal and Steel (RFCS). She currently works at the Jean Lamour Institute (France), a joint University of Lorraine-CNRS laboratory, where she leads the research team on bio-sourced materials. Vanessa has over 330 scientific publications, an h-index of 62 and extensive experience in the field of porous carbon materials for energy and environmental applications. She received the Charles E. Pettinos Prize from the American Carbon Society in 2019 and the CNRS Silver Medal in 2020.

# Attempts to Enhance Surface Area and Graphitization Degree of Activated Carbon from Biomass Waste

### Ratna Frida Susanti\*

Chemical Engineering Department of Parahyangan Catholic University, Ciumbuleuit 94, Bandung, West Java, Indonesia

### **Abstract:**

Activated carbon has gained its popularity in energy storage application as an electrode for supercapacitor and hybrid capacitor. It is cheap, abundant, high carbon content, large surface area, unique pore characteristics and high oxygen functional group. However, its properties are highly depending on its precursor and synthesize methods. In order to control its properties, several methods have been attempted to modify the properties of activated carbon. This is including variation of the synthesize method, used of various activating agent, heteroatom doping, utilization of carbonization catalyst and graphitization.

In this talk, we highlight the effect of hydrothermal carbonization condition (catalyst, temperature, doping) and graphitization into the properties of activated carbon. Produced carbons were characterized by BET, SEM-EDX, XRD, Raman and FTIR to investigate its properties. Thus, biomass waste derived activated carbon could meet the criteria of carbon used in energy storage application. In addition, the environment problem due to those waste could be solved properly.

### **Biography:**

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

# Insights into Electronic Structure and Transport in Single Wall Carbon Nanotube-single Layer Graphene Hybrid Nanostructures

### Anshu Gaur<sup>\*</sup> and Juhi Srivastava

Materials Science and Engineering, and Samtel Centre for Display Technologies Indian Institute of Technology Kanpur, Uttar Pradesh, India

### Abstract:

Allotropes of sp2 hybridized carbon in form of 1D – single wall carbon nanotubes (SWCNT), and 2D – single layer graphene (SLG) are interesting prototypes for studying physics of lowdimensional nanostructures. Hybrid structures of SWNTs and SLGs are also being investigated for potential technological applications. In this work, we have focused on fundamental understanding of electronic structure and transport through hybrid nanostructures of SWCNT and SLG using atomistic simulations using tight-binding density functional method (DFTB) and non-equilibrium Green's function (NEGF) approach. Our calculations show that the electronic structure of the hybrid nanostructure is modified due to interactions between atoms of SWCNT and SLG. The modification in the band structure is strongly dependent on the separation between SWCNT and SLG and the relative placement of electronic bands in E-k space and inturn affects the electronic transport through these hybrid nanostructures. In this work we present the correlation between modifications in electronic structure and electronic transport with increasing interaction between components. We will also discuss the effect of screening of transverse (gate) field by components in hybrid nanostructures in an external electric field.

### **Biography:**

Anshu Gaur is an associate professor in the department of Materials Science and Engineering at Indian Institute of Kanpur, India. Hs research interests includes carbon nanostructures, amorphous semiconductors, device physics, and computational materials science.

### Mass and Microporosity Contribution of Hemicellulose, Cellulose and Lignin in Activated Carbons Made from Agricultural Residues by Chemical Activation

### Paixan Samba<sup>1</sup>, Stéphanie de Persis<sup>2</sup>, Pauline Sidoli<sup>3</sup>, Benoît Cagnon<sup>1\*</sup>

<sup>1</sup>ICMN (Interfaces Confinement Matériaux Nanostructures) – CNRS (UMR 7374) - Université d'Orléans, France

<sup>2</sup>ICARE (Institut de Combustion Aérothermique Réactivité et Environnement) – CNRS (UPR 3021), France

<sup>3</sup>BRGM Orléans, France.

### Abstract:

The control of the activation yield and of the activated carbon porous texture requires the control of each stage of the activation procedure and the knowledge of the raw lignocellulosic materials composition. In the case of chemical activation, the economic and environmental constraints force to decrease as well as possible the quantities of activating agent, of energy and waters used. This can be carried out by optimizing the thermal treatment. The study of the lignocellulosic residues requires the knowledge of the raw material (chemical composition, elemental analyses...). The study of the experimental parameters is not sufficient to control pyrolysis as well as the final solid material obtained after the heat treatment. The objective of the study is to optimize the heat treatment of chemical activation procedure by H3PO4 of lignocellulosic precursors (rape straw and sunflower husks). The contents of hemicelluloses (H.), cellulose (C.), and lignin (L.) were determined for each sample. The TGA analyses of the heat treatment with and without the activating agent were carried out on all the lignocellulosic precursors and on the three pure compounds (H.,
C., L.) to estimate their respective contribution in the final mass of the char and of the activated carbons to establish the predictive calculation. The predictive calculation was established using the experimental results to evaluate the heat treatment yields with and without the activating agent and the respective contributions of H., C., L. to the chars and to the activated carbons in term of weight fraction.

#### **Biography:**

Benoît Cagnon is associate professor in Chemical Engineering Process at the University of Orleans. He works at the Laboratory ICMN (Interfaces, Confinement, Materials and Nanostructures – UMR 7374 CNRS) on the adsorption process in liquid phase and on the study of different Advanced Oxidation Processes to the removal and the mineralization of organic pollutants. He also works on the elaboration of activated carbons from biomass and tries to control the textural and the chemical properties of the adsorbents obtained. He is author of 49 publications, 2 book chapters and more than 100 conference proceedings.

#### Resolving the Structural and Electronic Properties of Graphene/Ge(110)

Luca Persichetti<sup>1,2\*</sup>, M. Galbiati<sup>3</sup>, L. Di Gaspare<sup>2</sup>, I. Pis<sup>4</sup>, F. Bondino<sup>4</sup>, V.-P. Veigang-Radulescu<sup>5</sup>, S. Hofmann<sup>5</sup>, P. Gori<sup>6</sup>, O. Pulci<sup>1</sup>, M. Bianchi<sup>7</sup>, J. Tersoff<sup>8</sup>, P. Hofmann<sup>7</sup>, M. De Seta<sup>2</sup>, L. Camilli<sup>1</sup>

<sup>1</sup>Department of Physics, Università di Roma "Tor Vergata", 00133 Rome, Italy;

<sup>2</sup>Department of Sciences, Roma Tre University, 00146 Rome, Italy

<sup>3</sup>Department of Physics, Technical University of Denmark, 2800 Kgs. Lyngby, Denmark

<sup>4</sup>IOM-CNR Laboratorio TASC Trieste I-34149, Italy

<sup>5</sup>Department of Engineering, University of Cambridge, Cambridge CB3 0FA, United Kingdom

<sup>6</sup>Department of Engineering, Roma Tre University, 00146 Rome, Italy

<sup>7</sup>Department of Physics and Astronomy, Aarhus University, 8000 Aarhus, Denmark; 8IBM Research Division, T.J. Watson Research Center, Yorktown Heights, 10598, USA

#### **Abstract:**

Investigating the interfacial properties between graphene and traditional semiconductors is crucial to develop novel electronic. In this framework, the Graphene/Ge(110) has recently received a great deal of attention [1]. However, no insights into the electronic properties of this interesting system are today available. Here, we investigate the evolution of the system's interface upon annealing in vacuum at different temperatures [2]. We use low-temperature STM to probe the surface structure with atomic precision. At each stage, images at different applied biases are collected and interestingly, graphene becomes transparent at high biases. When growing graphene by chemical vapour deposition, hydrogen that is used during growth passivates the Ge surface, stabilizes the (1x1) phase (i.e., unreconstructed surface). Annealing the sample at 350°C leads to desorption of hydrogen and STM and low energy electron diffraction (LEED) reveal that the surface of Ge(110) reconstructs into a (6x2) phase, never observed for bare Ge. Upon further annealing above 700°C, STM shows that the Ge surface modifies forming a different surface reconstruction with a symmetry close to the bulk truncated surface. To gain insights into the electronic properties, we perform angle resolved photoemission spectroscopy (ARPES) after each thermal annealing step. The ARPES data show how graphene's doping changes upon thermal annealing, signature of a different interaction with the Ge substrate. Data obtained by ARPES are correlated to Raman, x-Ray Photoelectron Spectroscopy and Near Edge x-ray Absorption Fine Structure Spectroscopy.

[1] J. Lee et al., Science, 344(2014).

[2] L. Persichetti, et al Appl. Surf. Science 499(2020).

#### **Biography:**

I have a Master in Material Science and Technology and a PhD in Physics obtained from the University of Roma "Tor Vergata" in November 2012. Since my PhD, my research activity has been focused on the investigation of surface systems/phenomena in ultra-high vacuum conditions using microscopy and spectroscopy techniques, in particular scanning probe microscopies and x-ray absorption and photoelectron spectroscopies. I was a postdoc at the Swiss Federal Institute of Technology ETH-Zurich from 2013 to 2018, being funded in part by Marie Curie Actions COFUND program. I am currently assistant professor at the Department of Physics of "Tor Vergata".

# Study of Isothermal Spin State Switching in Spin Crossover Molecular Thin Film

#### Ruihua Cheng\* and Saeed Yazdani

Department of Physics, Indiana University Purdue University Indianapolis (IUPUI), Indianapolis, IN 46202, USA Presenter

#### Abstract:

Using spectroscopy characterization, it is evident that the spin state of the spin crossover molecular complex [Fe{H2B(pz)2}2(bipy)] (pz = tris (pyrazol-1-1y)-borohydride, bipy = 2,2'-bipyridine) depends on the ferroelectric polarization of an adjacent thin film of the polymer ferroelectric polyvinylidene fluoride-hexafluoropropylene (PVDF-HFP). The UV-Vis spectroscopy reveals that room temperature switching of [Fe{H2B(pz)2}2(bipy)] molecules in bilayers of PVDF-HFP/[Fe{H-2B(pz)2}2(bipy)] as a function of ferroelectric polarization. The electric polarity dependence of bilayers of PVDF-HFP/[Fe{H2B(pz)2}2(bipy)] shows a strong dependence on the thickness of the PVDF-HFP layer. The PVDF-HFP/[Fe{H2B(pz)2}2(bipy)] interface may affect polarization retention in the PVDF-HFP thin film limit.

#### **Biography:**

Ruihua Cheng is currently working at the Department of Physics of Indiana University-Purdue University-Indianapolis (IUPUI) as an associate professor. She received her Ph.D in Physics at University of Nebraska-Lincoln in 2002. Then she conducted her postdoctoral research in the magnetic thin film group of materials science division at Argonne National Laboratory. In 2005, she joined the Department of Physics at IUPUI. Her current research is focused on molecular magnetic materials characterization, particularly spin crossover molecular manipulation and their applications in molecular based devices.

# Accelerating the Prediction of Large Carbon Clusters *via* Structure Search: Evaluation of Machine-learning and Classical Potentials

#### Bora Karasulu<sup>1\*</sup>

Department of Chemistry, University of Warwick, United Kingdom

#### Abstract:

From as small as single carbon dimers up to giant fullerenes or amorphous nanometer sized particles, the large family of carbon nanoclusters holds a complex structural variability that increases with cluster size. Capturing this variability and predicting stable allotropes remains a challenging modelling task, crucial to advance technological applications of these materials. While small cluster sizes are traditionally investigated with first principles methods, a comprehensive study spanning larger sizes calls for a computationally efficient alternative.

Here, we combine the stochastic ab initio random structure search algorithm (AIRSS) with geometry optimisations based on interatomic potentials to systematically predict the structure of carbon clusters spanning a wide range of sizes. We first test the transferability and predictive capability of seven widely used carbon potentials, including classical and machine-learning potentials. Results are compared against an analogous dataset generated via AIRSS combined with density functional theory optimizations. The best performing potential, GAP-20, is then employed to predict larger clusters, overcoming the computational limits of first principles approaches. Our datasets describe the evolution of topological properties with cluster size, capturing the complex variability of the carbon cluster family. As such, the dataset includes ordered and disordered structures, reproducing well-known clusters, like fullerenes, and predicting novel isomers.

#### **Biography:**

Bora Karasulu is an Assistant Professor and an EPSRC Early-Career Fellow at the Department of Chemistry, University of Warwick (United Kingdom). He is an expert in computational solid-state chemistry and physics and materials science. His current research focuses on the ab initio material design for the next-generation all-solid-state batteries and supercapacitors towards sustainable energy technologies. Dr. Karasulu received his PhD degree in theoretical chemistry/biochemistry from the Max-Planck-Institute for Carbon Research (Muelheim-Ruhr, Germany). Following his PhD, he worked as a post-doctoral researcher at Eindhoven University of Technology (TU/e, the Netherlands) and the University of Cambridge (UK).

# Synthesis, Functionalization and Assembly of Carbon Nanomaterials into 1D, 2D and 3D Structures

#### **Rina Tannenbaum\***

Stony Brook University, USA

#### Abstract:

Carbon nanomaterials (CNMs) are emerging as materials of interest in energy-related and biomedical applications. In particular, the surface decoration and functionalization of such CNMs with a variety of organic or metallic reactive moieties may impart new properties or provide enhancement of existing properties. Moreover, these surface modifications may facilitate the assembly of powerful signal enhancement in several tissue imaging techniques. Graphene oxide based CNMs (GO-CNMs) possess notable geometrical variants, such as flat sheets, tubes, scrolls and spheres, and form stable and easilyprocessable aqueous solutions. Furthermore, the presence of oxygen containing functional surface groups in GO-CNMs provide potential locations for attachment of drugs, disease targeting groups as well as decoration with metal nanoparticles, making them viable theranostics platforms. We synthesized mesoscale crumpled graphene oxide roses (GO roses) by using colloidal graphene oxide (GO) variants as precursors for a hybrid emulsification/rapid evaporation approach. This process produced 3D rose-like, spherical, reduced mesostructures of colloidal graphene oxide, with corrugated surfaces. This synthesized GO roses. We investigated the morphology and chemical properties of the synthesized GO roses and studied the possible applications of these synthesized mesostructures, together with their 1D and 2D counterparts, as potential theranostics platforms for cancer remediation as MRI contrast, tissue delineation and drug delivery agents.

#### **Biography:**

Tannenbaum received her B.Sc. in chemistry and physics from the Hebrew University, her M.Sc. in physical chemistry from the Weizmann Institute of Science and her D.Sc. in chemical engineering from the Swiss Federal Institute of Technology in Zürich. Dr. Tannenbaum is currently a full professor in the Department of Materials Science and Chemical Engineering, a member of the Stony Brook Cancer Center and a member of the Institute of Gas Innovation and Technology at Stony Brook University in New York. To date she has published over 200 peer-reviewed articles, reviews and conference proceedings. She is the recipient of numerous and a member of the editorial board of several professional journals. Dr. Tannenbaum's areas of interest are soft matter and complex fluids, bio-based functional materials, carbon nanostructures, nanocomposites from renewable resources, plastics recycling and catalysis.

#### Evidence for Flat Band Dirac Superfluid Originating from Quantum Geometry

Marc Bockrath<sup>1\*</sup>, Haidong Tian<sup>1</sup>, Shi Che<sup>1</sup>, Tianyi Xu<sup>2</sup>, Patrick Cheung<sup>2</sup>, Kenji Watanabe<sup>3</sup>, Takashi Taniguchi<sup>4</sup>, Mohit Randeria<sup>1</sup>, Fan Zhang<sup>2</sup>, Chun Ning Lau<sup>1</sup>

<sup>1</sup>Department of Physics, The Ohio State University, Columbus, OH 43221.

<sup>2</sup>Department of Physics, The University of Texas at Dallas, 800 West Campbell Road, Richardson, Texas 75080-3021, USA

<sup>3</sup>Research Center for Functional Materials, National Institute for Materials Science, 1-1 Namiki, Tsukuba 305-0044, Japan

<sup>4</sup>International Center for Materials Nano architectonics, National Institute for Materials Science, 1-1 Namiki, Tsukuba 305-0044, Japan

#### Abstract:

The group velocity vF of the electrons in a flat band superconductor is extremely slow, resulting in quenched kinetic energy. Superconductivity thus appears impossible, as conventional BCS theory implies a vanishing superfluid stiffness, coherence length, and critical current. Using twisted bilayer graphene (tBLG), we explore the profound effect very small vF in a superconducting Dirac flat band system. Non-linear transport studies, we measure vF via the Schwinger effect, yielding an extremely slow vF ~ 1000 m/s for filling fraction n between -1/2 and -3/4 of the moiré miniband. This same velocity yields a new limiting mechanism for the superconducting critical current, with analogies to a relativistic superfluid. We estimate the superfluid stiffness, which determines the electrodynamic response of the superconductor, showing that it is not dominated by the kinetic energy, but by the interaction-driven superconducting gap, consistent with recent theories on quantum geometric contributions. We study the BCS to Bose-Einstein condensation (BEC) cross-over via coherence length measurements, finding an unprecedented ratio of the superconducting transition temperature to the Fermi temperature exceeding unity, illustrating how this can arise for very strong coupling superconductivity in ultra-flat Dirac bands.

### **Biography:**

Bockrath received his PhD from UC Berkeley in 1999, then after a postdoc at Harvard moved to Caltech as an assistant professor in 2002. In 2010, he moved to UC Riverside and is currently at Ohio State University. Bockrath's research interests include nanoscale transport phenomena, nanomechanics, and low-dimensional materials. He has published over 80 works in these areas.

# Nanostructure Characterization and Thermal Stability of Ultrathin Films of Amorphous Carbon Synthesized by Filtered Cathodic Arc and Their Applicability as Protective Overcoats in Heat-assisted Magnetic Recording

#### Kyriakos Komvopoulos\*

Department of Mechanical Engineering, University of California, Berkeley, CA 94720, USA

#### Abstract:

Constantly growing demands for ultrathin (a few nanometers thick) amorphous carbon (a-C) films as protective overcoats in various emerging technologies, such as computer storage devices, microelectronics, microdynamic systems, and photonics, have increased the importance of their thermomechanical properties and structural stability. Nevertheless, the profound decrease of the film thickness raises a concern about the quality and protective capability of these films, especially for devices operating under elevated temperature conditions, such as the hard-disk drives of the emerging data storage technology known as heat-assisted magnetic recording. In general, a-C films with higher sp3 atomic carbon hybridization demonstrate higher density, better mechanical, tribological and corrosion properties, and increased structural stability. There is strong dependence of the sp2 and sp3 contents on the film growth conditions. Compared to deposition methods that use neutral carbon atoms as film-forming precursors, filtered cathodic arc (FCA), the prime method for depositing sub-5-nm thick a-C films, uses energetic ions as film precursors, which is advantageous for depositing ultrathin and perfectly smooth films with superior nanomechanical properties and good thermal stability. This presentation will elucidate the effects of important FCA process parameters, such as the substrate bias voltage that controls the ion energy, on the nanostructure and thermal stability of ultrathin a-C films in the context of microanalysis results and molecular dynamics simulations.

#### **Biography:**

Kyriakos Komvopoulos is Distinguished Professor in the Department of Mechanical Engineering at the University of California, Berkeley. He is also the founder and director of the Surface Sciences

and Engineering Laboratory and the Computational Surface Mechanics Laboratory, and holds the positions of Faculty Scientist, Materials Sciences Division, Lawrence Berkeley National Laboratory, Principal Investigator, Center for Information Technology in the Interest of Society, and Principal Investigator, The Berkeley Stem Cell Center. Professor Komvopoulos is internationally known for pioneering research in surface nanosciences and nanoengineering, with important implications in several emerging technologies including communications, microelectronics, information storage, and biotechnology.

# Kinetic Modelling of Hydrothermal Carbonization of Tea Processing Waste

#### **Basar Caglar\***

\*Izmir Institute of Technology, Turkey

#### Abstract:

Hydrothermal carbonization process (HTC) is recognized as an important technology to be deployed in the future for the treatment of lignocellulosic biomass, as well as biomass waste and residues, in relation to the interesting properties of the reaction products in the gas phase (syngas), the solid phase (biochar) and the liquid phase (VOC, furfural derivatives). Kinetic modelling studies on HTC are scarce in the literature and there is no a clear definition of reaction mechanism due to the formation of multitude intermediates and the complexity of chemistry. In this study, we propose a lumped reaction networks for kinetic modelling of HTC of tea processing waste in which it is converted into char and gaseous products in 5 steps: (1) The formation of liquid products via hydrolysis, (2) Gaseous products formation, (3) Char formation via dehydration and decarboxylation, (4) Decomposition of liquid intermedediates to CO and CO2 via decarbonylation and decarboxylation, (5) Secondary char formation via polymerization and condensation. The first 4 reactions were considered as first order reactions while the order of reaction 5 involving secondary char formation was determined by fitting experimental and model results. The kinetic equations will be solved numerically using Runge-Kutta method allowing to estimate the kinetics parameters (pre-exponential factor (k) and reaction order (n)) on the basis of experimental data. The effect of process parameters (temperature, reaction time, biomass composition, the type of catalyst, water/ biomass/catalyst ratio) on the char and gas yield was determined and an optimum conditions were formulated based on model results.

#### **Biography:**

Basar Caglar is an experienced researcher working in the fields of reaction engineering, catalysis, surface science, spectroscopy and electrochemistry. His research mainly focuses on the development of sustainable energy solutions in energy-chemistry nexus. His current research interests are thermochemical and electrochemical conversion technologies, energy storage systems, energy systems modelling and performance evaluations. He received his doctorate degree from Eindhoven University of Technology (Netherlands) in 2014 and then he continued his studies in both academia and industry in different disciplines. Dr. Caglar is a reviewer for several journals listed in ISI-Web of Science and an expert evaluator for H2020 calls.

# Adsorption of Rhodamine B and Congo Red dyes on Bioadsorbent: Carpobrotus Edulis Plant (HCI-treated and NaOH-treated)

# Abdelkader Dabagh<sup>\*</sup>, Ridouan Benhiti<sup>\*</sup>, M'hamed Abali, Abdeljalil Ait Ichou, Fouad Sinan, Mohamed Zerbet

Laboratory LACAPE, Faculty of Science, Ibn Zohr University, BP. 8106, Hay Dakhla, Agadir, Morocco

# Abstract:

This study assesses the ability of low-cost adsorbents made from waste of Carpobrutus edulis plant treated with HCI (HMCE) and its NaOH-treated analog (NMCE) for the removal of two dyes Rhodamine B (RB) and Congo Red (CR) from aqueous solutions. The adsorbent was characterized by SS, SEM, EDX, FT-IR, pHZ, COD, and BOD5. The adsorption of dye onto the adsorbents was studied as a function of adsorbent dose (0.08-1 g), contact time (up to 180 min), pH solution (2-10), initial concentration (20-1000 mg/L), ionic strength of salt NaCl (0.05-0.5 M), and temperature (25, 30, and 35 °C). The influence of these parameters on adsorption capacity was studied using the batch process. The pretreatment of the C.edulis plant significantly reduces the amount of soluble organic matter released into the aqueous solution by the biomaterial. The kinetic data revealed that adsorption of tow dyes onto the adsorbents closely follows the pseudo-second-order kinetic model. The results show that the data correlated well with the Langmuir isotherm. The maximum adsorption capacities of RB and CR onto HMCE were found to be 90 and 27 mg/g, and onto NMCE, the adsorption capacities were 103 and 31 mg/g, respectively. The positive  $\Delta H^{\circ}$  and  $\Delta S^{\circ}$  values for both dyes lead to an endothermic process, and it is a spontaneous process. The regeneration results indicate that the biomaterial was efficiently recycled with 75.49% and 55% uptake for RB and CR dyes, respectively, after 5th cycles of desorption-adsorption.

#### **Biography:**

The aim of this study was therefore to explore the potential of the modified Carpobrotus edulis plant as a low-cost adsorbent to remove dye from aqueous solutions using the batch equilibration technique. The effects on dye adsorption rates of the adsorbent dose, contact time, ionic strength, and solution pH were investigated. The adsorption kinetics, isotherm, thermodynamic, and the regeneration were also evaluated and reported.

# Graphene - A Laboratory for Electronic Analogues of Optics, Only Better

# Avik Ghosh

Dept. of Electrical and Computer Engineering and Dept. of Physics, University of Virginia, Charlottesville 22904, USA

# Abstract:

The topological properties of electrons in graphene, in particular the windings of its pseudospins (bonding-antibonding combinations of its dimer pz orbitals) arise from its symmetry properties. As a result, electrons in graphene mimic photons, except they can reach material limits not readily achieved in optoelectronics. The conservation of transverse momentum at a split-gated PN junction enforces Snell's laws and total internal reflection, except the refractive index can be negative, leading to Veselago focusing. Magnetic resonance measurements in Hall bar geometries can directly probe such a sign flip of the angle of refraction. The reflectivity follows the equivalent of Fresnel equations, except they show perfect normal reflection (Klein tunneling) for odd number of Bernally stacked layers, perfect normal transmission (anti-Klein tunneling) for even number, a prominent set of intermediate Brewster angles, and the equivalent of Malus' law for polarizer-analyzer pairs. All these effects are driven by symmetry constraints, and have been seen numerically as well as experimentally, such as with Corbino geometries and angled graphene junctions. I will discuss the impact of these unconventional transmissions on electronic switching devices, such as sub-thermal binary switching, as well as current saturation and RF gain in analog graphene devices.

#### **Biography:**

Avik Ghosh is Professor in the Dept of Electrical and Computing Engineering and Dept of Physics at the University of Virginia. He is the site-director of an NSF Center on Multifunctional Integrated Systems Technology and team leader of a Defense program on skyrmions. Ghosh has authored 150+ papers and two books in the area of computational nano-electronics. He has given over 150 invited lectures worldwide. He is Fellow of the Institute of Physics, senior member of the IEEE, winner of an IBM Faculty Award, the NSF CAREER Award, a best paper award, and UVA's All University Teaching Award.

#### Beyond Graphene; the Novel Nanomaterials Graphyne, Graphene and ATQG

#### Per A. Löthman<sup>(1,2)</sup>

Foviatech GmbH<sup>(1)</sup>, Hamburg, Germany; Kaiserslautern University of Applied Sciences<sup>(2)</sup>, Germany

#### **Abstract:**

Ever since the Nobel Prize for the discovery of Graphene there has been a continuous development in research and applications based upon graphene. Graphene's exceptional carrier transport characteristics that arise from the unique  $\pi$ -electron system in their conjugated carbon network structure is one of its extraordinary properties. To complement zero-bandgap graphene, material scientists have devoted considerable effort to identifying 2D carbon materials but it is a challenge to prepare large-sized single-crystal 2D carbon materials even with only moderate bandgaps. A novel single-crystal 2D carbon material, namely monolayer quasi-hexagonal-phase fullerene (C60), with a large size via an interlayer bonding cleavage strategy. Here monolayer polymeric C60, cluster cages of C60 are covalently bonded with each other in a plane, forming a regular topology that is distinct from that in conventional 2D materials and it offers an moderate band gap. An alternating twist quadrilayer graphene (ATQG) with twist angles of 1.96° and 1.52°, which are slightly removed from the magic angle of 1.68° is another promising new carbonmaterial. At the larger angle, signatures of correlated insulators only when the ATQG is hole doped, and no signatures of superconductivity, and for the smaller angle we find evidence of superconductivity. The third novel material is graphyne, a periodically sp-sp2-hybridized carbon allotrope, synthesized in bulk via a reversible dynamic alkyne metathesis of alkynyl-substituted benzene monomers to yield crystalline y-graphyne. Additionally, the ABC staggered interlayer stacking of the graphyne was revealed using powder X-ray and electron diffraction. Finally, the folding behaviour of the few-layer graphyne was also observed on exfoliation, and showed step edges within a single graphyne flake with a height of 9 nm which is extraordinary in this context.

#### **Biography:**

Per A. Löthman obtained his Ph.D. degree from Twente University, The Netherlands in the field of Magnetics and Self-assembly, conducted research in Canada, France and Germany on carbon nanotubes, Graphen and related 2D nanomaterials. His research is interdisciplinary and involve sensors and sensing, 2D advanced materials, BioNanotechnology including DNA, S-layers, Viruses (archaea, bacteriophages), Biomolecular Architecture, Botany and functional surfaces. Löthman has published over 80 scientifical articles, several book chapters and serves as a reviewer and he is on the editorial board for several journals such as Nature, Nature Materials, Journal of Bioanalytical and Analytical Chemistry, Journal of Colloid and Interface Science, Thin Solid Films, Sensors and Actuators, Microsystems Technologies, Biophysical Reviews and Letters and International Journal of Applied Mathematics and Theoretical Physics (IJAMTP). Löthman is CSO (Chief Scientifical Officer) at Foviatech GmbH in Hamburg, Germany, a young innovative high-tech company in the field of advanced materials and artificial intelligence, and a senior lecturer in "Nanomedicine, Nanopharmacy" and "Sensors and Sensing in Engineering, Biology and Medicine" (Kaiserslautern University) and "Mechatronics Systems and Design" (Hamburg University), Germany and "Interdisciplinary Manufacturing Engineering" (HTW Berlin) Germany.

#### Engineering Nano-biomaterials for Tissue Fabrication and Regenerative Medicine

#### Su Ryon Shin\*

Division of Engineering in Medicine, Department of Medicine, Brigham and Women's Hospital, Harvard Medical School, Boston, MA 02139, USA

# Abstract:

Tissue engineering holds great promise as an alternative therapy by creating biomimetic materials that can reestablish the structure and function of the injured tissue. Living tissues are complex, multicellular, and composed of microscale repeating units in a well-defined 3D matrix along with vessel networks. Therefore, the intricate heterogeneity in biological structures and the physical properties of native tissues/organs has galvanized a need for multi-material and multi-cellular hybrid designs. Advances in biomanufacturing techniques that can manipulate the structure of the engineered biomaterials are emerging as powerful techniques to recapitulate biological systems with adequate levels of functionality for tissue/organ remodeling and regeneration. To achieve in vivo-like biological functions of 3D tissue constructs, advanced biomaterials are required to develop mimicking biological and physical properties of native extracellular matrices (ECMs). Herein, we developed nanoparticle-incorporated biomaterials to improve the nanofibrous morphology and electrical and mechanical properties while maintaining biomaterials' beneficial properties, such as high porosity, biocompatibility, and biodegradability to resemble native ECMs. To create highly organized and complex 3D tissue constructs using these hybrid biomaterials, we developed an advanced multi-material bioprinting platform that employs colloidal gels as self-healing, non-sacrificial, and biodegradable supporting baths and a programmable microfluidic device, which can quickly switch between different materials, reagents, and cells. The versatile 3D bioprinting technique and novel hybrid bioinks have produced highly viable and functional in vitro constructs with excellent resolution. These works present a strategy for advanced hybrid biomaterials and 3D bioprinting techniques, which may find widespread application for creating artificial muscles, bio-hybrid actuators, and organs.

#### **Biography:**

Su Ryon Shin, Ph.D., is an Assistant Professor of Medicine at Harvard Medical School in the Division of Engineering in Medicine at the Brigham and Women's Hospital. Her interdisciplinary approach has earned her a growing international reputation for her work in nanomaterials science, bioprinting, organs-on-a-chip, biosensors, regenerative medicine, and tissue engineering. Dr. Shin has received grants from the National Institutes of Health, American Heart Association, Air Force Office of Sponsored Research, U.S. Department of Defense, etc. In addition, she has published over 148 papers in peer-reviewed journals with an h-index of 64 and >15,000 citations.

# POSTER

# Liquid Quench Method to Obtain the Molecular Structure of Char Samples by Means of Reaxff

#### Valentina Sierra<sup>1\*</sup>, Farid Chejne<sup>2</sup>, Manuel Garcia-Peréz<sup>1</sup>

<sup>1</sup>Washington State University, USA

<sup>2</sup>Universidad Nacional de Colombia, Colombia

#### **Abstract:**

Carbon molecular representations are based on characterization data, being simpler for coal samples consisting just of carbon and hydrogen, and more complicated for chars that usually are composed of carbon, hydrogen, oxygen, nitrogen, and sulfur. Model char structure by means of molecular dynamics and quantum chemistry techniques is an advantageous tool for predicting and understanding how these complex structures affect the reaction mechanism of char gasification with different oxidant agents such as O2, CO2, and H2O. This work addressed a methodology to construct a molecular representation of an amorphous char, which was used in further analysis to analyze the gasification processes. The methodology to construct the char structure was done using Lammps, where several thermostats were applied to perform the liquid quench method and give energy to the chemical system. In addition, because modeling both bond breaking and formation were necessary to obtain the final molecular structure of the amorphous char, a reactive force field ReaxFF was used. The molecular structure obtained was accurately validated with experimental data, such as molecular composition, radial distribution function, aromaticity, hybridization, density, and surface area, with errors of less than 5-10%. After validation, the molecular structure of char was oxidized, simulating the gasification process, and the results were compared with experimental data. This work developed a methodology, which is precise, faster, and cheaper than experimental analysis, to research the gasification process.

# **Biography:**

J. P. Mathews and A. L. Chaffee, "The molecular representations of coal – A review," Fuel, vol. 96, pp. 1–14, Jun. 2012, doi: 10.1016/J.FUEL.2011.11.025.

D. Hong, L. Liu, C. Wang, T. Si, and X. Guo, "Construction of a coal char model and its combustion and gasification characteristics: Molecular dynamic simulations based on ReaxFF," Fuel, vol. 300, no. February, p. 120972, 2021, doi: 10.1016/j.fuel.2021.120972.

R. Ranganathan, S. Rokkam, T. Desai, and P. Keblinski, "Generation of amorphous carbon models

using liquid quench method: A reactive molecular dynamics study," Carbon N. Y., vol. 113, pp. 87–99, Mar. 2017, doi: 10.1016/J.CARBON.2016.11.024.

#### Thermal Stability of Thermally Reduced Graphene Oxide

# Maksym Barabashko<sup>1</sup>, Marek Drozd<sup>2</sup>, Razet Basnukaeva<sup>1</sup>, Alexander Dolbin<sup>1</sup>, Nicolay Vinnikov<sup>1</sup>

<sup>1</sup>B. Verkin Institute for Low Temperature Physics and Engineering of the National Academy of Sciences of Ukraine, 47 Nauky Ave., Kharkiv 61103, Ukraine

<sup>2</sup>Institute for Low Temperatures and Structure Research Polish Academy of Sciences, ul. Okólna 2, Wrocław 50-422, Poland

#### Abstract:

Thermal stability of the thermally reduced graphene oxide (TRGO) has been studied. Modified Hummers method was used for obtaining the initial graphite oxide (GO) from graphite powder. The thermal exfoliation of the graphene oxide powder has been performed in the vacuum conditions at 300°C. For partial graphene hydrogenation, TRGO has been treated by pulsed high-frequency discharge in a hydrogen atmosphere that leads to structural changes in the carbon planes and the formation of C-H sp3 bonds. The TGA measurements of the mass loss have been carried in a nitrogen atmosphere from room to 1000°C. Kissinger's multiple heating rate method has been used to determine the activation energy for decomposing substances. Obtained activation energies have been compared with the energies of the activation of thermal defunctionalization of multi-walled carbon nanotubes (MWCNTs). Obtained experimental results are useful for further proposing the kinetic model of the mechanism of the most probable reaction of TRGO decomposition.

#### **Biography:**

M.S. Barabashko is a researcher in the B. Verkin Institute for Low-Temperature Physics and Engineering of the National Academy of Sciences of Ukraine, Kharkiv. The research field of interest includes the investigation of the properties of carbon nanomaterials and carbon-based nanocomposites for biomedical applications. In 2020/2021 was supported by the National Research Foundation of Ukraine (Grant No.197/02.2020).

#### Carbon Nanotube Thin-film Sheet for Low-voltage Heating Applications

#### Megha Chitranshi<sup>1</sup>, Peter Kosel<sup>1</sup>, Marc Cahay<sup>1</sup>, Mark Schulz<sup>1</sup>

#### **Abstract:**

Carbon Nanotube (CNT) is a multifunctional material and have been researched for many applications. The floating catalyst chemical vapor deposition (FCCVD) method was used to synthesize CNT thin-film sheet. In this method, a liquid feedstock consisting of a carbon source, catalyst and sulphur as a growth promoter is injected at the inlet of the high-temperature furnace. The CNT sock or web is collected at the other end of the tube and wrapped on a rotating drum to form a sheet. The FCCVD method is a continuous process and can produce large-scale CNT sheet. However, the as-synthesized CNT sheet contains gaps and randomly aligned nanotubes. This issue is solved by using a post-treatment to improve the packing density and make CNTs more aligned to improve the overall performance of the material. In this work, I will discuss the Chlorosulfonic Acid (CSA) stretching as a post-treatment method to improve the densification and alignment for electrothermal application of thin-film CNT sheet. This presentation discusses synthesis of CNT sheet using the FCCVD method, post-treatment to improve the performance of the material. Furthermore, the optimized stretching ratio for flexible and low-voltage heating applications for CNT sheet are discussed.

Keywords: carbon nanotubes, CSA-stretching, electrothermal application.

**Acknowledgements:** This research study is supported by the National Institute for Occupational Safety and Health (NIOSH) through the Pilot Research Project Training Program of the University of Cincinnati Education and Research Center Grant #T42OH008432.

# DAY 5 FRIDAY, OCTOBER 14, 2022 Virtual Presentations

# $\pi$ -Structures with Different Topologies: Synthesis, Aromaticity and Electronic Properties

### Chunyan Chi\*

Department of Chemistry, National University of Singapore, Singapore

#### **Abstract:**

Carbon-based nanostructures have shown revolutionary influence in the area of chemistry, physics and materials science. Recent efforts have been focused on novel topological structures of sp2 -carbons such as carbon nanohoops, nanobelts, molecular cages, and open-shell nanographenes, which provoked new chemistry and materials. However, synthesis of this kind of molecules is extremely challenging mainly due to strain or intrinsic high reactivity. Another issue is that most of these carbon nanostructures have a localized aromatic character; that means, the  $\pi$ -electrons are not globally delocalized along the backbone, which limits their optical and electronic properties and applications. Herein, the synthesis of a series of novel pi-structure with different topologies will be introduced, and their physical properties, aromaticity and diradical character will be discussed.[1-5] References [1] J.-J. Shen, Y. Han, S. Dong, H. Phan, T. S. Herng, T. Xu, J. Ding, C. Chi, Angew. Chem. Int. Ed. 60. (2021) 4464. [2] Y. Han, S. Dong, J. Shao, W. Fan, C. Chi, Angew. Chem. Int. Ed. 60. (2021) 2658. [3] Y. Han, Z. Xue, G. Li, Y. Gu, Y. Ni, S. Dong, C. Chi, Angew. Chem. Int. Ed. 59. (2020) 9026. [4] S. Dong, T. Y. Gopalakrishna, Y. Han, H. Phan, T. Tao, Y. Ni, G. Liu, C. Chi, J. Am. Chem. Soc. 141. (2019) 62. [5] Q. Wang, T. Y. Gopalakrishna, H. Phan, T. S. Herng, S. Dong, J. Ding, C. Chi, Angew. Chem. Int. Ed. 56. (2017) 11415.

#### **Biography:**

Chunyan Chi received her PhD degree from the Max-Planck Institute for Polymer Research and conducted her postdoctorate research in the University of California at Santa Barbara. She is now an associate professor in the Department of Chemistry, National University of Singapore. Her research interests are synthesis of extended  $\pi$ -electron systems with novel structures, aromaticity, organic diradicaloids and functional materials for organic electronics. She received Asian Core Program Lectureship Awards from Japan (2013), China (2014), Taiwan (2014) and Hong Kong (2019), Young Chemist Award from Department of Chemistry, NUS in 2016, Distinguished Lectureship Award from Chemical Society of Japan in 2017.

# Proposal of Braiding Pattern of Carbon Nanotubes for the Fabrication of Fabric Composites and Consideration of Basic Mechanical Properties

#### Fumio Ogawa

Tohoku University, Japan

#### Abstract not Available!!

# The Utilization of Waste Gelatin to Enhance the Performance of Bendable MnO<sub>2</sub>/PAN Anode Membranes for the Flexible Lithium Ion Battery

Supacharee Roddecha<sup>1\*</sup>, Katechanok Pimphor<sup>1</sup>, Wisallaya Phumeekrong<sup>1</sup>, Saksit Thavonviriyakul<sup>1</sup>, Witchaya Witoonrat<sup>1</sup>, Siriphorn Boonyarattanasathaporn<sup>1</sup>

<sup>1</sup>Department of Chemical Engineering, Faculty of Engineering, Kasetsart University, Bangkok 10900, Thailand

#### Abstract:

Flexible lithium-ion batteries (FLIBs) are considered as the promising electrical generating and storage device for using in various smart electronics, regarding to its high energy density, durability and relatively long lifespan. The key component that determines the performance of FLIBs is the anode material. Currently, the great concern of health care pushes the rapid growth of the food and pharmaceutical industry that ultimately results in the vast amount of the gelatin waste from their manufacturing process. Therefore, this work was aimed to utilize the waste gelatin to enhance the electrochemical performance of the flexible anode membrane for the FLIB. The anode membrane was prepared from different compositions of manganese dioxide (MnO2), and the polyacrylonitrile (PAN) combining with the gelation derived carbon xerogel. The SEM equipped with EDS analysis in conjunction with N2 adsorption isotherm revealed their mesoporous structure with the confirmed uniform distribution of nitrogen functional groups. It was found that the synergistic effect between the addition of MnO2, polyacrylonitrile, and gelation derived carbon played an essential role in enhancing the ionic capacity of the electrode membrane. In particular, the gelatin-based carbon has shown to promote the ionic capacity of anode membranes and reduce the interfacial resistance between the electrode surface and electrolyte. All the obtained free-standing bendable anode showed higher ionic capacity compared to that of the theoretical capacity of the graphite anode. The best anode membrane sample exhibited average discharge capacity of 523 mAh.g-1 at 0.5 C-rate with great coulombic efficiency nearly 100%.

#### **Biography:**

Supacharee Roddecha is a faculty and researcher of Chemical Engineering at Kasetsart University, Bangkok, Thailand. She received her PhD in Chemical Engineering from University of Rochester, USA in 2012. She worked as a Postdoctoral Researcher in the Department of Chemical Engineering at University of Rochester from 2012 to 2013. Then, she joined the Faculty of Engineering, Kasetsart University (Thailand) in 2013. Currently her research interests focus on electrochemical energy-storage materials and devices.

# Generation of Various Nanocarbon Allotropes in the Gas Phase During Diamond Hot Filament Chemical Vapor Deposition

#### Nong-Moon Hwang

Seoul National University, South Korea

#### Abstract not Available!!

# Soft Stretchable Electronics using Self-healable Nanocomposite Conductor for Skin-like Wearable Sensors

# Sungjun Lee<sup>1,2\*</sup>, Ki Jun Yu<sup>2</sup>, Hyungmin Kim<sup>1,6</sup>, Donghee Son<sup>3,4,5</sup>

<sup>1</sup>Center for Bionics, Biomedical Research Institute, Korea Institute of Science and Technology, Republic of Korea

<sup>2</sup>School of Electrical and Electronic Engineering, Yonsei University, Republic of Korea

<sup>3</sup>Department of Electrical and Computer Engineering, Sungkyunkwan University (SKKU), Republic of Korea

<sup>4</sup>Center for Neuroscience Imaging Research, Institute for Basic Science (IBS), Republic of Korea

<sup>5</sup>Department of Superintelligence Engineering, Sungkyunkwan University (SKKU), Republic of Korea

<sup>6</sup>Division of Bio-Medical Science & Technology, University of Science and Technology, KIST School, Republic of Korea

# Abstract:

Soft wearable sensors capable of monitoring electrophysiology or tactile information with stable electrical performance have pursued the ultimate electronic skin system and skin-prosthetics. Although massive efforts have been made to the skin-like, skin-conformal wearable electronics based on soft stretchable material strategies, securing stable electrical performance under repetitive deformation causing stress and fatigue still remain challenging. Here, we report unconventional soft stretchable wearable devices using mechanically self-healable, electrically self-recoverable nanocompoite conductors that can prevent its electrical degradation induced by repetitive strain. These functionalities originate from unique polymeric-material properties and nano-scale behaviors of self-healing polymer (SHP): i) spontaneous reconstruction of dynamic hydrogen bonding in a SHP and ii) dynamic rearrangement of electrical pathway by percolation of conducting nanoparticles. We developed self-healing composite conductor film s for skin-like soft electrodes capable of stable electrophysiology monitoring, demonstrated precise robot arm control and we implemented sinter-free printable self-healing composite conductors for bio-inspired sensory-neuromorphic system.

# **Biography:**

Sungjun Lee, Ph.D Candidate Year Education 2015 Computer science and electrical engineering, Handong Global University (B.S) 2018 Engineering of green energy and environment, Handong Global University (M.S) 2019 ~(current) Center for Bionics, Biomedical Research Institute, Korea Institute of Science and Technology (Student Researcher) School of Electrical and Electronic Engineering, Yonsei University (Ph.D Candicate).

# High-ampacity Freestanding CNT-Cu Composite Film with Controllable Fabrication

# Nilüfer Çakmakçı<sup>\*</sup>, Myunggyu Shin, Huiyeon Jung, Jeongyun Lee, Hyeonjun Song and Youngjin Jeong

Department of Organic Materials and Fiber Engineering, Soongsil University, Seoul 06978, Korea

# Abstract:

Alternative conductive materials have been studied for replacing metal with lighter ones to reduce the weight of portable electronic devices and electric vehicles. Carbon nanotubes (CNT) have attracted great interest as a matrix of light conductors combined with copper (Cu) thanks to their low density, high theoretical electrical conductivity, and high ampacity. Here we show a simple and effective method for producing CNT-Cu composite using freestanding CNT film. The CNT-Cu composite was successfully produced with the bottom-up filling mechanism using the suppressor polyethylene glycol (PEG) and accelerator bis-(3-sodiumsulfopropyl disulfide) (SPS) with hydrochloric acid. The uniformly Cu-plated CNT film has higher ampacity and lower density than copper foil, making it usable for daily life applications.

#### **Biography:**

Nilüfer Çakmakçı received her Master's degree from Istanbul Technical University in 2017. She is currently a Ph.D. student under the supervision of Prof. Youngjin Jeong at Soongsil University in South Korea. Her research interests focus on carbon nanotube, lithium-ion batteries and anode-free batteries.

# Solubilities of 4-Aminoazobenzene in Supercritical Carbon Dioxide and Development of New Semiempirical Model

# Ratna Surya Alwi<sup>1\*</sup>, Kazuhiro Tamura<sup>2</sup>, and Chandrasekhar Garlapati<sup>3</sup>

<sup>1</sup>National Research and Innovation Agency (BRIN), Indonesia

<sup>2</sup>Division of Natural System, Graduate School of Natural Science and Technology, Kanazawa University, Kakuma-machi, Kanazawa, 920-1192 Japan

<sup>3</sup>Department of Chemical Engineering, Puducherry Technological University (Formerly Known as Pondicherry Engineering College), Puducherry 605014, India

# Abstract:

Solubilities of 4-aminoazobenzene in supercritical carbon dioxide (ScCO2) were measured by flow type apparatus at temperatures ranges of 323.15-383.15 K and pressures ranges of 10 - 25 MPa. The measured solubilities of 4-aminoazobenzenein in mole fraction were ranged between 1.30 × 10-5 and 11.3 × 10-5. Twelve existing semi-empirical models were considered to correlate experimental data of 4-aminoazobenzene with 3 to 6 adjustable constants. The solubilities of 4-amino-azobenzene were also analysed thermodynamically by PREoS combined with vdW2. Moreover, solubilities of 4-aminoazobenzene were correlated by a new semiempirical model. The effective-ness of the model proposed were evaluated by comparing with twelve existing models and tested with azobenzene and anthraquinone dye compounds. According to the results, it was observed that all types of models accurately represent the solubility data of 4-aminoazobenzene in ScCO2. Additionally, the solvation and sublimation enthalpies of 4-aminoazobenzene were determined thermodynamically.

# **Biography:**

Ratna Surya Alwi currently works at the National Research and Innovation Agency (BRIN), Indonesia. She is a researcher in supercritical carbon dioxide. She focused on the measurement and correlation of solubility of compounds in supercritical carbon dioxide.

# Possible Metallization of Mn-DNA Based on the First-principles Calculation

# Takuya Sekikawa\*, Hiroyuki Kawai, Yoshiaki Ōno

Department of Physics, Niigata University, Japan

# Abstract:

We investigate the electronic states of Mn-DNA where hydrogen bonds of Guanine-Cytosine base pairs in the poly(GC) are replaced by Mn atoms on the basis of the first-principles calculation using OpenMX code. Due to the Mn-doping, a considerable number of new energy bands (in-gap bands) appear in the energy gap of O(3eV) which is originally observed in the non-doped poly(GC). When 80% of hydrogen bonds are replaced by Mn atoms, the in-gap bands are almost flat and the Fermi level sits in the energy gap between the flat bands resulting in the insulating ground state. On the other hand, when 100% of hydrogen bonds are replaced by Mn atoms, the in-gap bands are narrow but have finite band widths and the Fermi level sits in a narrow band with the width of 0.01eV indicating the metallic ground state. The narrow in-gap bands mainly consist of Mn-3d orbitals but the contributions from the Guanine and Cytosine are also relevant via the hybridization with Mn. As the coulomb interaction between the 3d electrons on the same Mn atom is of order of several eV and is much larger than the band width of the in-gap band across the Fermi level, the actual ground state is considered to be the Mott insulator where the Mn-3d electrons behave as localized spins of S=5/2 with small kinetic exchange interactions. This is consistent with the measured magnetic susceptibility of the Mn-DNA exhibiting Curie-Weiss law of S=5/2 spins with a small negative Weiss temperature.

# **Biography:**

Takuya Sekikawa is a third-year doctoral student of the Graduate School of Science and Technology, Niigata University and is supported by Research Fellowship of the Japan Society for the Promotion of Science for Young Scientists. He is working on condensed matter theory in Ōno's group, especially focusing on the electronic state and the superconductivity based on the first-principles and quantum many-body calculations.

# Functionalization of MWCNTS Using Phosphoric Acid for Immobilization of Cellulase

# Balakrishnan Kunasundari<sup>1\*,</sup> Hasnol Azahari Natasha Yasmin<sup>1</sup>, Siew Hoong Shuit<sup>2</sup>, Sandrasekaran Naresh<sup>2</sup>

<sup>1</sup>Fakulti Teknologi Kejuruteraan Kimia, Universiti Malaysia Perlis, Kompleks Pusat Pengajian Jejawi 3, Kawasan Perindustrian Jejawi, 02600 Arau, Perlis, Malaysia

<sup>2</sup>Department of Chemical Engineering, Lee Kong Chian Faculty of Engineering and Science, Universiti Tunku Abdul Rahman, Sungai Long Campus, Jalan Sungai Long, Bandar Sungai Long, Cheras, 43000, Kajang, Selangor, Malaysia.

# Abstract:

In this paper, functionalization of multiwall carbon nanotubes (MWCNTs) using phosphoric acid (H3PO4) was attempted. Based on the One Factor at a Time (OFAT) analysis, 8 M of H3PO4, 8

h of reflux time and 80 °C were identified as an ideal condition for the acid oxidation process. Successful functionalization of MWCNTs using H3PO4 was revealed from Fourier Transform Infrared Spectroscopy (FTIR) peaks. The resulting fMWCNTs were immobilized with cellulase via adsorption. The optimum temperature for free cellulase was at 50 °C and for immobilized cellulase was at 60 °C. The optimum pH was at 5 for both free and immobilized cellulase. Higher thermal stability was achieved with immobilized cellulase in which 39% of its activity was retained at 80 °C compared to free cellulase. Reusability study of immobilized cellulase depicted 28 % of remaining activity after 5th cycles of analysis using model substrate (filter paper Whatman No. 1). These results suggest that H3PO4 which is a mild acid is a promising substitution for functionalization of MWCNTs.

#### **Biography:**

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

# Synthesize and Characterization of Beta Cyclodextrin Modified Chitosan for Adsorption of Aspirin

#### Norzita Ngadi<sup>1\*</sup> and Muhammad Asyiq Azman

School of Chemical and Energy Engineering, Faculty of Engineering, Universiti Teknologi Malaysia, 81310, Skudai, Johor, Malaysia

#### Abstract:

In adsorption study, chitosan is a very promising material as it can be used to adsorb a variety of waste such as dyes, metal ions and pharmaceutical. This particular ability can be attributed to the presence of amino and hydroxyl group in its molecules. However, these reactive groups tend to form hydrogen bond with each other and greatly reduces the adsorption efficiency of chitosan. Therefore, in this study, chitosan was modified with  $\beta$ -cyclodextrin to improve its efficiency. The response for this study was the removal of aspirin in an aqueous solution. This study was conducted to synthesize and characterize chitosan modified with β-cyclodextrin, to determine the adsorption performance of the adsorbent for aspirin removal and analyze the adsorption mechanism of the adsorbent for aspirin removal. Chitosan was modified without using any harmful and hazardous chemical. The characterization of the adsorbents was conducted using Fourier transform infrared spectroscopy, point of zero charge, carbon, hydrogen, nitrogen and sulphur analysis, Field emission scanning electron microscopy and Brunauer-Emmett-Teller analysis. The adsorption kinetics were studied using the pseudo-first and pseudo-second order kinetic model and Elovich equation. The adsorption isotherm was studied using the Freundlich, Langmuir, Temkin and Dubinin-Radushkevich isotherm model. The adsorption thermodynamics was determined by studying the changes in enthalpy, changes in standard entropy and Gibbs free energy. The result shows an improvement in adsorption capacity when chitosan was modified with  $\beta$ -cyclodextrin. The maximum adsorption

capacity of chitosan was 236.97 mg/g while the maximum adsorption capacity for  $\beta$ -cyclodextrin modified chitosan was 359.87 mg/g which is an increase of 51%. The best condition for the removal of aspirin is 10 minutes of contact time, pH 3, 30 °C temperature, 500 mg/L initial concentration of aspirin and 0.05 g of adsorbent. The results of the model fitting showed that the adsorption of aspirin onto the adsorbent occurs via physical adsorption.

#### **Biography:**

Norzita Ngadi is an Associate Professor in School of Chemical and Energy Engineering, Faculty of Engineering, Universti Teknologi Malaysia (UTM), where she has been a faculty member since 2002. She received her Ph.D. degree from University of Canterbury, New Zealand in 2010. She obtained her M.Eng in Chemical Engineering from UTM in 2002, after completion of her undergraduate study in Universiti Sains Malaysia. Her research interest includes wastewater treatment, catalytic reaction, renewable fuel and surface coating. She has published over 200 articles in journals and conference papers.

# Conductive 2D Metal-organic Framework for High-performance Cathodes in Aqueous Rechargeable Zinc Batteries

Kwan Woo Nam<sup>1</sup><sup>\*</sup>, Sarah S. Park<sup>2</sup>, Roberto dos Reis<sup>2</sup>, Vinayak P. Dravid<sup>2</sup>, Heejin Kim<sup>3</sup>, Chad A. Mirkin<sup>2</sup>, and J. Fraser Stoddart<sup>2</sup>

<sup>1</sup>Ewha Womans University, Republic of Korea

<sup>2</sup>Northwestern University, USA

<sup>3</sup>Korea Basic Science Institute, Republic of Korea

#### Abstract:

The battery community is paying increasing attention to post-lithium (Li)-ion batteries, which can transcend current Li-ion batteries with respect to key electrochemical properties, cost, and safety. Cost and safety concerns have become more serious as grid-scale energy storage systems (ESSs) are emerging for the efficient and balanced distribution of electricity generated from renewable energy sources (e.g., solar, wind, etc.). As promising alternatives, aqueous rechargeable zinc batteries (ARZBs) are gaining considerable attention since they can take advantage of increased capacity resulting from the divalent charge of their carrier ions. In addition, they are cost-effective, environmentally benign, and subject to reduced fire hazards. ARZBs, however, still linger at the research stage, requiring cathode materials with enhanced performance. The main challenge in developing the cathode materials of divalent batteries is associated with the dual positive charge that induces stronger electrostatic interactions with the host framework, impeding the diffusion of divalent ions. The presence of these positively charged metal ions also imposes a higher dehydration energy penalty when divalent ions pass through the electrode-electrolyte interface, constituting an additional barrier in the overall cell operation. In this talk, I will introduce the development background and reaction mechanism of conductive 2D metal-organic framework (MOF). Cu3(HHTP)2, a 2D MOF with large one-dimensional channels, as a zinc battery cathode. Owing to its unique structure, hydrated Zn2+ ions which are inserted directly into the host structure, Cu3(HHTP)2, allow high diffusion rate and low interfacial resistance which enable the Cu3(HHTP)2 cathode to follow the intercalation pseudocapacitance mechanism. Cu3(HHTP)2 exhibits a high reversible capacity of 228 mAh g-1 at 50 mA g-1. At a high current density of 4000 mA g-1 (~18 C), 75.0% of the initial capacity is maintained after 500 cycles. These results provide key insights into high-performance, 2D conductive MOF designs for battery electrodes.

#### **Biography:**

Kwan Woo received his B.S degree in Materials Science Engineering in 2010 from Hanyang University in Korea. After graduation, he moved to Korea Advanced Institute of Science and Technology and received M.S. in 2012. During M.S. course, he developed graphene- based catalysts for PEM-FC under the supervision of Prof. Jung Ki Park. In 2016, he received his Ph.D under the supervision of Prof. Jang Wook Choi. During Ph.D course, his research focused on the hydrated cathodes for high performance sodium and magnesium rechargeable batteries. After finishing Ph.D course, he entered LG Chem and then developed commercial separators for iPhone and advanced separators such as all solid type separators during 2016.02~2018.08. In September 2018, he joined to the Stoddart group in Northwestern University as a postdoctoral fellow, working on the design and synthesis of organic cathode materials for rechargeable batteries. Currently, he is currently working as an assistant professor in the Department of Chemical Engineering and Materials Science at Ewha Womans University.

# Desorption and Reduction Studies of Graphitic Carbon Nitride Supported Nickel Catalyst for CO Methanation

#### Wan Nor Roslam Wan Isahak\* and Khairul Naim Ahmad

Department of Chemical and Process Engineering, Faculty of Engineering and Built Environment,

Universiti Kebangsaan Malaysia, 43600 UKM Bangi, Selangor, Malaysia.

#### **Abstract:**

Graphitic carbon nitride (g- C3N4) has attracted much attention due to its unique polymeric structure of carbon and nitrogen in the form of heptazine units. In this study, a nickel catalyst supported on graphitic carbon nitride was prepared by a facile impregnation method. Ni/g-C3N4 desorption and reduction behaviour with carbon monoxide (CO) was investigated by temperature- programmed desorption (TPD) and reduction (TPR). The as-prepared Ni/g-C3N4 catalyst was also characterized by X- ray diffraction (XRD), N2 phy-sisorption, and X-ray photoelectron spectroscopy (XPS). It was found that the utilization of g-C3N4 as a catalyst support enhances the complete reduction of Ni species and CO desorption.

This can be attributed to the role of g-C3N4 support as a reducing agent for Ni, as well as its basicity owing to the richness of nitrogen functional group. The good performance of Ni/g-C3N4 catalyst towards CO methanation can be ascribed to the improvement in adsorption and activation of CO molecules on the active sites and the number of surface basic sites.

#### **Biography:**

Wan Nor Roslam Wan Isahak received his PhD (2014) in Chemistry (Catalysis) from National University of Malaysia (UKM). His academic career started at UKM, where his group studied catalysis involved in development heterogeneous catalysts and adsorbents for CO2 utilization and hydrogen production. Currently, he is Associate Professor of catalysis and reaction engineering in the

Department of Chemical and Process Engineering, UKM.

He has coauthored more than 80 refereed papers including high rank journals in SCIE and patents. He has co-supervised more than 20 post-graduate students in the field of catalysis in energy and environment, and advanced materials development.

#### Graphene Supported on Ru (0001) as Catalyst in Processes Involving Organic Molecules

#### **Cristina Díaz**

Departamento de Química Física, Facultad de CC. Químicas, Universidad Complutense de Madrid, 28040 Madrid, Spain

#### Abstract:

Deposits of graphitic carbon on transition metals (TM) have historically been studied as poisons of transition metal catalysts due to their chemical inertness and physical blocking of the active site of the catalyst [1]. However, a complete graphene (Gr) monolayer adsorbed on a transition mental substrate behaves very different from this poisoning carbon deposits, boosting new chemical mechanisms. For example, Gr/TM can be used to isolate molecules from the TM preventing the formation of hybridized metal-molecule orbitals, allowing the study of upperturbed molecular orbitals [2], the formation of two-dimensional structures of unperturbed organic molecules [3], or the growth of three-dimensional molecular crystals [2] to name a few phenomena. Among the different Gr/TM systems, Gr/Ru(0001) is especially relevant because due to its moiré structure [5] it is a very versatile template for the formation of new organic molecule structures and the promotion of chemical processed involving organic molecules [6]. Here, we focus on two of this phenomena, namely: (i) the reversible formation of a C-C bonds [7] between cyanomethylene groups (-CH2CN), anchored covalently at specific positions on the graphene surface, and 7,78,8-tetracyano-p-quinodimethane (TCNQ), able to diffuse at room temperature; (ii) the photogeneration of nonacene from  $\alpha$ -bisdiketone precusors [8], where, a 100% conversion has been observed due to the presence of an unoccupied surface state, spatially localized in the regions where the precursors are adsorbed, which is energetically accessible in the region of the electromagnetic spectrum where the n- $\pi^*$  transitions take place.

#### **Biography:**

Cristina Diaz is currently working as an associate professor in the faculty of Chemical sciences, Complutense of Madrid, Spain.

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# POSTER

# Synthesis of Heterogeneous Catalysts from Metal Complexes by the High-pressure High-temperature Method

#### Ichiro Yamane<sup>1\*</sup>, Teruki Ando<sup>1</sup>, Seiya Yokokura<sup>1</sup>, Taro Nagahama<sup>1</sup> and Toshihiro Shimada<sup>1</sup>

<sup>1</sup>Hokkaido University, Japan

#### Abstract:

Metal complexes have gained attention as precursors of heterogeneous catalysts because the metal atoms and organic linkers can be pyrolyzed into the catalytic particles and carbon carriers in one step. However, in this method, the particles become relatively large and easy to aggregate by the diffusion of metal atoms during pyrolysis. In this work, we attempt to solve the problem by pyrolyzing the complexes under high pressure, taking advantage of the diffusion suppression of atoms under high pressure. Thus, we synthesize metal/carbon composite materials by high-pressure high-temperature (HPHT) treatment to metal complexes and evaluate the catalytic activity.

We used W(NO)2CI2(C5H5N)2 as the precursor and applied HPHT treatment at 5 GPa/500 °C. It was observed that the precursor was decomposed to the nanoparticles of <5 nm diameter embedded in the carbonaceous matrices. These particles consisted of WO3 and WC. It indicated that the diffusion of tungsten atoms was inhibited successfully during pyrolysis under high pressure. In addition, it was revealed that the carbon support had low degrees of graphitization.

The electrochemical catalytic performance on the ORR of the product was evaluated by linear sweep voltammetry (LSV) using rotating disk electrode in O2-saturated 0.1 M KOH aqueous solution at a scan rate of 5 mV s-1. The LSV curve at 1600 rpm exhibited the onset potential for the ORR of 0.78 V vs. RHE. The electron transfer number was 2.98, indicating a four-electron pathway and two-electron pathway for the ORR. This would suggest that the product contains two kinds of active sites.

#### **Biography:**

Ichiro Yamane is a PhD student at Hokkaido University. He was born in Kanagawa in 1995 and raised in Hokkaido, Japan. He received bachelor's and Master's degrees from Hokkaido University in 2018 and 2019, respectively. His research interest is the high-pressure synthesis of functional materials from organic compounds and metal complexes.

# Electrochemical Dearomative Carboxylations of Heteroaromatics with Highly Negative Reduction Potentials

#### Tsuyoshi Mita\*

WPI-ICReDD, ERATO, Hokkaido University, Japan

#### Abstract:

The dearomative dicarboxylation of stable heteroaromatics using CO2 is highly challenging but represents a very powerful method for producing synthetically useful dicarboxylic acids, which can potentially be employed as intermediates of biologically active molecules such as natural products

and drug leads. However, these types of transformations are still underdeveloped, and concise methodologies with high efficiency (e.g., high yield and high selectivity for dicarboxylations) have not been reported. We herein describe a new electrochemical protocol using the CO2 radical anion (E1/2 of CO2 = -2.2 V in DMF and -2.3 V in CH3CN vs SCE) that produces unprecedented trans-oriented 2,3- dicarboxylic acids from N-Ac-, Boc-, and Ph-protected indoles that exhibit highly negative reduction potentials (-2.50 V to -2.94 V). Based on the calculated reduction potentials, N-protected indoles with reduction potentials with up to -3 V smoothly undergo the desired dicarboxylation. Other heteroaromatics, including benzofuran, benzothiophene, electron-deficient furans, thiophenes, 1,3- diphenylisobenzofuran, and N-Boc-pyrazole also exhibit reduction potentials more positive than -3 V, and served as effective substrates for such dicarboxylations. The dicarboxylated products thus obtained can be derivatized into useful synthetic intermediates for biologically active compounds in few steps. We also show how the dearomative monocarboxylation can be achieved selectively by choice of the electrolyte, solvent, and protic additive; this strategy was then applied to the synthesis of an octahydroindole-2-carboxylic acid (Oic) derivative, which is a useful proline analogue.

#### **Biography:**

Keio University (M.Sc. 2002, Prof. Tohru Yamada). Ajinomoto Co., Inc. (Researcher 2002-2004). The University of Tokyo (PhD 2007, Prof. Masakatsu Shibasaki). Harvard University (Postdoctoral Fellow 2007-2009, Prof. E. N. Jacobsen). Faculty of Pharmaceutical Sciences, Hokkaido University (Assistant Professor 2009-2019). WPI-ICReDD, Hokkaido University (Associate Professor 2019-present). A group leader in the organic chemistry group of the JST ERATO "MAEDA Artificial Intelligence in Chemical Reaction Design and Discovery Project" (2019-present). [Field of research] Synthetic Organic Chemistry, Organometallic Chemistry, Computational Chemistry, and Medicinal Chemistry.

#### **Graphite as Negative Electrodes for K-Ion Batteries**

L. Monconduit<sup>1,2,4\*</sup>, Phuong Nam Le Pham<sup>1,2,4</sup>, Vincent Gabaudan<sup>1,2,4</sup>, Lorenzo Stievano<sup>1,2,4</sup>, Patrik Johansson<sup>3,5</sup>, Lénaïc Madec<sup>2, 4</sup>, Badre Larhrib<sup>2,4</sup>, Hervé Martinez<sup>2,4</sup>

<sup>1</sup>ICGM, Univ. Montpellier, CNRS, Montpellier, France

<sup>2</sup>RS2E, CNRS, Amiens, France

<sup>3</sup>Department of Physics, Chalmers University of Technology, Göteborg, Sweden

<sup>4</sup>Universite de Pau et des Pays de l'Adour, E2S UPPA, CNRS, IPREM, Pau, France

<sup>5</sup>Alistore-ERI, CNRS FR 3104, Amiens, France

#### Abstract:

Recently potassium-ion batteries have been proposed as a promising next generation battery owing to cost effectiveness as well as a wide range of options for electrode materials and electrolytes. [1] Graphite is a very promising negative electrode for such batteries. The volume expansion of graphite (60%) remains, however, a major limitation to its practical use as negative electrodes material for KIBs. We worked on the graphite electrode formulation by playing on the electrode porosity and the amounts of conductive additive and binders as well as the type of binders. Thanks to this optimization, graphite electrodes reached a capacity of 256 mAh/g at 5C rate with a capacity retention of 240 mAh/g after 55 cycles. Then we have studied the electrochemical mechanism as function of the electrolyte type and concentration, by using operando XRD and Raman spectroscopy coupled with computational chemistry. The K+ solvation heavily depends on the salt concentration and strongly affects the electrochemistry of electrode materials.[2] When using KFSI in DME, pure K+ intercalation occurs when using a high concentration, while co-intercalation is dominant for less concentrated electrolyte. These mechanisms are easily distinguished by their galvanostatic curves as well as by operando XRD. Reduced solvation numbers (SN) were obtained for HCE, resulting in a thermodynamically more favored desolvation at the graphite surface leading to intercalation, whereas the higher SN of conventional electrolytes leads to cointercalation, with a strong influence on the cycle life of the battery. [1] T. Hosaka et al, Chem. Rev. 120 (2020) 6358. [2] J. Touja et al Chem. Commun. 56 (2020) 14673

#### **Biography:**

Laure Monconduit is CNRS research Director in ICGM (CNRS) in Montpellier, where she currently leads the group of Batteries. Her research directions include the synthesis and characterization of new electrodes materials for Li-ion, and for post-Li systems: Na-, K-, Ca- ion batteries, improvement of their performance and understanding of the electrochemical mechanism through operando characterization technics (XRD, IR-ATR, Raman, Mössbauer spectroscopy).

# Highly Oriented Pyrolytic Graphite (HOPG) Anion Intercalation Followed *In-situ* and In Real Time by an Innovative Combined Raman Spectroscopy and Electrochemical Atomic Force Microscopy System

Gianlorenzo Bussetti<sup>1\*</sup>, Marco Menegazzo<sup>1</sup>, Sergey Mitko<sup>2</sup>, Chiara Castiglioni<sup>1</sup>, Matteo Tommasini<sup>1</sup>, Andrea Lucotti<sup>1</sup>, Luca Magagnin<sup>1</sup>, Valeria Russo<sup>1</sup>, Andrea Li Bassi<sup>1</sup>, Martina Siena<sup>1</sup>, Alberto Guadagnini<sup>1</sup>, Samuele Grillo<sup>1</sup>, Davide Del Curto<sup>1</sup>, Lamberto Duò<sup>1</sup>

<sup>1</sup>Politecnico di Milano, Italy

#### <sup>2</sup>NT-MDT BV, Netherlands

#### **Abstract:**

The intercalation of anions inside the stratified structure of highly oriented pyrolytic graphite (HOPG), which can be obtained inside an electrochemical cell and with diluted mineral acids (such as sulfuric acid), represents a model system to understand intercalation mechanisms at the molecular length-scale [1]. The complex physical-chemical processes occurring at the electrode-electrolyte interface require the use of both microscopic and spectroscopic techniques [2,3]. Generally, these studies are not directly comparable: atomic force microscopy (AFM) is coupled with a potentiostat to follow morphological evolutions of the electrode surface when different electrochemical (EC) potentials are applied to the HOPG; Raman spectroscopy is able to perform a chemical analysis during the different steps of the intercalation process. The comparison between experiments is only possible by exploiting the EC analysis that, however, does not always exactly use the same parameters in microscopic and spectroscopic experiments. Here, we discuss the HOPG anion intercalation by exploiting an innovative experimental set-up, which is able to combine Raman spectroscopy and AFM together and inside an EC cell. The proposed set-up allows to correlate morphological images with chemical maps, as extracted from Raman data, during the oxidation

process of graphite. This system thus plays a crucial role when chemical reactions, both reversible and non-reversible, are studied step by step during EC processes and/or when local chemical analysis is required.

#### **Biography:**

[1] C.A. Goss et al. Anal. Chem. 65, 1378 (1993) [2] G. Bussetti et al. J. Phys. Chem. C 120, 6088 (2016) [3] R. Yivlialin et al. Appl. Surf. Sci. 504, 14440 (2017)

# Synthesis of Nickel Nanostructured Microwires and their Composites with Carbon Nanotubes for Electrochemical Applications

#### Mikhail Morozov<sup>1\*</sup>, Svetlozar Ivanov<sup>2</sup>

<sup>1</sup>Kazan National Research Technical University named after A.N. Tupolev-KAI (KNRTU-KAI), Russia

<sup>2</sup>Technical University Ilmenau, Germany

#### **Abstract:**

The approach for the synthesis of electrodes based on nickel nanostructured microwires and their composites with carbon nanotubes is presented. The introduction of carbon nanotubes resulted in increasing of the specific surface area of the composite material. Also, it is shown that nickel microwires can be as effective scaffolds for electrochemical applications. Binder free Ni/NiO microwire hybrid network with a nanostructured surface is synthesized by employing a facile and low-cost method, involving one-pot synthesis of Ni microwires, followed by their partial oxidation in air atmosphere. A combination of imaging, diffraction, thermodynamic and electrochemical methods has been applied to reveal the impact of the synthesis conditions on the energy storage performance of the Ni/NiO microwire networks. The thermal conditions for the synthesis have been optimized by means of thermogravimetric (TGA/DSC) analysis, where an appropriate temperature (T=400oC) for obtaining a low defect NiO phase has been determined. The performed electrochemical characterisation of the materials has shown that setting a low temperature for the synthesis enables high reversible capacity and better cycling stability of the binder free materials. When the Ni/NiO network structures are deposited by a conventional slurry-based technology, involving polymer binder and conductive additive, the high capacity and cycling stability of the anodes are preserved, independent on the temperature conditions of synthesis. The presented approach may have wide applications in electrochemistry, especially for creation of electrodes for rechargeable batteries and for electrocatalysis.

#### **Biography:**

Mikhail Morozov is an Associate Professor in Chair of Nanotechnologies in Electronics at Kazan National Research Technical University named after A.N. Tupolev-KAI (KNRTU-KAI), Kazan, Russia. He has 14 years of research experience and his areas of interest includes materials science, synthesis of nickel-based nanostructured microwires and rechargeable batteries. He has established his research group and research laboratory. He was a visiting researcher in several prestigious German universities. He has published 11 research papers in International Journals.

## Fabrication of a Stable CdS Photoanode for CO<sub>2</sub> Reduction under Visible-light Irradiation

#### Masanobu Higashi<sup>1\*</sup>

<sup>1</sup>Research Center for Artificial Photosynthesis (ReCAP), Osaka Metropolitan University, Japan

#### **Abstract:**

Metal sulfides are promising visible-light photocatalysts for CO2 reduction. However, available sulfide photocatalysts are limited because of their instability in aqueous solutions under photoirradiation. In this study, we investigated the fabrication of a stable CdS photoanode for CO2 reduction. The CdS photoanode prepared by the chemical bath deposition method was subjected to N2 calcination, which significantly affected its stability. Calcination up to 300 °C did not significantly change the surface morphology of the CdS photoanode. In contrast, the CdS electrode calcined at 400 °C had a smoother surface, with lower surface area of the electrode, which consequently reduced the CdS photocorrosion. K2Cd[Fe(CN)6] (particle size ~10 nm) was densely formed on the CdS surface via photocorrosion, and it effectively scavenged photogenerated holes in CdS and enabled the oxidation of [Fe(CN)6]4– to [Fe(CN)6]3–. Thus, we demonstrated stable CO2 reduction to CO over the CdS photoanode system in an aqueous solution under visible-light irradiation, along with the oxidation of [Fe(CN)6]4– to [Fe(CN)6]3–.

#### **Biography:**

2022.04-Present Associate Professor, Osaka Metropolitan University

2019.04-2022.03 Associate Professor, Osaka City University

2012.11-2019.03 Assistant Professor, Graduate School of Engineering, Kyoto University 2012.04-2012.10 Postdoctoral Fellow, Graduate School of Engineering, Kyoto University 2008.08-2012.03 Postdoctoral Fellow, Catalysis Research Center, Hokkaido University 2005.04-2008.03 Ph.D. Chemical System Engineering, The University of Tokyo (Domen Lab.)

#### Glassy Carbon Paste as a Promising Electrode Material for Stripping Voltammetry

#### Agnieszka Królicka<sup>\*</sup> and Anna Szczurkowska

Department of Building Materials Technology, Faculty of Materials Science and Ceramics, AGH University of Science and Technology, Mickiewicza 30, 30-059 Krakow, Poland

#### Abstract:

Working electrodes are the most important components of an electrochemical cell used for voltametric research. Among the variety of modern electrode materials, one is widely used, which is synthetic glassycarbon (GC). Because of its advantages, such as good electrical conductivity, fast and reversible electron transport, and a wide window of accessible potentials, glassy carbon is a material of choice for disc electrodes used in various fields of electrochemistry and electroanalysis.

In addition to solid materials, asemiliquid carbon paste has also found many applications. Classic carbon paste electrodes (CPEs) are prepared by mixing spectrally pure graphite and a Water-immiscible liquid, e.g. paraffin oil, to form a carbon paste which is filled in the electrode body. The working surface of the electrode is refreshed by removing the top layer of the paste. CPE elec-

trodes can be modified by depositing a layer of modifier not only on the surface but also on the mass because the modifier in the form of a sparingly water-soluble compound can be dispersed in paste at the stage of its preparation. Due to the CPE modifications, the sensitivity of the recorded signals can be increased. In the work, a new formula of the paste for CPE electrodes was developed using ground natural glassy carbon as the main component and polydimethylsiloxane as the binder. The replacement of graphite paste with glassy carbon paste improved the quality of the stripping voltametric signals recorded for catechol derivatives. An additional enhancement of the properties of the new CPE electrodes was achieved by adding lanthanum, ytterbium, and yttrium oxides to the paste. The newpaste electrode and its oxide-modified versions have been successfully used to test organic compounds such as catechin, epigallocatechin gallate, chlorogenic acid, and caffeic acid contained in plant extracts.

**Acknowledgement:** Research was carried out using the 'Financing of research carried out as part of the preparation of a doctoral dissertation at the Faculty of Materials Science and Ceramics at AGH.

#### **Biography:**

Agnieszka Królicka, assistant professor, received her Ph.D. in analytical chemistry from the 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 include various aspects of electroanalytical methods and nanotechnology.

# Biochar/Zinc Oxide Composites as Effective Catalysts for Electrochemical CO<sub>2</sub> Reduction

Juqin Zeng<sup>1\*</sup>, Mirtha A. O. Lourenço<sup>1\*</sup>, Pravin Jagdale<sup>1</sup>, Micaela Castellino<sup>2</sup>, Adriano Sacco<sup>1</sup>, Candido F. Pirri<sup>1,2</sup>

<sup>1</sup>Istituto Italiano di Tecnologia - IIT, Centre for Sustainable Future Technologies (CSFT), Italy

<sup>2</sup>Department of Applied Science and Technology (DISAT), Politecnico di Torino, Italy

#### Abstract:

Catalysts play a vital role in the electrochemical reduction of CO2 to value-added products. Only based on an effective catalyst, the CO2 electrolysis process can be advanced toward industrial application.

Novel electrocatalysts based on zinc oxide (ZnO) and biochars are prepared through a simple and scalable route and are proposed for the electrocatalytic reduction of CO2 (CO2RR). Materials with different weight ratios of ZnO to biochars, namely, pyrolyzed chitosan (CTO) and pyrolyzed brewed waste coffee (CBC), are synthesized and thoroughly characterized. The physicochemical properties of the materials are correlated with the CO2RR to CO performance in a comprehensive study. Both the type and weight percentage of biochar significantly influence the catalytic performance of the composite. CTO, which has pyridinic- and pyridone-N species in its structure, outperforms CBC as a carbon matrix for ZnO particles, as evidenced by a higher CO selectivity and an enhanced current density at the ZnO\_CTO electrode under the same conditions. The study on various ZnO to CTO weight ratios shows that the composite with 40.6 wt % of biochar shows the best performance, with the CO selectivity peaked at 85.8% at -1.1 V versus the reversible hydrogen electrode (RHE) and a CO partial current density of 75.6 mA cm-2 at -1.3 V versus RHE. It

also demonstrates good stability during the long-term CO2 electrolysis, showing high retention in both CO selectivity and electrode activity.

#### **Biography:**

J. ZENG is a post-doc. researcher in Center for Sustainable Future Technologies @POLITO, Istituto Italiano di Tecnologia, Italy. Her research activities have been mainly focused on carbon-based and metal oxide-based electrocatalysts toward oxygen reduction and carbon dioxide reduction reactions for the applications in Li-O2 batteries, fuel cells and carbon dioxide valorisation. During her career, J. Zeng has won the award of PHD "Fondazione De Nora" (awarded by the Society of italian chemistry). She has been involved as First/Corresponding author of 20 articles and co-author of 15 articles in international peer-reviewed journals and authored 2 patents.

#### Honeycomb Structure Made Out of Protein: A Promising Biomaterial for Nanotechnology

#### Elise Jacquier<sup>1\*</sup>, Grégory Si Larbi<sup>2</sup>, Renaud Dumas<sup>2</sup> & Pierre-Henri Elchinger<sup>3</sup>

<sup>1</sup>Univ. Montpellier, CNRS, INSERM, Institut of Functional Genomic, 34000 Montpellier, France

<sup>2</sup>Univ. Grenoble Alpes, CNRS, CEA, INRAE, IRIG-DBSCI-LPCV, 38000 Grenoble, France

<sup>3</sup>Univ. Grenoble Alpes, CEA, CNRS, IRIG-DIESE-SYMMES, 38000 Grenoble, France

# Abstract:

Achieving nanopatterning of a surface is a key point in fields covering microelectronics, photovoltaic, biomedial and biosensors. The purpose of nanopatterning a surface is to increase the surface specificity to improve, for example, nanotechnological devices sensitivity. As cutting-edge technics are reaching physical limitations and become more and more expensive, light has been put on bottom-up methods. This approach relies on the organization of small building blocks to create supramolecular 2D lattices. Nowadays, constructing 2D lattices for nanopatterning is mainly based on self-assembly process with an emphasis on biological self-assembled building blocks. However, these 2D lattices depict thin height which limits their grafting capability and thereby their wider use in nanotechnological field.

In this work, we present a self-assembled protein oligomerization domain able to create large 3D honeycomb lattice based on the natural ability of the protein to self-assemble through head-tail interaction. With electron microscopy analysis, we showed that the orientation of the honeycomb structure on carbon or SiO2 surface can be modulated. Atomic force microscopy measurements revealed a height of 30 nm corresponding to 40-stacked protein for one pore of the honeycomb. Furthermore, we showed that the amino acid sequence of the protein can be modulate without altering the honeycomb structure. Noteworthy, depending on the amino acid present inside the honeycomb pores, we also showed a specific metal chelation inside the pore.

Altogether, these characteristics make this protein-based 3D lattice a grafting platform never described until now paving the way to design adaptive self-assembled structure for nanotechnological purpose.

#### **Biography:**

She holds a master's degree in Structural Biology and Biochemistry from Claude Bernard Univer-

sity in Lyon, France. For her PhD project, she chooses to work in an interdisciplinary environment mixing biochemistry, material science and physics on developing a biomaterial based on protein. From this work, one patent and one article were already published. As her main field of interest is the use of electron microscopy on biological sample, she moved to Montpellier for a Post-Doctoral position at the IGF to work on the resolution of the structure of membrane proteins involved in schizophrenia by CryoEM.

# Synthesisation of Graphene Oxide: TiO<sub>2</sub> Nanorod/Nanourchin Via a Single-step Facile Sonicated Aqueous Chemical Route

Mohd Firdaus Malek<sup>1,2,3,\*</sup>, Musa Mohamed Zahidi<sup>4</sup>, Mohamad Hafiz Mamat<sup>4</sup>, Suriani Abu Bakar<sup>5</sup>, Mohd Khairul Ahmad<sup>6</sup>, Tetsuo Soga<sup>7</sup>, Mohamad Rusop Mahmood<sup>1,4</sup>

<sup>1</sup>NANO-SciTech (NST) Laboratory, Centre for Functional Materials and Nanotechnology (FMN), Institute of Science (IOS), Universiti Teknologi MARA (UITM), 40450 Shah Alam, Selangor, Malaysia

<sup>2</sup>Electroactive Material Research (EMR) Laboratory, Centre for Functional Materials and Nanotechnology (FMN), Institute of Science (IOS), Universiti Teknologi MARA (UiTM), 40450 Shah Alam, Selangor, Malaysia

<sup>3</sup>Faculty of Applied Sciences, Universiti Teknologi MARA (UiTM), 40450 Shah Alam, Selangor, Malaysia

<sup>4</sup>NANO-ElecTronic Centre (NET), Faculty of Electrical Engineering, Universiti Teknologi MARA (UiTM), 40450 Shah Alam, Selangor, Malaysia

<sup>5</sup>Nanotechnology Research Centre, Department of Physic, Faculty of Science and Mathematics, Universiti Pendidikan Sultan Idris (UPSI), 35900, Tanjung Malim, Perak, Malaysia

<sup>6</sup>Microelectronic and Nanotechnology–Shamsuddin Research Centre (MiNT-SRC), Faculty of Electrical and Electronic Engineering, Universiti Tun Hussein Onn Malaysia (UTHM), 86400, Parit Raja, Batu Pahat Johor, Malaysia

<sup>7</sup>Department of Electrical and Mechanical Engineering, Nagoya Institute of Technology (NITech), Showa-ku, Gokiso-cho, Nagoya, 466-8555, Japan

# Abstract:

The development of graphene oxide:TiO2 nanorod/nanourchin is beneficial, especially to the research community. In this project, graphene oxide:TiO2 nanorod/nanourchin thin film was deposited by a single-step facile sonicated aqueous chemical route on FTO-coated glass substrates. The influence of graphene oxide on the properties of TiO2 thin films was investigated. A meticulous study on the film would be worthwhile and can impart pragmatic information regarding the defect evolution, which is very important for a better understanding and improvement of the quality of the film and for the fabrication of TiO2-based devices such as sensors and solar cells.

#### **Biography:**

Mohd Firdaus Malek obtained Ph.D. from Universiti Teknologi MARA (UiTM), Malaysia in 2017. He received his B.Sc. (Hons.) in Physics and masters in electrical engineering from UiTM, Malaysia in 2008 and 2012, respectively. He is currently a senior lecturer and research fellow at the faculty of

Applied Sciences and Institute of Science (IOS), UiTM, respectively. His field of research covers nanomaterials and nanodevices. He has authored over 100 journal articles and conference proceedings.

#### Reduced Graphene Oxide-based Inverter Applied to Ion Detection in Aqueous Media

### Nicolas Battaglini<sup>1\*</sup>, Rassen Boukraa<sup>1</sup>, Giorgio Mattana<sup>1</sup>, Benoît Piro<sup>1</sup>

<sup>1</sup>ITODYS, Université Paris Cité, Paris, France

#### Abstract:

Graphene-based transistors are becoming promising building blocks in the large field of Chemical Logic but also for application as biosensors, requiring highly stable materials in aqueous and biological media. The low-cost fabrication process of reduced Graphene Oxide Electrolyte-Gated Transistors (rGO-EGFETs) from homemade formulation of surfactant-free Graphene Oxide (GO) ink paves the way to the development of cheap and competitive graphene-based logic gates, operating at low-voltage thanks to the thin double layer capacitance forming at the electrolyte/ conductive layer interfaces.

In this work, we investigate the conception of a complementary-like inverter from two rGO-EG-FETs, with different doping states induced either by changing the reduction charge amount or the nature of the electrolyte itself. In both cases, the system of coupled transistors is analogous to two resistors in series. The switch between high and low levels occurs when the value of one resistor becomes significantly lower than the other one, while changing the applied gate voltage. We further investigate such rGO-based logic gates as ion-sensors through the functionalization of the gate with an ionophore-based membrane: A sufficient change of the Gate/Electrolyte capacitance, induced by the accumulation of the targeted ion (e.g. K+), could lead to a shift of the electrical properties of one transistor and trigger the switch.

#### **Biography:**

Nicolas Battaglini is assistant professor in the chemistry department (ITODYS lab, team Bioelectronics and Smart Surfaces) of Université Paris Cité (France). He obtained his PhD degree in the field of physics of materials from Aix-Marseille Université (France) in 2004, followed by a postdoctoral stay at Université Paris Diderot (France). His current research activities focus on electronic properties of assemblies of functional organic and graphene-based materials for printed electronics applications.

#### Reactivity of Nanodiamond Aqueous Suspension Under Illumination

#### Hugues A. Girard

Université Paris-Saclay, CEA, CNRS, NIMBE, CEDEX, 91 191 Gif-Sur-Yvette, France

#### **Abstract:**

Among the nano-carbon family, nanodiamonds (NDs) possess unique properties and have been intensively studied over the past 20 years. Synthesized either by detonation-based techniques or by milling of macroscopic synthetic or natural material, NDs can be obtained in the form of 2-10

nm spherical particles or 2-100 nm faceted particles, respectively. They exhibit at the nanometric scale most of the electronic, optical and mechanical properties of bulk diamond combined to a versatile carbon-based surface chemistry, which can be efficiently adjusted via wet chemistry and/ or gas-phase treatments (annealing, plasma). Furthermore, playing on the functional groups present at their surface, NDs behave colloidal properties in aqueous or organic media, with cationic or anionic behaviors, without any help of surfactants. Thanks to the association of these surface and core -related properties, NDs are nowadays studied for a wide range of applications in medical, energy-related or quantum-related domains.

This contribution will focus on the behavior of aqueous suspensions of NDs under irradiation from UV to Gamma Rays. The influence of their surface chemistry, their source or their colloidal characteristics on water decomposition and the associated production of oxidizing/reductive reagents will be detailed. Indeed, for photocatalytic and nanomedical applications, the way NDs can promote or inhibit the production of reactive oxygen species and/or solvated electrons is essential to understand and will be discussed here.

#### **Biography:**

Hugues Girard, Dr, HDR, holds more than ten years' expertise in the field of the diamond particles toward biomedical or energy-related applications. Among his current research topics, he drives the development of boron-doped diamond core/shells particles and works on nanodiamond hybrid systems toward energy-related application. He is also involved in more fundamental studies linked to the behavior of nanodiamonds during radiolysis processes. He has authored or co-authored more than 60 publications in refereed journals, and deposited 7 patents.

#### The Nv-…N+ Charged Pair in Diamond: A Quantum-mechanical Investigation

#### Anna Maria Ferrari

University of Torino Dipartment of Chemistry Via P. Giuria 5 10125 Torino Italy

#### **Abstract:**

The NV...N+ charged pair in diamond has been investigated by using a Gaussian-type basis set, the B3LYP functional, the supercell scheme and the CRYSTAL code. It turns out that: (i) when the distance between the two defects is larger than 6–7 Å, the properties of the double defect are the superposition of the properties of the individual defects. (ii) The energy required for the reaction NVO + Ns - NV + N+ is roughly 1.3 eV at about 12 Å, irrespective of the basis set and functional adopted, and remains negative at any larger distance. (iii) These results support the observation of a charge transfer mechanism through a Ns - NVO donation occurring in the ground state, through a tunnelling process, without irradiation. (iv) The IR spectrum of the two subunits is characterized by specific peaks, that might be used as fingerprints. (v) Calculation of electrostatic interaction permitted an estimate of the effective charge of the defects.

# How Disordered are Disordered ${\rm sp}_2\mbox{-}{\rm based}$ Carbons? Insights from Wide-angle Neutron-Scattering Analysis.

#### **Bernd Smarsly**

Justus-Liebig-University, Germany

#### Abstract not available!!

# Revealing The Nature of Optical Activity in Carbon Dots Produced from Different Chiral Precursor Molecules

Elena V. Ushakova<sup>\*1</sup>, Ananya Das<sup>2</sup>, Evgeny V. Kundelev<sup>1</sup>, Anna A. Vedernikova<sup>1</sup>, Sergei A. Cherevkov<sup>1</sup>, Denis V. Danilov<sup>3</sup>, Aleksandra V. Koroleva<sup>3</sup>, Evgeniy V. Zhizhin<sup>3</sup>, Anton N. Tsypkin<sup>1</sup>, Aleksandr P. Litvin<sup>1</sup>, Alexander V. Baranov<sup>1</sup>, Anatoly V. Fedorov<sup>1</sup>, and Andrey L. Rogach<sup>4,5</sup>

<sup>1</sup>ITMO University, Russia

<sup>2</sup>University of Rochester Medical Center, USA

<sup>3</sup>Research Park, Saint Petersburg State University, Russia

<sup>4</sup>Department of Materials Science and Engineering, and Centre for Functional Photonics (CFP), City University of Hong Kong, Hong Kong SAR, China

<sup>5</sup>Shenzhen Research Institute, City University of Hong Kong, China

#### Abstract:

Carbon dots are emissive nanoparticles promising for bio-applications due to the ease of fabrication, low toxicity, and attractive optical properties. Optical chirality, on the other hand, is an intrinsic feature inherent in many objects in nature, and it can play an important role in the formation of artificial complexes based on carbon dots for enantiomer recognition, asymmetric catalysis, etc. We developed two methods to synthesize chiral carbon dots from the commonly used precursors together with a set of different chiral precursors. First method is based on chiral shell formation on the carbon dots by carbodiimide chemistry. The fabricated chiral carbon dots demonstrate significantly improved photoluminescence compared to intrinsic nanoparticles. Moreover, those carbon dots show signals in circular dichroism spectra in the region of their absorption bands. Another method is a one-step hydrothermal synthesis where L-isomers of cysteine, glutathione, phenylglycine, and tryptophan are added in the reaction mixture. The resulting carbon dots exhibit superior optical properties: high photoluminescence quantum yields reaching 57%, chiral optical signals in the UV and visible spectral regions, and two-photon absorption. The optical characteristics of these carbon dots, which can easily be dispersed in solvents of different polarities, remained stable during pH changes in the environment and after UV exposure for more than 400 min, which opens a wide range of bio-applications. This work was financially supported by Priority 2030 Federal Academic Leadership Program and the Russian Science Foundation (RSF22-13-00294).

#### **Biography:**

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

# Fungal Biosorbents: Smart Tools for Environmental Applications

### Aslı Göçenoğlu Sarıkaya\*

Bursa Uludag University, Faculty of Science&Art, Department of Chemistry, Bursa, Turkey

#### Abstract:

Increasing industrialization leads to an increase in environmental problems all around the world. Industrial effluents like heavy metals, textile dyes, pharmaceuticals, are known to show toxicity to human, animals, plants, and microorganisms. Hence, these effluents in wastewater from industrial, agricultural and domestic discharge cause various diseases for living species. Different treatment methods like physical, chemical and biological have been developed to remove effluents from aqueous solutions. Traditional methods are expensive, ineffective and not allow to reusability. Biosorption is an alternative process of the chemical-physical methods because micro/biosorbents (bacteria, fungi, algae, yeast) are low cost and ecofriendly.

Fungal organisms are widely investigated to use as a biosorbent for remove various effluents from aqueous solutions. Dead and living fungal biomass can be used for biosorption and bioaccumulation, respectively. Fungal biosorbents can be effectively biosorbed some effluents like textile dyes, heavy metals, antibiotics, and endocrine disruptors. These sorbents can be used either native or pretreated. Reusability of these sorbents also make some advantages to scale-up process to industrial applications.

#### **Biography:**

Aslı Göçenoğlu Sarıkaya received her BS degree (2007) and MSc. degree (2009) in biochemistry from Ege University. She won an education scholarship from the European Union Commission for 1 year to study in Universidad de Miguel Hernandez in Spain. She received her Ph.D. degree from Bursa Uludag University in 2016. Her research interests are molecularly imprinted polymeric (MIP) biomaterials and biosensors, micro/nano materials and their applications, cryogels, removal of tox-ins from aqueous solutions by biosorbents, fungal seconder metabolites and their applications in textile and antimicrobial pigment production.

#### **CFx Electrodes and CFx-based Batteries**

#### **GUERIN ARAUJO DA SILVA**

Clermont Auvergne University, France

Abstract not available!!

#### **Biomimetic Polymer Capsules for Drug Delivery and Imaging**

#### Beata Miksa<sup>1\*</sup> and Małgorzata Sierant<sup>1</sup>

Centre Molecular and Macromolecular Studies Polish Academy of Science in Lodz, Poland

#### Abstract:

Biomimetic polymer capsules (PC) are prepared on a liposome framework. Liposomes, due to their high intercellular penetration and a binary encapsulation system (for hydrophobic as well as lipophilic molecules) can encapsulate bioactive agents and they have been used in pharmacology as efficient drug nanocarriers. The mechanical and chemical instability of assembled liposomes is eliminated by swelling lipid bilayers with monomers which can be in situ polymerized under UV light irradiation or a redox system. The fundamental idea of mapping the morphology of liposomes used as templates to carry out the polymerization reaction inside the lipid bilaver, has led to obtain their polymeric replicates i.e. capsules with a polymer wall with higher chemical and mechanical stability. Capsules with a synthetic nanoporous membranes are capable of exchanging molecules between their interior and surrounding environment. The diffusion process can be controlled by reactive functional groups introduced into the polymer membrane, which are sensitive to external factors e.g. light, temperature, and pH environment. In our work we synthesized photosensitive PC with the reversible cross-linked poly[2-ethylhexyl methacrylate-co-7-(4-trifluoromethyl)coumarin acrylamide] wall designed as nanocarriers for 5-fluorouracil used as an anticancer drug (New J. Chem. 2015, 39, 1506). Moreover, the intermolecular (interchain) cross-linking by dimerization of two coumarin groups exposed to light at 350 nm enabled polymer chains to bind increasing polymer density with fluorescent properties (Coll. Sur. B: Biointerfaces 2013, 111, 571). Furthermore, PC with poly(pyrrole-phenosafranin) fluorescent wall (Macromol. Chem. Phys. 2021, 2000396) can be used for variety of applications such as encapsulation of nucleotides or enzymes.

#### **Biography:**

Beata Miksa is working in CMMS PAS in Lodz, Poland. From 2007 to 2008 year she had postdoc. position at The University of Memphis. In 2006 - 2007 year she worked as research assistant at the Kansas State University in Manhattan. She interested in materials science especially polymer capsules as nanocarriers for the drug delivery system. Moreover, she synthesized phenazine analogues which can be used as potential anticancer drugs and theranostic agents.

#### Carbon Dots Derived from Biomass Sources and Their Biosensor Applications

#### Saliha Dinç\*, Meryem Kara

Selcuk University, Turkey

#### Abstract:

Carbon dots, emerging as a glowing star in the field of fluorescent nanomaterials, exhibit outstanding properties including low toxicity, biocompatibility, synthesizing by green methods, etc. so they are considered as an alternative to traditional quantum dots. Till now, carbon dots have found many applications in biosensors, bioimaging, drug delivery, etc. Recently, bioinspired techniques for the fabrication of multifunctional nanomaterials have garnered attention in many areas as in the synthesis of carbon dots. Biomass sources containing various heteroatoms such as N, P, S, etc., and abundant biorecognition and therapeutic agents provide to design heteroatom-doped multifunctional carbon dots with green, renewable, biocompatible, high throughput as well as environment-friendly properties. One of the wide applications of biomass-derived carbon dots is the development of biosensors for the detection of amino acids, enzymes, vitamins, metal ions, drugs, pesticides, etc. This talk will present an overview of biomass-derived carbon dots, synthesis, and

#### biosensor applications.

#### **Biography:**

I graduated from the University of Hacettepe with a bachelor's degree in food engineering in 1995. After working at cookie and chocolate factories, I completed my MSc thesis at Food Engineering Department in 2001 and my Ph.D. thesis at Bioengineering Department at Hacettepe University in 2012. Currently, I am working at Cumra School of Applied Sciences as an Associate Professor, at Selcuk University since 2011. My research interests mainly are the green synthesis and applications of carbon dots, molecular imprinting, and liquid and gas chromatography.

#### Utilization of Surfactants to Augment Decolorization Process by Biosorbents

#### Ülküye Dudu GÜL<sup>1\*</sup>

<sup>1</sup>Department of Bioengineering, Faculty of Engineering, Bilecik Seyh Edebali University, Bilecik, TURKEY

#### Abstract:

The development of the textile industry significantly impacts the country's economy, but also the wastewater of this industry causes some environmental problems such as water pollution. Unfortunately, textile dyes are the most important pollutants in the aquatic environment. The inexpensive treatment technologies for textile effluents continuously save their importance in order to prevent water pollution. The aim of this study is to investigate the potential of biosorbents modified by surfactants for the treatment of dye-contaminated solutions. Biological waste material was modified with surfactants to enhance biosorption capacity in this study. The effects of pH, contact time, and surfactant concentration were determined. The cationic surfactant-modified biosorbents performed higher decolorization activity than unmodified biosorbent. It is concluded that surfactants can be utilized to augment the decolorization capacity of inexpensive and eco-friendly waste biosorbents for the treatment of textile dye-contaminated water.

#### **Biography:**

Ülküye Dudu GÜL was graduated from the biology department of Ankara University, where she was also awarded her Ph.D. During her master's degree studies, she completed an internship program at Iowa State University, the USA as a Fulbright Scholar. Currently, she is a professor at the Department of Bioengineering in Bilecik Seyh Edebali University, Turkey. Her research interests are environmental biotechnology, wastewater treatment technology, biosorption, bioremediation, surfactants, microbiology, industrial microbiology, fungal and algae technology.

# Production of Delafossite CuCoO<sub>2</sub> Nanoparticles and Their Use in Photocatalysis Applications with Semiconductors for the Removal of Pollutants in Wastewater

#### Sami Dursun<sup>1\*</sup>

<sup>1</sup>Konya Technical University, Turkey



#### Abstract:

Photocatalysis is considered as one of the important technologies that can be a solution to many environmental problems, including wastewater. n-type semiconductors with high oxidation properties are used in various photocatalytic applications such as removal of organic pollutants and toxic chemicals from wastewater. However, there are limitations such as wide band gap, recombination of electron-hole pairs, and poor separation of charge carriers, which prevent these semiconductors from displaying high photocatalytic properties. In this study, it is aimed to eliminate the mentioned limitations and thus to improve the photocatalytic activity of the semiconductor. For this, heterostructured semiconductor photocatalysts were obtained by decorating delafossites CuCoO2 with p-type electrical conductivity on the semiconductor metal oxide in the narrow band gap. The structural, morphological, optical and electrical properties of both semiconductor nanofibers and heterostructured materials were studied in detail. In photocatalytic measurements, methylene blue (MB) dye was used in wastewater samples. The effect of CuCoO2 nanoparticle amount on photocatalytic performance in heterostructured photocatalysts was systematically investigated. The heterostructure with the highest photocatalytic performance was obtained with 0.35% by weight CuCoO2 and containing compositions. The degradation rate constants were found to be 83% higher compared to the semiconductor nanofiber.

#### **Biography:**

The author has been working in the Metallurgical and Materials Engineering Department of Konya Technical University in Turkey since 2014. He received his Master's (2017) and Doctorate degrees (April 2021) from the Metallurgical and Materials Engineering Department. In his master's thesis, he worked on the synthesis and characterization of new covalent organic polymers (COPs) for environmental applications. In his PhD, he synthesized photocatalysts suitable and efficient for photocatalytic applications, including the degradation of toxic chemicals and organic pollutants from wastewater, and used them in environmental applications.

#### Energy Storage in Super-activated Carbon-based Materials from Agrifood Wastes

Chiara Milanese<sup>1\*</sup> Ilaria Frosia<sup>1,2</sup>, Alessandro Girella<sup>1</sup>, Simone Puoti<sup>1</sup>, Vittorio Berbenni<sup>1</sup> Giacomo Magnani<sup>3</sup>, Daniele Pontiroli<sup>3</sup>, Mauro Riccò<sup>3</sup> Adele Papetti<sup>2</sup>

<sup>1</sup>Pavia Hydrogen Lab, C.S.G.I. & Chemistry Department, Università di Pavia, Italy

<sup>2</sup>Pavia FoodLab, Drug Science Department, Università di Pavia, Italy

<sup>3</sup>Nanocarbon Laboratory, DSMFI, Università di Parma, Italy

#### Abstract:

Recently biochar, the carbon side-product in the pyrolysis/gasification of residual waste biomasses, started to receive a widespread attention in the field of energy-storage, thanks to its hierarchical porous structure inherited from biomass precursors, its excellent chemical and electrochemical stability, high conductivity, high surface area and inexpensiveness. In particular, biochar converted to activated carbon (SSA > 1000m2 /g) through a chemical treatment with KOH appears to be a new cost-effective and environmentally-friendly carbon material with great application prospect in the field of energy-storage. We report here on the preparation of novel hierarchically-porous super-activated carbon materials originating from biochar derived by the pyrolysis of agrifood
wastes such as rice bran and husk, and melon and pumpkin peels. The chemical activation process proved to be efficient to remove the majority of impurities other than carbon, stabilizing highly porous hierarchical structures with local graphene-like morphology. The porous compounds obtained by rice bran and husk mixtures demonstrated to behave as excellent electrode materials for high-performance symmetric supercapacitors (SCs), reaching interestingly high specific capacitance. On the contrary, the materials obtained by rice bran or the vegetable peels, having specific surface area up to 3000 m2 /g, show a very good hydrogen storage ability, adsorbing up to 4.5 wt % of hydrogen in around 20 seconds at 77K and around 1.5 wt% at room temperature. Work is in progress to optimize the pyrolysis and activation conditions and to improve the performance of the materials by decoration with transition metals.

#### **Biography:**

Chiara Milanese is associate Professor at the Physical Chemistry Section of the Chemistry Department – Pavia University, where she is the scientific coordinator of the Pavia Hydrogen Laboratory. Her main research activities regard the preparation and characterization of innovative materials for solid state hydrogen storage and energy storage and topic linked to circular economy. She is Italian expert of the task 40 "Energy storage and conversion based on hydrogen" activated by IEA and member of the International Hydrogen Carrier Alliance. She is author of more than 215 papers on materials science topics on high impact factor journals (h index 33).

## Electrochemical Sensors Based on Green Ionic Liquid Nanocomposites for Determination of Environmental Pollutants

#### **Reena Saxena\* and Amit Lochab**

Department of Chemistry, Kirori Mal College, University of Delhi, Delhi - 110007, India

#### **Abstract:**

Development of environment friendly nanocomposite for the treatment of environmental pollutant is of extreme importance all over the world. Numerous anthropogenic activities like industrialization, food security and globalization have resulted in release of various environmental pollutants (toxic metal ions, drugs and pesticides). World Health Organization (WHO) has given a maximum permissible limit in water for these toxic pollutants, above which, it is hazardous for both human beings and animals. Numerous techniques are available for the detection of these environmental pollutants like FAAS, ICP-MS and HPLC etc. which are bulky, costly, time consuming and require proper training. However, electrochemical sensors are fast, portable and can execute simultaneous analysis of analyte. Selectivity can be introduced in these electrochemical sensors by fabricating with various nanocomposites having a number of functional groups. Currently, inclination towards use of greener materials in analytical field is growing day by day for the development of electrochemical sensors. Ionic liquids having low toxicity, non-volatility, wide potential window, conductivity and high electrochemical stability have presented itself as sustainable electrochemical sensing platform. Ionic liquids nanocomposite as electrochemical sensor has been extensively employed in the determination of various environmental pollutants. This presentation provides a review of different ionic liquid nanocomposite based electrochemical sensors for the detection of various environmental pollutants.

#### **Biography:**

Reena Saxena, Professor, Department of Chemistry, Kirori Mal College, University of Delhi has done her PhD from Indian Institute of Technology (IIT), Delhi, India. She is Fellow Royal Society of Chemistry (FRSC), London. Her area of research involves the separation and detection of trace heavy metal ions and organic contaminants and speciation of chromium in water samples, with the use of functionalized nanoadsorbents and polymeric materials. She is working on Green synthesized nanomaterials based colorimetric sensors and electrochemical sensors for environmental pollutants.

# Biomimetic Calcium-deficient Hydroxyapatite Deposited on a Carbon Cloth Substrate as a Biomaterial used to Accelerate Bone Regeneration

#### Florian Olivier<sup>1</sup>, Nathalie Rochet<sup>2</sup>, Sylvie Bonnamy<sup>1\*</sup>

<sup>1</sup>CNRS, Univ. Orléans, ICMN, F-45071 Orléans, France

<sup>2</sup>Univ. Côte d'Azur, CNRS, Inserm, Institut de Biologie Valrose, F-06107 Nice, France

#### **Abstract:**

This work is focused on the use of a carbon cloth substrate (CCS) as a patch, for its application in the bone regeneration field. To improve the CCS biological properties, different treatments were performed. At first, the CCS surface was coated with different biomimetic calcium phosphates phases in using a sono-electrodeposition process. An optimization of the electrochemical parameters allowed to get an uniform biomimetic carbonated calcium-deficient hydroxyapatite (CDA) coating. Then, the carbonated CDA coating was doped with bioactive strontium ions leading to biomimetic carbonated strontium-substituted CDA (Sr-CDA) coatings. We also took benefit of the CCS microporosity to adsorb bioactive molecules such as aspirin into the CCS/CDA composite biomaterial. The biocompatibility of the different composite biomaterials was studied in performing in vitro biological tests using primary human osteoblasts. It was shown a positive and dose-dependent effect of strontium addition on osteoblast activity and proliferation. An increase of the human osteoblasts viability on biomaterial was also observed with adequate drug adsorption. In vivo experiments were performed in a model of rat femoral defect. The bone defects were investigated by X-ray micro-computed tomography in order to analyze the kinetic of bone regeneration. Results highlighted the efficiency of Sr-substituted CDA/CCS biomaterials for accelerating bone defect reconstruction and improving bone healing.

#### **Biography:**

Sylvie Bonnamy is Director of Research at CNRS, ICMN-Orleans. She is internationally renowned for her expertise in the multiscale characterization (HR-TEM) and the physicochemical studies of carbon materials (carbon-based biomaterials, nanotubes, porous carbons, carbon fibers, C/C composites). She was recipient of Carbon Schunck award in Berlin in 2000. She directed 18 PhD. A track-record of 85 publications in peer-reviewed journals, 5 patents, 9 book chapters, 28 invited lectures/keynotes and about 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.

#### Functionalization of Carbon Materials for Pollution Detection and Remediation

**Mohamed Habila** 

King Saud University, Saudi Arabia

Abstract not Available!!

# Nitrogen Doped Activated Carbon Derived from Marula Nutshell Waste for use in High Performance Supercapacitors

Manoko Maubane-Nkadimeng<sup>1,2\*</sup>, Bokome Shaku<sup>1,2</sup>, Thapelo Mofokeng<sup>1,2</sup>, Neil Coville<sup>1,2</sup>, Kenneth Ozoemena<sup>1,2</sup>

<sup>1</sup>University of the Witwatersrand, South Africa

<sup>2</sup>DSI-NRF Centre of Excellence in Strong Materials, South Africa

#### Abstract:

This study reports on the valorisation of marula nutshell waste into a valuable electrode material for supercapacitors. Marula nutshell waste, a brown hard residue from marula fruits was valorised into a nitrogen-doped activated carbon (N-ACs) by KOH treatment and using melamine as a nitrogen source. The microporous and mesoporous nature of N-ACs exhibited a high surface area of 1427 m<sup>2</sup>/g and pore volume of 0.31 cm3 /g. Three electrode measurements were done in 6 M KOH and 2.5 M KNO3 aqueous electrolytes, to examine the materials in alkaline and neutral medium. The N-ACs exhibited a capacitance of 350 F/g in 6 M KOH and 248 F/g in 2.5 KNO3 electrolyte. Due to low toxicity and wider operating voltage (~2 V) of 2.5 KNO3, the material was further analysed in a symmetric device. The high surface area, the efficient presence of micropores and mesopores, defects, and the high content of nitrogen (5.1%) revealed that the material produced an outstanding energy density of 28.4 Wh/kg and a power density of 499 W/kg in 2.5 M KNO3 electrolyte. The conversion of marula nuts waste into N-ACs thus provide a means of converting biomass waste into a useful energy storage material for supercapacitors.

#### **Biography:**

Manoko Maubane-Nkadimeng is a Senior Instrument Scientist and a Researcher at the University of The Witwatersrand (Wits) in Johannesburg, South Africa. She holds a PhD degree and a Postgraduate Diploma in Higher Education from Wits University. Her research interests are in material sciences, in particular; structured carbon nanomaterials, focusing on their properties and applications in devices. Dr Maubane-Nkadimeng chaired the first virtual National Nanotechnology Young Resercher's Symposium in 2021, she is the deputy chairperson of the Employment Equity committee at Wits and the Advisory Board Member of the Faculty of Education at the University of Pretoria.

# Lithium Superoxide Stabilization through $Ir_3Li/rGO$ and Implication Toward High Energy Capacity Li-O<sub>2</sub> Batteries

#### **Hsien Hau Wang**

Argonne National Laboratory, Lemont, IL, USA

#### Abstract not Available!!

#### Atomic Layer Deposited Nickel Nanoparticle Catalysts for Dry Reforming of Methane

#### Xinhua Liang<sup>1\*</sup>, Baitang Jin<sup>1</sup>, and Shiguang Li<sup>2</sup>

<sup>1</sup>Missouri University of Science and Technology, USA

<sup>2</sup>Gas Technology Institute, USA

#### Abstract:

Highly dispersed nickel (Ni) nanoparticle (NP) catalysts were prepared by atomic layer deposition (ALD) using bis(cyclopentadienyl)nickel and hydrogen as precursors at 300 °C. Porous y-Al2O3 particles and four-channel  $\alpha$ -Al2O3 hollow fibers were used as the substrates. For comparison, Ni NPs supported on porous  $\gamma$ -Al2O3 particles were also prepared by the incipient wetness (IW) method using an aqueous solution of Ni(NO3)2.6H2O. The Ni/alumina catalyst was employed to catalyze the reaction of dry reforming of methane (DRM). The ALD Ni NPs were much more active and stable than the Ni NPs synthesized by the IW method. The greater stability could have been due to the formation of NiAl2O4 spinel during the ALD coating process, which could limit the sintering of the Ni NPs and, thus, inhibit coking during the reaction. The high catalytic activity was due to the high dispersion of Ni NPs deposited by ALD and the reduction of NiAl2O4 spinel to Ni during the DRM reaction at 850 °C. MgO and CeO2 prepared by traditional incipient wetness method were used to promote the performance of ALD-prepared Ni NPs supported on  $\alpha$ -Al2O3 hollow fibers for DRM. CeO2 could help release NiO from inactive NiAl2O4, therefore a large proportion of NiAl2O4 could be gradually reduced to metallic nickel by the reaction products of DRM at high temperature. MgO could introduce surface oxygen and enhanced the adsorption of CO2. The reduction of NiO-MgO solid solution provided the metal-support interface for CO2 activation.

#### **Biography:**

Xinhua Liang is the Linda and Bipin Doshi Associate Professor in the Doshi Department of Chemical and Biochemical Engineering at Missouri University of Science and Technology. He joined the Doshi Department as an Assistant Professor in 2012 and was promoted to Associate Professor with tenure in 2017. He attended the Chemical Engineering program at Tianjin University, earning B.S. in 2001 and M.S. in 2003. He received Ph.D. in Chemical Engineering from the University of Colorado Boulder in 2008. His research interests are in nanostructured materials synthesis and functionalization by atomic/molecular layer deposition for energy and environmental applications.

### Use of Piperidine for CO<sub>2</sub> Capture

#### Qinghua Lai<sup>1</sup>, Samir Budhathoki<sup>1</sup>, Maohong Fan<sup>1,\*</sup>

<sup>1</sup>College of Engineering and Applied Sciences, University of Wyoming, Laramie, WY, 82071, USA

#### Abstract

People are increasingly interested in capturing CO<sub>2</sub> with different amines. The performance of

piperidine on  $CO_2$  capture was evaluated under different conditions, and compared to that of monoethanolamine (MEA) conventionally used for  $CO_2$  capture. The stability of the piperidine was evaluated via cyclic  $CO_2$  sorption and desorption tests. Also, the reaction kinetics of piperidine was derived by using experimental data. The study results show that piperidine is a promising CO2 capture agent.

#### **Biography:**

Maohong Fan is the Carrell Endowed Chair and School of Energy Resources Professor in Chemical and Petroleum Engineering at the University of Wyoming, and Adjunct Professor at Georgia Tech. Dr. Fan has led and worked on many projects in the areas of chemical production, clean energy generation and environmental protection, which have been supported by various domestic and international funding agencies such as NSF, DOE and EPA, USGS and USDA in the US, New Energy and Industrial Technology Development Organization (NEDO) in Japan, the United Nations Development Programme (UNDP), and industrial companies such as Siemens and Caterpillar. He has helped various chemical, environmental and energy companies to overcome their technical challenges.

#### Triboelectric Nanogenerators for Energy Harvesting and Self-powered Sensing

## Yanguang Zhang<sup>1,\*,</sup> Shiyu Hu1, John Weber<sup>1</sup>, Shoude Chang<sup>1</sup>, Gaozhi Xiao<sup>1</sup>, Jianping Lu<sup>1</sup>, Jun Gao<sup>2</sup>, Weihong Jiang<sup>1</sup>, and Ye Tao<sup>1</sup>

<sup>1</sup>National Research Council Canada, Canada; 2Queen's University, Canada Affiliation

#### Abstract:

Tribiboelectric nanogenerators (TENGs) operate based on the conjunction of contact electrification and electrostatic induction. The former provides static surface charges, and the latter transforms the motion of the charged surface or the spatial redistribution of surface charges into electricity. This operating mechanism renders TENGs natural candidates for energy harvesting and self-powered sensing devices. TENGs with various material selections, structural designs, and working modes, have been developed to harness mechanical motions in different application scenarios. The major applications can be categorized into four areas: micro/nanopower sources, large-scale blue energy harvesting, self-powered sensors, and high voltage (HV) sources for specific systems. Self-powered sensors that have been demonstrated include, among others, tactile touch sensors, acoustic sensors, motion and acceleration sensors, chemical sensors, strain sensors, and temperature sensors. In recent years, research efforts that pursues the shape adaptability/stretchability of TENGs (stretchable TENGs) and cost reduction measures (low-cost TENGs), have emerged and grown rapidly. The development of stretchable TENGs is driven by their potential applications in wearable/implantable electronics, electronic skin, epidermal electronics, and human-machine interfacing (HMI) for internet of things (IoT). Research efforts on low-cost TENGs are aimed for improving technological competitiveness and facilitating their market proliferation to niche areas. The market size of triboelectric nanogenerators is expected to reach US\$ 134.119 million in 2025. This presentation summarizes our recent efforts at NRC on stretchable TENGs and low-cost TENGs.

#### **Biography:**

Yanguang Zhang was born in Northeast of China, in 1977. He received the B.E. degree in electrical engineering from Jilin University in China in 2000, and the Ph.D. degree in physics from Queen's University, in Canada, in 2009. He joined National Research Council Canada (NRC) after his graduation as a PhD. He has been working on many projects covering the area of organic solar cells, inorganic nanocrystals solar cells, thin-film transistors, organic thin-film memories, piezoelectric and triboelectric nanogenerators. Zhang is currently a research officer at NRC. His current research is about energy harvesting and sensing with the focus on piezoelectric and triboelectric nanogenerators.

#### The Unique Electrochemical Performance of Rotated Multilayer Graphene

#### Tereza M. Paronyan

HeXalayer LLC, Louisville, KY, USA

#### Abstract:

Carbon structures are the commonly used anode material in current commercial Li-ion batteries (LIBs) due to several advantages including high power capacity, environmental stability, and long-term cycling performance. However, the improvement of the rechargeable battery energy density remains a challenge for many battery applications.

Hexalayer develops a new class of unconventional layered carbon anode material containing slightly rotated high-quality graphene layers called incommensurate multilayer graphene (IMLG). We study the correlation of original graphene interlayer rotation to the specific capacity of LiBs applied as an anode material. The weekly interaction of graphene layers is caused by slight rotation to each other due to the synthesis process making available for an intense diffusion of Lithium atoms into storing active material/anode and providing up to five-fold (~1800 mA/g) reversible capacity improvement throughout long-term cycling. This new Innovative technology promises a new generation of lightweight high energy density secondary batteries.

#### **Biography:**

Tereza M. Paronyan is a Chief Scientist and Co-Founder of HeXalayer, LLC, she is also a Professor of Physics at Bellarmine University, KY, USA. Dr. Paronyan earned her Doctorate degree in Applied Physics in 2003 and has many years of postdoctoral experience working on nanomaterials and Energy storage areas. Her current focus is developing graphene structures as an advanced material for rechargeable batteries. She is currently leading Hexalayer's projects to commercialize her innovative technology for next-generation high-energy batteries and other energy storage. Her innovations and monographs have been published in high-impact journals and in Encyclopedias, and handbooks as well.





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