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Keynote Session

Strategies for Regeneration of Hard Tissues

Jonathan Knowles

Department of Biomaterials and Tissue Engineering, Eastman Dental Institute, Royal Free Hospital, Rowland Hill Street, London NW3 2PF, United Kingdom

Abstract:

Regeneration of bone is a critical process in dentistry and orthopaedics, to restore function. It is my view that it is always important to consider the health economics (or cost benefit analysis) when developing a new implant material. We can develop very complex devices, but if these devices are too expensive for the benefit, they will not succeed in their market area. With this in mind, I will describe some of the ways we have tried to approach the problem of bone regeneration. This presentation will describe the structure of bone and how some of these properties have been mimicked in bone graft materials. Our current work utilizes controlled release glass systems to provide ion at levels that will stimulate new bone formation. I will also describe some work utilizing fusion protein technology and couplgin this with 3D printed scaffolds for rapid regeneration of bone defects. Current work has also focused on developing new resins for 3D printing of custom fit bone graft materials and how we went about designing a new light curable degradable resin. We will also present some of our current work on developing stratified tissue such as bone and cartilage interfaces.

Health Impacts Assessment of Graphene Related Materials a Prerequisite for a Safe and Sustainable Biomedical Use

Peter Wick*, Savvina Chortarea, Daria Korejwo, Daina Romeo, Govind Gupta, and Tina Buerki-Thurnherr

Empa, Swiss Laboratories for Materials Science and Technology, Laboratory for Particles-Biology Interactions, St. Gallen, Switzerland

Abstract:

Graphene and graphene related material have attracted tremendous interest since the isolation of atomically thin sheets of graphene in 2004, due to the specific and versatile properties of these materials. However, the increasing production and use of 2D materials necessitate a thorough evaluation of the potential impact on human health. The present paper provides a compact survey of acute and long-term effects of freshly produced as well as processed graphene e.g. in graphene reinforced polymers, applications. The lung as the most sensitive organ when exposed to airborne particles was investigated mostly among the classical exposure routes like ingestions or skin interactions. Drawing from these obtained data together with recent meta-analysis and machine learning based data analysis, a comprehensive and consolidated current state of art is provided.

3D Interconnected Carbon Nanostructures for Filter Capacitor Applications

Bingqing Wei[a]* and Guowen Meng[b], Fangming Han[b], and Gan Chen[b]

[a]Department of Mechanical Engineering: University of Delaware, Newark, DE 19711, United States
[b]Key Laboratory of Materials Physics, and Anhui Key Laboratory of Nanomaterials and Nanostructures: Institute of Solid State Physics, HFIPS, Chinese Academy of Sciences, Hefei, 230031, P. R. China

Abstract:

Filter capacitors play a critical role in ensuring the quality and reliability of electrical and electronic equipment, especially memory devices and computers. Circuit filtering has been dominated by aluminum electrolytic capacitors (AECs), which, unfortunately, are always the largest electronic component due to their low volumetric capacitances. Therefore, developing new small-size filter capacitors is highly desirable to meet current and emerging digital circuits and portable electronics demands. The high areal and volumetric capacitance nature of

electric double-layer capacitors should make them ideal miniaturized filter capacitors, but they are hindered by their slow frequency responses.

We report the development of interconnected and structurally integrated carbon tube grids based electric double-layer capacitors with high areal capacitance and rapid frequency response. The grid with truly interconnected and structurally-integrated vertical and lateral carbon tubes can provide high structural stability, superior electrical conductivity, and effective open porous structure. They exhibit excellent line filtering of 120 Hz voltage signal and volumetric advantages under low-voltage operations for digital circuits, portable electronics, and electrical appliances.

Additive Manufacturing of Carbon Based Materials

David Tilve Martinez, Wilfrid Neri, Julien Roman, and Philippe Poulin*

Centre de Recherche Paul Pascal, CNRS University of Bordeaux, France

Abstract:
We present 3D carbon based structures processed by Digital Light Processing (DLP) and Direct Ink Writing (DIW), two additive manufacturing technologies. DLP offers high speed and high resolution. However, this method, which consists in photopolymerizing layers of polymers, is generally limited to transparent resins. The requirement for transparency limits the incorporation of electrically conductive fillers, hindering the fabrication of 3D objects with sensing, actuating, or communicating functionalities. Our research addresses the challenge via two approaches. In the first approach, we use Graphene Oxide (GO) as a UV transparent precursor dispersed in polymer resins. GO, which is electrically insulating, is further *in-situ* thermally reduced into conductive particles after 3D printing. In a second approach, we use thin and long carbon nanotubes that form electrically conductive percolated networks at low concentration. The achievement of conductivity for a low carbon content ensures maintaining a sufficient transparency to UV light for efficient 3D printing. The present approaches appear therefore as ways to reconcile the fast and accurate DLP technology with the manufacturing of 3D conductive objects. Example of applications will be discussed. Additionally, we will show how graphitic structures can be 3D printed via DIW of lignin-GO solutions. These solutions are processed in 3D before drying and carbonization. By tuning the relative fraction of GO and lignin, it is possible to change the density, graphitic order, and thereby the electrical and mechanical properties of the printed materials. This allows for the development of graphitic 3D materials with tunable properties.

Macromolecular Hybrid Materials and Nanostructures Based on Polysaccharides

Stergios Pispas

Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation, Athens, Greece

Abstract:
Polymeric materials and nanostructures based on natural polysaccharides, covalently or non-covalently interlocked at the molecular level with synthetic polymers are presented. The RAFT polymerization process is used to facilitate the covalent attachment of functional polymer chains on polysaccharides, creating hybrid synthetic-biological polymers with new functionalities and properties. Nanostructures through non-covalent co-assembly of (co)polymers, prepared by RAFT polymerization, with natural polysaccharides using mainly electrostatic interactions are formed and studied in aqueous solutions. Physicochemical characterization using a gamut of techniques provides information on the structure and properties of the designed materials and nanostructures. The obtained sustainable polymeric nanomaterials are expected to find applications in the biomedical field and environmental technology.

Anisotropic Nano-MOFs

Chengzhong Yua,b

aAustralian Institute for Bioengineering and Nanotechnology, University of Queensland, Australia
bSchool of Chemistry and Molecular Engineering, East China Normal University, Shanghai, China

Abstract:
Metal-organic frameworks (MOFs) are an appealing class of porous crystalline materials. The compositional and structural control of single MOFs has enjoyed great success. Construction of purpose-designed nanostructure MOF-based composites holds promise to further improve their functions and applications. MOFs have intrinsic molecular and nanoscale anisotropy, the latter is significantly amplified via nanosizing and control over facet exposure. The combination of both molecular and nanoscale engineering is expected to be a new strategy to enhance the functions of anisotropic nano-MOFs, yet this research area is still at its infancy. In this talk, we demonstrate the design of anisotropic nano-MOFs with highly controllable nanoarchitectures and compositions. We have developed a number of strategies to increase atomic anisotropy (e.g., mixed metal ions / ligands, modulating ligands) and nanoscale anisotropy (e.g., facet control and amorphization). By further using multiple site-selective growth, various unique MOFs nanocomposites and their derivates have been fabricated, e.g., MOF-on-MOF superstructures. Thanks to the precisely controlled structures and compositions at atomic and nano-scale, the resultant materials exhibit superior catalytic performances in various photo- and electro-catalytic reactions such as two or four-electron oxygen evolution and reduction reactions. Moreover, new understandings of structure-function relationship have been generated, such as the impact of heterojunction coverage on the 2e-oxygen reduction reaction performance of nano-MOF composites.

Nanoscale Carbon Materials for Emerging Battery Electrodes and Their *In Situ* Characterization

Jang-Kyo Kima,b

Department of Mechanical & Nuclear Engineering, Khalifa University, P.O. Box 127788, Abu Dhabi, United Arab Emirates
School of Mechanical & Manufacturing Engineering, University of New South Wales, Sydney, NSW 2052, Australia

Abstract:
This talk reports the recent development of novel electrodes for high-performance rechargeable batteries, such as Li-ion, Li-sulfur, Li-metal, Na-ion and Na-metal batteries. An in-depth discussion is made of the synthesis of composite electrodes consisting of active materials and nanocarbon supporters and substrates, including graphene, carbon nanotubes and electrospun carbon nanofibers. The influences of pores and cavities of various sizes and distributions, surface area, graphitizing sacrificial metals, activation and functionalizing agents on characteristics of nanocarbon materials and the electrochemical performance of the electrodes are discussed. Special focus is placed on in-depth demonstration of the underlying reaction mechanisms and the kinetics probed by real-time characterization, including *in-situ* TEM and *in-situ* XRD, depth profiling XPS and SIMS, together with theoretical analyses based on the density functional theory and molecular dynamic simulations.

References:
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[3] S. Yao, J. Cui, J. Huang, J.Q. Huang, W.G. Chong, L. Qin, J.K. Kim. Rational assembly of hollow microporous carbon spheres as P hosts for long-life sodium ion batteries. Adv. Energy Mater. 8(7) (2018) 1702267.
[4] N. Mubarak, F. Rehman, M. Ihsan-Ul-Haq, M. Xu, Y. Li, Y. Zhao, Z.T. Luo, B. Huang, J.K. Kim. Highly sodiophilic, defect-rich, lignin-derived skeletal carbon nanofiber host for sodium metal batteries. Adv. Energy Mater. 12 (2022) 2103904.

Recent Progress in the Development of Materials for Reversible Solid Oxide Cells

Meilin Liu

School of Materials Science and Engineering, Georgia Institute of Technology, 771 Ferst Drive, Atlanta, GA, USA

Abstract:

Reversible solid oxide cells show promise as the most efficient and cost-effective choice for green hydrogen production and electricity generation. However, the efficiency and longevity of these systems depend on advancements in materials development. This includes the creation of proton conductors with superior tolerance to high concentrations of steam, CO_2, and other contaminants, along with the development of electrode or catalyst materials for both the oxygen reduction reaction (ORR) and oxygen evolution reaction (OER) in dual-mode operation. In this presentation, we will start with an overview of the critical scientific challenges in advancing materials and the strategies aimed at significantly improving proton conductivity, electro-catalytic activity, and durability. We will then highlight our recent progress in the creating novel electrolyte, electrode, and catalyst materials,[1-7] with a focus on our endeavors to uncover the mechanism of transport and electrode processes. This exploration involves a combination of modeling and *in situ/operando* characterization conducted under well-controlled conditions.

Nanozeolites with Controlled Defect Sites and Structural Flexibility: Future Materials for Selective Gas Separation and Biomedicine

Svetlana Mintova

Laboratory of Catalysis and Spectrochemistry, CNRS, ENSICAEN, Normandy University, Caen, France

Abstract:

Zeolites, a class of nanoporous crystalline inorganic materials, are among the most versatile catalysts, playing a pivotal role in advancing sustainable chemistry, separation technologies, and emerging processes including biomedicine. This presentation will explore recent advancements in the field of nanosized zeolites, focusing on their synthesis, advanced characterization, and wide-ranging applications. Special emphasis will be placed on how structural defects in these materials serve as a foundation for creating future materials with enhanced reactivity and selectivity in both gas separation and biomedical applications.

The presentation will delve into the intriguing role of these imperfections, examining how they contribute to the framework's flexibility and their critical importance in the reaction centers of nanozeolites.

The utilization of nanosized zeolites in adsorption processes including gas separation ($CO_2/CH_4/H_2O$) and biomedical applications for controlled delivery of gases in hypoxic tumor (O_2/CO_2) where the selectivity and stability of the materials in colloidal suspensions is of great importance will be presented.

Symposium I: Future Biomaterials-Biomedical, Medicine and Other Applications

Session 1: Biomaterials for Cancer Treatments

Tumor Eradication by Boron Neutron Capture Therapy Using 10-boron Enriched Nanoparticles

Naoki Komatsu

Graduate School of Human and Environmental Studies, Kyoto University, Sakyo-ku, Kyoto 606-8501, Japan

Abstract:

Boron neutron capture therapy (BNCT) is a non-invasive cancer treatment with little adverse effect utilizing nuclear fission of 10B upon neutron irradiation. While neutron source has been developed from a nuclear reactor to a compact accelerator, only two kinds of drugs, boronophenylalanine (BPA) and sodium borocaptate (BSH), have been clinically used for decades despite their low tumor specificity and/or retentivity. To overcome these challenges, various boron-containing nanomaterials, or "nanosensitizers", have been designed based on micelles, (bio)polymers and inorganic nanoparticles. Among them, inorganic nanoparticles such as boron carbide (10B4C) and boron nitride (10BN) can include much higher 10B content [1], but successful *in vivo* applications are very limited [2, 3]. In this talk, I will present our successful results to eradicate tumor in cancered mouse by BNCT using 10-boron containing nanoparticles under neutron irradiation.

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Investigating the Complexation Propensity of Self-assembling Dipeptides with the Anticancer Peptide-drug Bortezomib: A Computational Study

Peter Divanach[a], Eirini Fanouraki[a], Anna Mitraki[a], Vagelis Harmandaris[b], and Anastassia N. Rissanou[c]*

[a]*Department of Materials Science and Technology, University of Crete, Voutes Campus Greece, Crete, Greece*
[b]*Department of Mathematics and Applied Mathematics, University of Crete, GR-71409, Heraklion, Crete, Greece*
[c]*Theoretical & Physical Chemistry Institute, National Hellenic Research Foundation,48 Vassileos Constantinou Avenue, 11635 Athens, Greece*

Abstract:

The investigation of potential self-assembled peptides as carriers for the delivery of the anticancer drug Bortezomib, using all-atom molecular dynamics simulations, is the topic of the present study. A series of dipeptides with a similar chemical formula to Bortezomib with hydrogel-forming ability are being investigated for their propensity to bind to the drug molecule. Dipeptides are divided into two classes, the protected FF (Fmoc-FF and Z-FF) and the LF-based (Cyclo-LF and LF) ones. The thermodynamic stability of the complexes formed in an aqueous environment, as well as key morphological features of the nanoassemblies are investigated at the molecular level. Binding enthalpy between Bortezomib and dipeptides follows the increasing order: LF < Cyclo-LF < Fmoc-FF < Z-FF under both van der Waals and electrostatic contributions. Protected FF dipeptides have higher affinity for the drug molecule, which will favor its entrapment, giving them an edge over the LF based dipeptides. By evaluating the various measures, regarding both the binding between the two components and the eventual ability of controlled drug release, we conclude that the protected FF class is more suitable for drug release of Bortezomib. The selection of the optimal candidates based on the present computational study will be a stepping stone for future detailed experimental studies, involving the encapsulation and controlled release of Bortezomib both *in vitro* and *in vivo*.

Assessment of Minimal Residual Disease in Acute Myeloid Leukemia Using Microfluidics, Nanosensors, Next Generation Sequencing and Artificial Intelligence Algorithms

Alexandra Teixeira[a], Ahmed Mahmoud[a], João Alves[b], Sara Abalde-Cela[a], Paula Ludovico[c], David Posada[b], and Lorena Diéguez[c]*

[a]INL - International Iberian Nanotechnology Laboratory, Braga, Portugal
[b]CINBIO, Universidade de Vigo, Vigo, Spain
[c]Life and Health Sciences Research Institute, Universidade do Minho, Braga, Portugal

Abstract:
Acute myeloid leukemia (AML) is the most common form of acute leukemia in adults and associated with poor prognosis. Unfortunately, most of the patients that achieve clinical complete remission after the treatment will ultimately relapse due to the persistence of minimal residual disease (MRD), that is not measurable using conventional technologies in the clinic. Despite advances in treatment, AML remains a highly fatal disease, with a 5-year survival rate of only 30 %, making essential to develop new tools for early assessment of MRD and treatment selection. In this talk, I will present our most recent work to tackle this issue.

We have developed microfluidic devices capable of concentrating leukemic blasts from peripheral blood. Blasts were later analysed using our very versatile plasmonic nanosensors based on surface enhanced Raman scattering spectroscopy (SERS), and classified using AI/ML algorithms. Finally targeting RNA-sequencing was performed on clinical samples demonstrating the significant relation between AML and autophagy and its relevance for patient prognosis.

Pt-based Nanostructured Coordination Polymers for Glioblastoma Treatment. The Resurgence of Platinum Drugs

Fernando Novio[a]*, Ramiro Pérez-Becher[a,b], Adrià Marañón Gràcia[a,b], Roger Gòmez Herrera[b], Daniel Ruiz Molina[b], Paula Alfonso Triguero[b,c], and Julia Lorenzo[c]

[a]Departament de Bioquímica i Biologia Molecular, Universitat Autònoma de Barcelona, 08193 Cerdanyola del Vallès, Spain
[b]Catalan Institute of Nanoscience and Nanotechnology, CSIC and BIST, Campus UAB, Bellaterra, 08193 Barcelona, Spain
[c]Institut de Biotecnologia i de Biomedicina, Departament de Bioquimica i Biologia Molecular, Universitat Autònoma de Barcelona, 08193 Cerdanyola del Vallès, Barcelona, Spain

Abstract:
One of the major challenges faced by the development of effective therapeutic strategies for glioblastoma (GB) remains in the presence of the blood-brain barrier which prevents the uptake of most drugs[1]. Cisplatin has been considered as a second-line therapeutic due to the restricted local bioavailability, lack of selectivity, and severe adverse effects. However, the use of Pt(IV) prodrugs open new challenges in the treatment of GB due to their therapeutic efficacy and limited systemic toxicity[2].
We propose a novel family of nanostructured coordination polymer made of a Pt(IV) prodrug derived from cisplatin that presents a notable *in vitro* therapeutic effect in GB cell lines (GL261). Moreover intranasal administration route was employed to evaluate the anticancer efficacy against orthotopic preclinical GB tumors *in vivo*[3].
Although higher intracellular uptakes of Pt-Fe NCPs were observed *in vitro* compared to cisplatin, the relative slow release and activation of Pt(IV) prodrug implies that the increase in effectiveness occurs over a long period of time with reduced systematic toxicity. Results gathered in this work *in vivo,* and other recent developments combining synergic drugs, open a future path for investigation of IN platinum derivatives for brain tumor treatment, which can be a suitable option to overcome BBB permeability challenges, even in high grade brain tumors such as GB.

References:
[1] Chaoyong Liu et al. *Front Pharmacol.* **2021**, *12*, 786700.
[2] S. E. Lawler et al., *J. Control Release* **2022**, *352*, 623-636.
[3] F. Novio et al. Nanomaterials **2022**, 12(7), 1221.

Exploring the Impact of Nanoparticle Stealth Coatings in Cancer Models: From PEGylation to Cell Membrane Coating Nanotechnology

Pablo Graván[a,b], Jesús Peña-Martínez[b], Julia López de Andrés[b], María Pedrosa[a], Martín Villegas-Montoya[a], Francisco Galisteo-González[a], Juan A. Marchal[b], and Paola Sánchez-Moreno*

[a]Department of Applied Physics, Faculty of Science, University of Granada, Granada, Spain
[b]BioFab i3D - Biofabrication and 3D (bio)printing laboratory, University of Granada, Granada, Spain

Abstract:
Nanotechnological platforms offer advantages over conventional therapeutic and diagnostic modalities. However, efficient biointerfacing of nanomaterials for biomedical applications remains challenging. In recent years, nanoparticles with different coatings have been developed to reduce non-specific interactions, prolong circulation time, and improve therapeutic outcomes. This study aims to compare various nanoparticle coatings to enhance surface engineering for more effective nanomedicines. We prepared and characterized polystyrene nanoparticles with different coatings of polyethylene glycol, bovine serum albumin, chitosan, and cell membranes from a human breast cancer cell line. The coating was found to affect colloidal stability, adhesion, and the elastic modulus of NPs. Protein corona formation and cellular uptake of NPs were also investigated, and a 3D tumor model was employed to provide a more realistic representation of the tumor microenvironment. The prepared NPs were found to reduce protein adsorption, and cell membrane-coated nanoparticles showed significantly higher cellular uptake. The secretion of proinflammatory cytokines of human monocytes after incubation with the prepared NPs was evaluated. Overall, the study demonstrates the importance of coatings in affecting the behavior and interaction of nanosystems with biological entities. The findings provide insight into bio-nano interactions and are important for the effective implementation of stealth surface engineering designs.

Iridium(III) Complexes as Potential Photosensitizers for Photodynamic Therapy

Wenfang Sun[a,b*], Bingqing Liu[b], Li Wang[b], Xinyang Sun[a], Ge Shi[c], S. Monro[d], C. G. Cameron[c], and Sherri A. McFarland[c]

[a]Department of Chemistry and Biochemistry, The University of Alabama, Tuscaloosa, AL, USA
[b]Department of Chemistry and Biochemistry, North Dakota State University, Fargo, ND, USA
[c]Department of Chemistry and Biochemistry, University of Texas at Arlington, Texas, TX, USA
[d]Department of Chemistry, Acadia University, 6 University Avenue, Wolfville, NS B4P 2R6, Canada

Abstract:
Iridium(III) complexes are promising photosensitizers for photodynamic therapy (PDT). We have synthesized several series of cationic or neutral Ir(III) complexes and evaluated their PDT effects toward melanoma cancer cells and/or breast cancer cells and tumors. The photophysics of these complexes were systematically investigated via UV-vis absorption, emission, and transient absorption spectroscopy. Singlet oxygen generation efficiencies of these complexes were investigated. A correlation between the photophysical parameters with their PDT effects was intended to be built up.

Session 2: Engineering Biomaterials

Graphene-based Hydrogels and Electrospinning: 3D Printing Techniques for Advanced Antibacterial Therapy

Cristina Martín[a,b,c*], Ariadna Bachiller[a], Andrea Ferreras[a], Juan Alcaide[b,c], Juan Pedro Fernández-Blázquez[d], Yuta Nishina[e,f], Ester Vázquez[b], and José Luis Jorcano[a,g]

[a]Department of Bioengineering, Universidad Carlos III de Madrid, 28911 Leganés, Spain
[b]Faculty of Chemical Science and Technology, University of Castilla La-Mancha, 13071 Ciudad Real, Spain
[c]Instito Regional de Investigación Científica Aplicada (IRICA), University of Castilla La-Mancha, 13071 Ciudad Real, Spain

[d]*Institute IMDEA Materials, 28906 Getafe, Spain*
[e]*Graduate School of Natural Science and Technology, Okayama University, 700-8530 Okayama, Japan*
[f]*Research Core for Interdisciplinary Sciences, Okayama University, 700-8530 Okayama, Japan*
[g]*Instituto de Investigación Sanitaria Gregorio Marañón, 28007 Madrid, Spain*

Abstract:
Extensive burns and chronic ulcers present severe challenges to the human body, often leading to immunosuppression and heightened susceptibility to infection. With an estimated 11 million new burn injuries annually requiring medical attention worldwide, and approximately 180,000 resulting in fatalities, there's a pressing need for effective skin-inspired dressings to mitigate infection risks. While collagen and fibrin hydrogels have been used for skin substitute synthesis, their mechanical stability and handling pose limitations. To address these challenges, graphene derivatives have emerged as promising additives to enhance hydrogel mechanical properties and combat infections due to their bactericidal effects. Meanwhile, advancements in bioprinting technologies offer opportunities to augment the regenerative potential of hydrogel-based constructs for wound dressing.

In this context, several hydrogels based on different polymers and containing various graphene derivatives, even functionalized to achieve bactericidal nanohybrids, have been fabricated in a pioneering way. Moreover, investigating the synergistic effects of photothermal activity and nanomaterial-mediated cell proliferation, the utilization of graphene-based materials to develop photoactive bioinks has been explored. Bioprinting experiments ensured the successful fabrication of intricate constructs, and the integration of graphene-based materials offered promising avenues for developing innovative strategies in 4D bioprinting, enabling the creation of smart tissue constructs with enhanced therapeutic capabilities, including drug delivery and bactericidal wound dressings.

Finally, electrospinning technology has gained significant attention as a versatile method for fabricating advanced wound dressings with enhanced functionalities. The fabrication of polyvinylpyrrolidone-based dressings through this novel technique and incorporating graphene oxide/zinc oxide nanocomposites as potent antibacterial agents has also been explored, resulting in final mats with unique properties, including broad-spectrum antibacterial activity for improved wound healing capabilities.

Biomedical Applications of Amorphous Calcium Carbonate Nanoparticles

Susana Carregal-Romero[a,b,c]*, Claudia Miranda-Pérez de Alejo[a,d], Marina Piñol-Cancer[a,b,d], Ainhize Urkola Arsuaga[a], Carlos Sanchez-Cano[c,e], and Jesús Ruíz-Cabello[a,b,c,f]

[a]*Center for Cooperative Research in Biomaterials (CIC biomaGUNE), Basque Research and Technology Alliance (BRTA), Donostia, Spain*
[b]*CIBER de Enfermedades Respiratorias, Madrid, Spain*
[c]*Ikerbasque, Basque Foundation for Science, Bilbao, Spain*
[d]*Euskal Herriko Unibertsitatea (UPV/EHU), Donostia, Spain*
[e]*Donostia International Physics Center, Donostia, Spain*
[f]*Departamento de Química en Ciencias Farmacéuticas, Universidad Complutense de Madrid, Madrid, Spain*

Abstract:

In nature, amorphous calcium carbonate nanoparticles (ACC NPs) serve as precursors in the formation of biogenic calcium carbonate, a key element in rocks, skeletons, and shells. The potential applications of these hydrated and metastable phases of $CaCO_3$ have been overlooked due to challenges in their manipulation and stability. However, recent years have witnessed significant progress in understanding the nucleation and crystal growth mechanisms of $CaCO_3$. These advancements have enhanced our comprehension of $CaCO_3$ biogenesis and facilitated the stabilization of ACC NPs, paving the way for new applications.

ACC nanomaterials are attractive materials for advancing in the biomedical field following the Safe and Sustainable by Design (SSbD) approach, in line with the vision of the European Chemicals Strategy for Sustainability (2020), due to their high abundance, biocompatibility, and biodegradability in innocuous subproducts. Remarkably, ACC NPs doped with Gd^{3+} have recently been applied for enhanced magnetic resonance imaging (MRI) contrast in preclinical studies.

In our work, we implemented these novel Gd-doped contrast agents for targeted imaging of atherosclerosis by decorating ACC NPs with specific ligands targeting key biomarkers of this prevalent disease. We completed our study with X-ray fluorescence analysis of arterial tissue to delve deeper into fundamental aspects of NP-targeted imaging. Additionally, we are implementing the use of ACC NPs doped with new metal ions to expand the library of applications in molecular imaging and future theranostics.

Development of Warping-free Polypropylene-based Elastomer Filament for 3D Printing of Medical Prosthesis

Bandar Almeshari[a], Mansour Alsowhib[a], and Abdulhakim Almajid[*a,b]

[a]Department of Engineering Management, College of Engineering, Prince Sultan University, PO BOX 66833, Riyadh 11586, Saudi Arabia
[b]Department of Mechanical Engineering, College of Engineering, King Saud University, PO BOX 800, Riyadh 11421, Saudi Arabia

Abstract:
The development of advanced materials for 3D printing of medical prosthetics is crucial to improving the comfort, functionality, and customization of these devices. Polypropylene is a popular material used in the manufacturing of prosthetic devices, particularly for the fabrication of prosthetic limbs and components. The combination of favorable physical properties, customizability, skin compatibility, and cost-effectiveness make polypropylene a widely used and preferred material in the field of prosthetic design and fabrication.

The use of crystalline polymers like polypropylene in 3D printing has been challenging due to warping and shrinkage of printed parts. This study presents the formulation and characterization of a novel polypropylene-based elastomer designed to reduce and mitigate warping in 3D printed parts. The elastomer combines the flexibility and resilience of a thermoplastic elastomer with the strength, chemical resistance, and biocompatibility of polypropylene.

The elastomer was developed through a systematic investigation of polymer blends and additive manufacturing process parameters. Key innovations include the incorporation of tailored elastomeric additives and the optimization of printing temperatures, bed adhesion, and cooling strategies. This approach aimed to reduce residual stresses and improve interlayer bonding, which are primary drivers of warping. Mechanical testing of the optimized elastomer composition revealed desirable properties, including high elongation at break (over 400%), low modulus (8-12 MPa), and good impact resistance.

The successful creation of this warping-resistant polypropylene elastomer represents an important advancement in materials science for 3D printing. It enables the fabrication of high-performance polymer parts with the desirable properties of polypropylene while addressing the challenges associated with printing crystalline polymers. This work has significant implications for expanding the application of additive manufacturing in industries requiring dimensional precision, such as aerospace, automotive, and medical device manufacturing.

The developed polypropylene-based elastomer enables the 3D printing of prosthetic devices that are customized to individual patient anatomy and offer improved comfort and functionality compared to traditional prosthetics. This work represents an important advancement in the field of medical additive manufacturing, providing a new material solution to enhance the quality of life for prosthetic users.

Advanced Magnetic Nanomaterials at the Frontier of the Wireless Neuromodulation

Danijela Gregurec

Friedrich Alexander University, Germany

Abstract:

Materials science plays a pivotal role in unlocking the transformative potential of converting magnetic fields into diverse neural manipulation mechanisms using nanomaterials. Magnetic materials are especially intriguing in the field of neuromodulation as they offer wireless interaction with external magnetic fields, without spatial limitations, as magnetic fields are transparent to biological tissues [1]. Firstly, the utilization of magnetic nanoparticles enables hysteresis-driven heating in high-frequency alternating magnetic fields (MFs), allowing for precise modulation of neural activity in the deep brain through activation of chemosensory ion channels [2]. Secondly, the development of novel anisotropic magnetite nanomaterials, such as magnetite nanodiscs (MNDs), has demonstrated the capability to generate piconewton torques under slow MFs through vortex magnetization-driven moments, facilitating selective activation of mechanoreceptors in neural tissues [3]. Lastly, the integration of anisotropic magnetite as ferromagnetic cores in 1D and 3D embedding enables efficient conversion of magnetic fields into electric potentials, opening avenues for wireless electrical neuromodulation [4]. Additionally, meticulous surface engineering allows for targeted interactions with neurobiological systems, combined with innovative material design, drives advancements with immense promise for revolutionizing neural interfaces and neurostimulation tools, offering less invasive and more precise interventions.

Significance of Soft Tissue Viscoelasticity in Energy Dissipation by Tissues

Frederick H. Silver[a,b]

[a]Department of Pathology and Laboratory Medicine: RWJMS, Rutgers, the State University of New Jersey, Piscataway, NJ 08854, USA
[b]OptoVibronex, LLC, Ben Franklin Tech Ventures, Bethlehem, PA 08015, USA

Abstract:
Viscoelasticity is an important physical property of all mammalian tissues. The ability to dissipate energy by tissues under mechanical loading prevents overstretching, permanent deformation, tearing, physical failure, and up- or down-regulation of mechanotransduction. For example, the stretching of skin over joints and the ability of the cornea to withstand blunt trauma depends on the ability of these tissues to store and then dissipate applied energy. The ability of these tissues to store energy elastically involves strong extensible collagen fibers in the papillary and reticular dermis of skin and in the corneal lamellae of the eye. Tissues dissipate energy effectively by reversible sliding of collagen fibers through a proteoglycan matrix and by hydrodynamic rearrange and flow of loosely bound water-molecules that surround collagen fibers and proteoglycan molecules. We have developed a new technique called vibrational optical coherence tomography to study the elastic and viscous properties of tissues *in vitro* and *in vivo*. This technique applies an acoustical-sinusoidal load at a fixed frequency and measures both the in-phase and out-of-phase deformation that results from the applied mechanical-force. The elastic and viscous contribution is determined from measurement of the resonant frequency (elastic) and the width of the decay of the deformation as a function of time (viscous). Published results for skin and cornea indicate that at loading frequencies approaching 10 Hz the viscous component of the deformation is as high as about 65% of the elastic component and decreases to about 5-10% of the elastic component above a frequency of 100 Hz.

Hybrid Inorganic-organic Materials for 4D Printed Dynamic *In vitro* Models

D. Jimenez de Aberasturi[a,b,c*], and U. Aizarna-Lopetegui[a,d] A. Urigoitia-Asua[a,d,e], and L. Valenzuela[a]

[a]CIC biomaGUNE, Basque Research and Technology Alliance (BRTA), Donostia, Gipuzkoa, 20014, Spain
[b]Centro de Investigación Biomédica en Red de Bioingeniería, Biomateriales y Nanomedicina (CIBER-BBN, ISCIII), Donostia, Gipuzkoa, 20014, Spain
[c]Ikerbasque, Basque Foundation for Science, Bilbao, 48009, Spain
[d]Department of Applied Chemistry, University of the Basque Country, Donostia, 20018, Spain
[e]POLYMAT, Basque Center for Macromolecular Design and Engineering, Donostia, 20018, Spain

Abstract:
Dynamic 4D-printed *in vitro* models can be excellent tools for studying the fundamental mechanisms governing

native tissue functions and pathophysiology, and to perform drug testing studies. However, the exact reproduction of organ motions realistically is highly challenging. For that, we have explored how incorporating inorganic nanoparticles (NPs) into organic matrixes that allow the fabrication of the models, we can generate such dynamism and can also facilitate their characterization using multimodal imaging techniques. We have demonstrated that by incorporating photo-responsive plasmonic NPs embedded within a thermoresponsive ink, highly controllable cyclic expansion-contraction changes can be achieved. Considering this, we have therefore developed a dynamic 3D printed pulmonary artery model that recreates the physical forces to which cells are exposed during arterial pulsation. We have also used a hybrid inorganic-organic mixture for the fabrication of an alveolar *in vitro* model, aiming to simulate realistic breathing motions. Developing these advanced models implies improvements in cell engineering techniques, in material designs, in 3D bioprinting techniques as well as advanced imaging tools to accurately characterize them. To address this, we are exploring the use of hybrid NPs included into the model which can also act as contrast agents for correlative imaging techniques.

Combinatory Use of Cell Secretome and Biodegradable Biomaterials for CNS Regenerative Medicine: Insights on Spinal Cord Injury and Parkinson's Disease

António J. Salgado[a,b]

[a]Life and Health Sciences Research Institute (ICVS), School of Medicine, University of Minho, Braga, Portugal
[b]ICVS/3Bs PT Associated Lab, Braga/Guimarães, Portugal

Abstract:
The low regeneration potential of the central nervous system (CNS) represents a challenge for the development of new therapeutic strategies. Mesenchymal stem cells (MSCs) have been proposed as a possible therapeutic tool for CNS disorders, namely due to the beneficial actions of their secretome. Indeed, the latter possesses a broad range of neuroregulatory factors that promote an increase in neurogenesis, inhibition of apoptosis/glial scar, immunomodulation, angiogenesis, neuronal and glial cell survival, as well as relevant neuroprotective actions into different pathophysiological contexts. Considering their protective action in lesioned sites, MSCs, and their secretome, might also improve the integration of local progenitor cells in neuroregeneration processes. In this sense their use could represent an important vehicle for the establishment of future CNS regenerative therapies. Previously we have shown that the administration of MSCs secretome in pre-clinical models of spinal cord injury (SCI) and Parkinson's Disease (PD) led to important motor and histological improvements. In order to further improve this, in the present talk we will discuss and present the outcomes of the combinatory use of MSCs secretome and biodegrable biomaterials, particularly self-assembling peptides, lypossomes and hydrogels in *in vitro* and *in vivo* models of SCI and PD.

Session 3: NanoSafety

Neural Nanotechnology: Advancing Safe Applications of Nanomaterials within the Central Nervous System

Mattia Bramini[a]*, Andrea Armirotti[b], Ester Vazquez[c], Paola Sánchez Moreno[d], Andrea Capasso[e], and Fabio Benfenti[f]

[a]Department of Cell Biology, Universidad de Granada, Granada, Spain
[b]Analytical Chemistry, Istituto Italiano di Tecnologia, Genova, Italy
[c]IRICA, Facultad de Ciencias y Tecnologías Químicas, Universidad de Castilla-La Mancha, Spain
[d]Department of Applied Physics, Universidad de Granada, Granada, Spain
[e]International Iberian Nanotechnology Laboratory, Braga, Portugal
[f]Center for Synaptic Neuroscience and Technology, Istituto Italiano di Tecnologia, Genova, Italy

Abstract:
The emerging interest toward applying nanomaterials for drug and gene delivery, biomedical imaging and diagnostic biosensors within the central nervous system prompted neuroscientists to focus on the effects of the interaction of nanostructures in contact with neural systems. This work intends to give an overview of the studies

we have carried out in the past recent years over the impact of nanotechnology to *in vitro* blood-brain barrier (BBB) model, primary neurons, astrocytes and microglia cells Mechanistic studies of nanoparticles trafficking through a human BBB *in vitro* model will be presented, guiding researchers toward the development of improved drug-delivery systems to the brain. Recently, we also challenged the BBB with innovative biomimetic lipid-based nanocarriers to potentially target glioblastoma tumour cells, with the goal of achieving higher accumulation of chemotherapeutics in deep brain tissue by minimally invasive technology. With regard to graphene-based materials for neuro-biomedical applications, the molecular mechanisms of graphene and graphene oxide bio-interaction with primary neurons and glial cells together with the possible inflammatory responses, and the possibility of using both 2D and 3D graphene-based supports as biocompatible scaffolds for biomedical applications will be extensively discussed. The final aim is to exploit the conductive properties of graphene to modulate and control the activity of neural networks grown in strict contact with such structures (focusing on both nanomedicine and nanosafety features).

Advanced Graphene Biomaterials for Cardiovascular and Antimicrobial Applications

Andreia Pereira[a], Patrícia Henriques[a], Ana Brites[a], Herbert Middleton[a], and Inês C. Gonçalves[a,b,*]

[a]i3S – Instituto de Investigação e Inovação em Saúde, Universidade do Porto, Porto, Portugal
[b]INEB – Instituto de Engenharia Biomédica, Universidade do Porto, Porto, Portugal

Abstract:
In an aging population with increasing health challenges, medical devices will need to substantially improve performance.
Making use of graphene-based materials' outstanding mechanical strength, high area/thickness ratio, conductivity and light absorption, and by playing with their properties (thickness, lateral size and oxidation), we are designing new biomaterials and medical devices with enhanced performance, with primary focus on antimicrobial and cardiovascular applications.
We explore conjugation of graphene, polymers/matrices and production techniques according to the desired application, and evaluate the interaction of the resulting graphene biomaterials with biological systems (mammalian cells, bacteria and blood components), both *in vitro* and *in vivo*. Some of the examples that will be presented are:
  i)   reinforced hydrogels for load bearing applications, that we are using to develop synthetic vascular prosthesis, such as the GO-graft for coronary bypass surgery;
  ii) energy harvesting systems for implantable electronic medical devices, that we are using to develop the iGraft, an intelligent self-powered vascular graft that generates electricity from blood flow;
  iii) light-activated antimicrobial surfaces, that we are using to develop disinfection systems like the GOcap, a disinfection cap to prevent catheter-related infections.

New Approach Methodologies (NAMs) Based on *In vitro* Ecotoxicity Models to Support the Development of Safe and Sustainable by Design (SSbD) Advanced Materials

Alberto Katsumiti*, Mikel Isasi-Vicente, Rita Ewela Ojo, Vanesa Benito, Isabel Rodríguez-Llopis, and Felipe Goñi de Cerio

GAIKER Technology Centre, Basque Research and Technology Alliance (BRTA), Zamudio, Spain

Abstract:
Currently, most approaches for environmental hazard assessment involve animal testing (i.e. OECD TG 203, 210, 230). However, for ethical reasons, society is progressing towards minimising or eliminating animal testing. New Approach Methodologies (NAMs) based on *in vitro* ecotoxicity models offer a great opportunity to reduce animal testing, while showing high sensitivity to identify the potential hazard of chemicals and materials to the environment. In addition to that, *in vitro* NAMs allow the identification of the mode of action (MoA) of these chemicals and materials. However, despite of these clear advantages, there is still a need to build up confidence on these tools and to increase robustness of these methods to make *in vitro* NAMs more predictive. Here we show

several examples on the application of *in vitro* NAMs for the environmental hazard assessment of Advanced Materials (AdMa). We also show how *in vitro* NAMs can be adapted to better reflect the environmental exposure scenarios and to become better predictors of the *in vivo* responses. For instance, some methods using fish cell lines *in vitro* may provide equivalent or similar results obtained with a standard acute fish study (OECD TG 203). Additionally, high throughput methods based on animal cell lines may allow a faster identification of potential hazard effects of AdMa, supporting an agile development of Safe and Sustainable by Design (SSbD) materials.

Sources of Biases in the *In vitro* Testing of Nanomaterials: The Role of Biomolecular Corona

Valentina Castagnola[a,b], Valeria Tomati[c], Luca Boselli[d], Clarissa Braccia[e], Sergio Decherchi[f], Pier Paolo Pompa[g], Nicoletta Pedemonte[h], Fabio Benfenati[a,b], and Andrea Armirotti[e]

[a]Center for Synaptic Neuroscience and Technology, Istituto Italiano di Tecnologia, Largo Rosanna Benzi 10, 16132 Genova, Italy
[b]IRCCS Ospedale Policlinico San Martino, Largo Rosanna Benzi 10, 16132 Genova, Italy
[c]UOC Genetica Medica, IRCCS Istituto Giannina Gaslini, Via Gaslini 5, 16147 Genova, Italy
[d]Nanobiointeractions & Nanodiagnostics, Istituto Italiano di Tecnologia, Via Morego 30, 16163 Genova, Italy
[e]Analytical Chemistry Facility, Istituto Italiano di Tecnologia, Via Morego 30, 16163, Genova, Italy
[f]Data Science and Computation Facility, Istituto Italiano di Tecnologia, via Morego, 30, Genova, 16163, Italy

Abstract:
The biological fate of nanomaterials (NMs) is driven by the specific interactions that biomolecules, naturally adhering onto their surface, engage with cell membrane receptors and intracellular organelles. The molecular composition of this layer, called biomolecular corona (BMC), depends on both the physical-chemical features of the NM and the biological media in which the NM is dispersed, and cells grow. In this work, we demonstrate that the widespread use of 10% fetal bovine serum (FBS) for *in vitro* assay is unable to recapitulate the complexity of an *in vivo* systemic administration, with NMs being transported by the blood. To this purpose, by using gold nanoparticles (GNP) and graphene oxide (GO) as test NM, we undertook a comparative journey involving proteomics, lipidomics, high throughput multiparametric *in vitro* screening, as well as single molecular feature analysis to investigate the molecular details behind this *in vivo/in vitro* bias. Our work indirectly highlights the need to introduce novel, more physiological-like media closer in composition to human plasma to produce realistic *in vitro* screening data for NMs. We also aim to set the basis to reduce this *in vitro-in vivo* mismatch, which currently limits the formulation of NMs for clinical settings.

Hazard Characterization of Hexagonal Boron Nitride at the Skin Level

Michela Carlin, Gaia Pavan, and Marco Pelin*

University of Trieste, Department of Life Sciences, Trieste, Italy

Abstract:
Hexagonal boron nitride (hBN) is a promising two-dimensional (2D) material that is attracting great interest in scientific and industrial fields thanks to its revolutionary physico-chemical properties. Since most technological applications of hBN are still at the experimental stage, the major risk for humans is mainly related to an occupational scenario, where cutaneous contact is one of the most feasible exposure routes for workers.

Hence, the toxicological potential of hBN at the skin level has been evaluated using an *in vitro* approach with different levels of complexity, both using simplified models, such as epidermal keratinocytes, and more predictive and complete systems, such a 3D model of human epidermis. The obtained results show a moderate toxic potential, that may be altered by some physico-chemical properties of the materials, such as shape and size of the flakes.

On the whole, these results contribute to elucidate the hazard posed by hBN at the skin level, with particular relevance for the definition of hBN safety.

Water-soluble Dendritic Antioxidants

Choon Y. Lee[a]*, Collins Antwi-Boasiako[a], Blessed Agbemade[a], Jaqueline H. Ko[a], Jemima Nyamogo[b], and Rebecca L. Uzarski[b]

[a]Department of Chemistry, Central Michigan University, Mount Pleasant, MI 48859, USA
[b]Department of Biology, Central Michigan University, Mount Pleasant, MI 48859, USA

Abstract:

Free radicals are produced by normal metabolic activities, stress, infection, inflammations, and other environmental factors. The excessive and persistent production of radicals can override the body's antioxidant defense capacity. These excess free radicals may attack cellular components and change the structural integrity of the molecules, resulting in a change in their cellular functions and oxidative stress. Oxidative stress may lead to health repercussions such as diabetes, arteriosclerosis, high blood pressure, cancer, inflammatory conditions, and neurodegenerative conditions. Polyphenols are well known for their health-related benefits including antioxidant activities. However, most of the phenolic antioxidants are not aqueous-soluble, decreasing their bioavailability. Therefore, our research focused on synthesizing water-soluble antioxidants in dendritic forms. In this presentation, we will present synthesis of water-soluble dendritic antioxidants as well as their antioxidant activities against 2,2-diphenyl-1-picrylhydrazyl (DPPH) radicals and protective effects on biomolecules against 2,2'-Azobis(2-amidinopropane) dihydrochloride (AAPH) radicals.

Session 4: Innovations in Sensing and Recognition

Towards Discovering Aggregation Inhibitors Against Light Chain Amyloidosis

Brotzakis Z. F.[a]*, Michoglou A[a]., Ricagno S.[b], Vendruscolo M.[c], and Skretas G.[a]

[a]Institute for Bioinnovation, BSRC Fleming, Vari, Greece
[b]Department of Biosciences, University of Milan, Milan, Italy
[c]Department of Chemistry, University of Cambridge, Cambridge, United Kingdom

Abstract:

Systemic light chain amyloidosis (AL) is a life-threatening disease caused by aggregation and deposition of monoclonal immunoglobulin light chains (LC) in target organs. Currently there is no pharmaceutical treatment targeting directly the formation of LC aggregates. In order to prevent this condition, we take an *in-silico* structure-based drug discovery approach and screen for cyclotide peptide binders that best target the primary nucleation site of the LC fibrils structure available by Cryo-EM. By using inverse folding algorithms and varying residue positions corresponding to the paratope-like loop-6 region of the kalata cyclotide, we select variants that best adopt the stable Kalata fold. These Kalata fold variants are further subjected to *in-silico* docking calculations and best binding variants are currently prioritised in GFP based assays to result in rescuing the misfolding of immunoglobulin LC aggregation.

PCR-free Sensing of Pathogen Nucleic Acid for Biomedical Applications

Emanuele Luigi Sciuto[a]*, Paolo Calorenni[a], Tommaso Gritti[b], Stefania Varani[b], Giovanni Valenti[b], Maria Vittoria Balli[b], Luca Prodi[b], and Sabrina Conoci[a,b,c]

[a]University of Messina, Messina, Italy
[b]University of Bologna, Bologna, Italy
[c]URT Lab Sens - CNR-DSFTM, Messina, Italy

Abstract:

Infectious diseases represent a crucial issue for public health, especially for those populations who live at low resource settings where undernutrition, poor hygiene practice, and underdeveloped health systems do not guarantee access to appropriate therapies and assistance. The recent pandemic of COVID-19, causing millions of

deaths and impacting dramatically the quality of life worldwide, increased this global threat leading to a huge demand of new diagnostic solutions that could be able to provide a reliable and massive molecular screening. The PCR-free sensing represents the most appealing approach since it could provide the molecular detection of a pathogen without the complex experimental procedures and system architectures required by the conventional PCR-based methods. In this contribution we present the PCR-free sensing of the *Leishmania* protozoan parasite, one of the main pathogens causing neglected tropical diseases. This novel tool is based on the electrochemical impedance spectroscopy (EIS) detection of the parasitic kinetoplast (k)DNA. The technology relied on a gold working electrode (WE) that has been modified with an array of thiol-modified oligonucleotide capture probes for the kDNA detection and quantification without the target amplification by PCR. In parallel, the effectiveness of the chemical protocol used for the WE surface functionalization has been validated by contact angle (CA) analysis. Results reported the ability of the technology to detect the genetic target down to 10 copies μL^{-1}, paving the way to develop new nanobiotechnological platform suitable for fast, time-/cost saving and sensitive diagnosis of infections in biomedical applications.

Novel Materials for an Emotion Recognition System Embedded in Fashion Items

A. Maffucci[a]*, S. Di Marco[b], L. Micheli[c], L. Sansone[d], and A. Moschitta[e]

[a]University of Cassino and Southern Lazio, Dept. of Electrical & Information Engin, Cassino, Italy
[b]Academy of Fine Arts, Frosinone, Italy
[c]University of Rome Tor Vergata, Dept. of Chemical Science and Technologies, Rome, Italy
[d]National Council of Research, Institute for Polymers, Composites and Biomaterials, Portici, Italy
[e]University of Perugia, Dept. of Bioenginnering and Medical Informatics, Perugia, Italy

Abstract:
The presentation describes the use of novel materials in a wearable sensing system integrated into fashion items, able to detect the emotional state. The system implements the paradigm of smart distributed sensors, with the front-edge made by novel sensors integrating into a portable potentiostat unit. This unit is connected to a data collector (back-edge) via Bluetooth technology, that in turns is linked to a central cloud via WiFi.

The emotional appraisal is expressed through from bodily changes triggered by the emotional events. Specifically, it is detected the presence in human sweat of chemicals like cortisol. To this end, techniques like voltammetry and electrical impedance spectroscopy are adopted, by using Screen Printed Electrodes (SPEs). Measurements are locally performed at the front-edge level, then the data are partly processed at the back-edge level and at the cloud level. Machine learning algorithms improve the selectivity of the system and its robustness against noise.

Novel materials are investigated to enhance the response of the sensing elements (SPEs), such as carbon-based nanomaterials like graphene as active electrodes or sustainable bio-materials as passive substrates.

The processed data are used to change the state (colors, shapes) of the fashion items by means of actuators. To this end, a fashion design research is investigating new active materials able to provide the desired response to the emotional state.

The activity is carried out in the frame of the project "STARGATE, Dress the future: novel combined wearable integrated systems", funded by Italian MUR under the PRIN-PNRR 2022 Program.

Chemically Programmable Bacterial Probes for the Recognition of Cell Surface Proteins

L. Motiei*, and D. Margulies

Department of Chemical and Structural Biology, Weizmann Institute of Science, Rehovot, Israel

Abstract:

In living cells, information is conveyed through a series of recognition and signaling events, often initiated by cell-surface receptors binding to extracellular signals. There has been growing interest in modifying cells with artificial receptors to impart new properties. We recently developed a method to decorate bacterial surfaces with self-assembled synthetic receptors based on modified DNA duplexes. Integrated with DNA nanotechnology, this approach allows precise modification of bacteria with nanostructures that are water-soluble, biocompatible, and programmable via self-assembly. We utilized this structural programmability to create bacterial probes (B-probes) capable of labeling different cancer cell types with distinct colors and to engineer highly fluorescent B-probes with minimized self-quenching.[1-3] Additionally, we demonstrated the versatility of this strategy by endowing bacteria with new functionalities, such as multicolor bioluminescence, surface adhesion, and interactions with proteins or cells, which hold promise for applications in cell imaging, living materials, therapeutics, and diagnostics.

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Insights into Molecular Details of Lipid-based Drug Delivery Systems from Liposomes to Lipid Nanoparticles

Mahmoud Moradi*, Ehsan Khodadadi, Ehsaneh Khodadadi, Fauzia Haque, Soheil Jamali, and Mortaza Derakhshani

Department of Chemistry and Biochemistry, Fayetteville, Arkansas, USA

Abstract:
Lipid-based drug delivery systems (DDS) are an important part of the pharmaceutical industry from the early cancer drug formulations based on drug delivery liposomes (DDLs) such as DOXIL in 1990s to recent lipid nanoparticle (LNP) based COVID vaccines. At the molecular level, however, there is little information on how DDLs, LNPs, and other lipid-based DDSs look like and how they interact with their environment or with the drugs they contain. The lipid composition plays a crucial role in the stability and function of DDLs and LNPs and the choice of lipids and their ratio has been mostly driven based in trial and error rather than a rational design approach, which is both costly and time-consuming. With the help of large-scale atomistic or near-atomic (i.e., MARTINI coarse-graining) modeling and state-of-the-art molecular dynamics simulations, we have investigated the role of lipid composition in the stability and other physical properties of both DDLs and LNPs. Our simulations reveal that cholesterol substantially alters the morphology and biophysical characteristics of both liposomes and DDLs across multiple time and length scales. These simulations provide comprehensive insights into the molecular interactions between cholesterol and other lipids, offering a nuanced understanding of DDS behavior at the atomic level. By bridging multiple time and length scales, our study advances the knowledge of lipid-based DDS mechanisms. It presents a robust computational framework for rationally designing and optimizing lipid-based DDS.

Wicking Prediction in Lateral Flow Assays: Establishing a Data-driven Structure-wicking Relationship for Porous Membranes

Kunz Willfried[a,b], Ernst Andrea[c], and Nestler Britta[a,b]

[a]Institute of Applied Materials – Microstructure Modelling and Simulation (IAM-MMS), Karlsruhe Institute of Technology (KIT), Strasse am Forum 7, 76131 Karlsruhe, Germany
[b]Institute of Digital Materials Science (IDM), Hochschule Karlsruhe - University of Applied Sciences, Willy-AndreasAllee 19 76133 Karlsruhe, Germany

*c*Sartorius Stedim Biotech GmbH, August-Spindler-Straße 11, 37079 Göttingen, Germany

Abstract:

The demand for rapid and user-friendly medical diagnostic devices, known as Point-of-CareTesting (POCT), has surged in recent years. Among these devices, lateral flow assays (LFAs) have gained popularity due to their affordability and simplicity. These assays operate by utilizing capillary-driven liquid movement—commonly referred to as wicking—through highly porous, open-pored diagnostic membranes to a designated reaction zone. However, despite their widespread use, especially in COVID-19 rapid tests, the detailed interaction mechanisms and microstructural properties of these membranes remain not fully understood. To address this gap in knowledge, we use a data-driven approach that establishes the linkages between the structure of highly porous open-pored polymeric membranes, and the capillarydriven fluid transport through them. Through the use of fluid flow simulations and image analysis, we generate a database of approximately 160 virtual membrane structures with varying geometric characteristics. By analyzing these structures, we aim to predict fluid propagation times based solely on the characteristics of porosity and ligament radius. Our findings could significantly speed up the development of new diagnostic membranes with optimized pore structures. By aligning this newly acquired knowledge with experimental data, we aim to deepen our understanding of the underlying mechanisms and microstructural features of these membranes. This, in turn, will advance the field of POCT and lead to improved healthcare outcomes.

Assembly of Double-Hydrophilic Block Copolymers Triggered by Metal Ions: Applications in Catalysis and Biology

Jean-Daniel Marty*, Stéphane Gineste, Laure Gibot, Diana Ciuculsecu-Pradines, Florence Benoît-Marquié, Barbara Lonetti, Nanccy Lauth-de Viguerie, and Christophe Mingotaud

SoftMat laboratory CNRS – University of Toulouse, France

Abstract:

Mixing double-hydrophilic block copolymers containing an ionizable complexing block and a neutral block with polyvalent metal ions (e.g., Cu^{2+}, Zn^{2+}...) leads to the spontaneous formation of polymeric colloids. Recently, we demonstrated that copolymers made of poly(acrylic acid) and poly(ethylene oxide) blocks interact efficiently with different ions (Gallium, Copper, Zyrconyl, Gadolinium...) and forms nano-objects with a diameter of 20 nm.[1-3]

These particles are biocompatible and surprisingly stable, even after dilution or under dialysis. Therefore, they were tested as contrast agent for magnetic resonance imaging (MRI). *In vivo*, these nano-objects are well tolerated by rats and show surprisingly good stability, fast urinary elimination, low RES uptake, and superior magnetic relaxivity properties even at high magnetic field. With long blood remanence this new type of Gd probe could be used for MRI at lower concentrations than currently used contrast agents. The easiness to elaborate such hybrid systems enables their use in various medical multimodal imaging techniques[1,4] or as catalysts by combining different ions with specific properties.[3] Additionally, these assemblies can be used as template leading to the formation of inorganic nanoparticles (GdPO4, iron oxide, Prussian blue...) with high colloidal stability and controlled morphology.[5]

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Utilization of Nanomaterials for Realization of Unconventional Wearables-wearables

Shideh Kabiri Ameri[a,b]*

[a]Department of Electrical and Computer Engineering, Queen's University, Kingston, Ontario, Canada
[b]Center for Neuroscience Studies, Queen's University, Kingston, Ontario, Canada

Abstract:
Wearables have found broad applications in mobile health care, Internet of Things (IoT) and Human Machine Interfaces (HMI). However, significant improvements in functionality, reliability and performance of wearable are required to enable their extended applications in and their integration with advancing smart lifestyle that we are rapidly moving towards. Nanomaterials possess extraordinary, electrical, chemical, optical and mechanical properties that can be utilized for the development of the next generation of wearables. In this talk different types of unconventional wearables enabled by utilizing nanomaterials for the applications in electroencephalography (EEG), electrocardiography (ECG), electromyography (EMG), Electrooculography (EOG), sensing skin temperature and hydration, human machine interface and IoT will be presented.

Young Researchers Presentations

Dissolvable Multistage Drug Release Microneedles for Skin Biofilm Treatment: Light Activate Killing, Anti-inflammation, and Healing

Haihan Chen*, Giacomo Reina, and Peter Wick

Particles-Biology Interactions Laboratory, Empa, Swiss Federal Laboratories for Materials Science and Technology, Lerchenfeldstrasse 5, 9014 St. Gallen, Switzerland

Abstract:
Antimicrobial resistance is a worldwide substantial threat that happened due to the horizontal transfer of antibiotic resistance between pathogens.1 This situation became more severe after COVID-19, due to the increased usage of antimicrobial drugs during the pandemic.2 Methicillinresistant Staphylococcus aureus (MRSA) is a kind of skin infection bacteria that has multi-drug resistance abilities. Traditional skin bacteria biofilm treatments (e.g. antibiotics in cream or patch formulations) have been limited due to poor drug penetration, which further leads to incomplete bacteria killing, biofilm reoccurring, and more importantly, drug resistance.3 For this study, we used light mediate generated reactive oxygen and nitrogen species (ROS and RNS) that can eradicate the. Moreover, current anti-biofilm studies are mainly focusing on antibacterial only and ignore the excessive inflammation that is triggered by bacteria death, which faces challenges such as delayed healing, impaired angiogenesis, and intravascular coagulation.4 Herein, we proposed a molecular-weight-related dissolvable microneedle patch that contains poly lactic-coglycolic acid (PLGA) nanoparticles with different molecular weights allowing multi-stage drugreleasing to treat biofilm and accompanying inflammation separately. By this, we combined a healing strategy to our microneedle system, to provide a system that can not only kill bacteria without inducing resistance and deal with inflammation.

Reactive Molecular Dynamics Simulations to Investigate Drug Delivery by Functionalized Nanoparticle

Cheherazade Trouki[a,b]*, Giovanni Barcaro[a], and Susanna Monti[c]

[a]CNR-IPCF, Institute of Chemical and Physical Processes, Pisa 56124, Italy
[b]Department of Pharmacy, University of Pisa, Pisa 56126, Italy
[c]CNR-ICCOM, Institute of Chemistry of Organometallic Compounds, Pisa 56124, Italy

Abstract:

This investigation shows how reactive molecular dynamics simulations can be used to predict the structure and dynamics of functionalized nanoparticles as drug delivery agents. Following the indications of our experimental coworkers, we focused on lipid-decorated ZnO nanoparticles and the Carfilzomib pseudo-peptide as an anticancer agent. After building appropriate models according to the experimental procedures, we simulated their behavior in various environments, representing the solvents in which they were assembled and the medium in which these vehicles released their cargo. By disclosing the details of the interaction of the metal oxide with surfactants and solvents at the atomic level and possible reactions, we could identify the crucial problems that directly affected the drug's stability, release, and performance. The experimental scientists then used these data to re-design newly tuned vehicles with calibrated shapes and appropriate functionalizations that rendered the release more efficient and controlled.

Improving Serotonine Detection: The Power of Molecular Imprinted Polymers

Adrián M. Abelairas[a]*, Giuseppe Misia[b], Juan P. Merino[c], Maurizio Prato[b], Jesús Mosquera[a], Alessandro Silvestri[d], and Alejandro Criado[a]

[a]Centro Interdisciplinar de Química e Bioloxía (CICA) and Departamento de Química, Facultade de Ciencias, Universidade da Coruña, 15071 A Coruña, Spain
[b]Center for Cooperative Research in Biomaterials (CIC biomaGUNE), Basque Research and Technology Alliance (BRTA), Paseo de Miramon 194, 20014 Donostia-San Sebastián, Spain
[c]Macromolecular Chemistry Research Group (labquimac), Department of Physical Chemistry, Faculty of Science and Technology, University of the Basque Country (UPV/EHU), 48940 Leioa, Spain
[d]Department of Molecular Sciences and Nanosystems, Ca' Foscari University of Venice, Venezia, 30170 Italy

Abstract:
Molecularly imprinted polymers (MIPs) represent a cutting-edge technology with immense potential in analyte detection. By creating synthetic binding sites within a polymer matrix, such as polypyrrole, MIPs offer a tailored approach for the detection of specific chemical species. However, the sensitivity of traditional MIPs may be compromised due to analyte diffusion through the polymer matrix. Neurotransmitters are pivotal for the optimal functioning of the brain. In recent years, there has been a growing interest in the electrochemical detection of these biological molecules, owing to its remarkable selectivity and sensitivity. This study investigates the optimization of the electrodeposition of molecularly imprinted polypyrrole on electrodes modified with Multi-Wall Carbon Nanotubes (MWCNTs), with the final aim to improve the selectivity toward the detection of monoamine neurotransmitters such as serotonin. The incorporation of the developed MIP in an electrochemical sensor enhanced specificity in serotonin detection, effectively reduced the interference from other compounds and inhibited the fouling of the electrode in protein enriched environment such as serum.

Development of Decellularized Magnet-driven Stem Cell Carriers for Cartilage Regeneration Therapy

Hanjin Huang[a]*, Junyang Li[b], Fei Pan[c], Cheng Wang[d], Liuxi Xing[a], Hua Tian[d], Feng Li[d], and Dong Sun[a]

[a]Department of Biomedical Engineering, City University of Hong Kong, Hong Kong SAR, China
[b]Department of Electronic Engineering, Ocean University of China, Qingdao, China
[c]School of Interdisciplinary Studies, Lingnan University, Hong Kong SAR, China
[d]Department of Orthopaedics, Peking University Third Hospital, Beijing, China

Abstract:
In the field of cartilage regeneration therapy, the use of cell carriers to deliver functional cells for regenerative purposes has drawn increasing attention. However, traditional cell carrier materials, typically synthetic polymers, have faced challenges in supporting desired cellular events, such as attachment, proliferation, and differentiation. This work presents the development of decellularized magnetic-driven stem cell carriers that can deliver stem cells for cartilage defect treatments in a minimal-invasive approach. Human bone marrow mesenchymal stem cells are selected for their therapeutic potential in cartilage defect treatments. The cell carriers are derived from

decellularized porcine cartilage ECM, and they have significantly preserved hyaline cartilage structures to temporarily create micro-environments similar to that of human cartilage for loaded cells during a cell delivery process. The carriers are driven by a gradient magnetic field and release cells spontaneously at the destination for over 20 days. Preclinical experiments show that cell carriers deliver stem cells to defect sites and result in better knee joint function recovery compared to control groups after surgery in a cartilage defect model. These findings highlight the potential of using decellularized microcarriers as a platform for targeted cell delivery and cartilage regeneration therapy.

Enhancing Lateral Flow Assay Sensitivity Through Computational Modeling

Farshid Jamshidi[a,b*], Andrea Ernst[c], and Britta Nestler[a,b]

[a]Institute of Digital Materials Science, Karlsruhe University of Applied Sciences (HKA), Moltkestraße 30, 76133 Karlsruhe, Baden-Württemberg, Germany
[b]Institute for Applied Materials - Microstructure Modelling and Simulation, Karlsruhe Institute of Technology (KIT), Straße am Forum 7, 76131 Karlsruhe, Baden-Württemberg, Germany
[c]Sartorius Stedim Biotech GmbH, August-Spindler-Straße 11, 37079 Göttingen, Niedersachsen, Germany

Abstract:
Lateral flow assays (LFAs) are essential diagnostic tools in resource-limited healthcare settings. Examples include pregnancy tests and rapid tests for the detection of coronavirus disease 2019 (COVID-19). These assays work by drawing a liquid sample through a porous membrane. As the liquid moves by capillary action, biochemical reactions occur that are influenced by factors such as fluid flow (convection), chemical interactions (reaction), and molecular spreading (diffusion).

The open-cell porous membrane directs the liquid and allows it to interact with specific components, such as antibodies, located at designated test and control zones. The resulting interaction between the liquid and the immobilized components produces visible color signals. The intensity of these signals indicates the presence and amount of the target substance. Accurate measurement of signal intensity is critical to determining the sensitivity of the assay. To achieve this, we need to understand the behavior of all the components involved.

In this study, we use a convection-diffusion-reaction model to assess LFA sensitivity. Our model captures the comprehensive dynamics of all LFA components, allowing for the quantification of sensitivity. In addition, the wetting properties (surface tension coefficient and contact angle) of the sample within the pore space of the membrane as well as the membrane characteristics (porosity, pore and ligament radii, permeability and tortuosity) can be integrated into the sensitivity model. In this way, we establish structure-sensitivity linkages in LFAs. This knowledge helps us design LFAs with improved sensitivity and reliability.

Blood Plasma Protein Interactions with Low-fouling Zwitterionic Polymer Brushes

Monika Spasovová[a,b*], Ivan Barvík[b], Filip Dyčka[c], Markéta Vrabcová[a,b], Michala Forinová[a,b], Dagmar Chvostová[a], Nicholas S. Lynn Jr.[a*], and Hana Vaisocherová-Lísalová[a]

[a]FZU - Institute of Physics of the Czech Academy of Sciences, Na Slovance 1999/2, 182 00 Prague, Czech Republic
[b]Charles University, Faculty of Mathematics and Physics, Institute of Physics, Ke Karlovu 5, 121 16 Prague, Czech Republic
[c]Faculty of Science, University of South Bohemia, Branišovská 1760, 370 05 České Budějovice, Czech Republic

Abstract:
Zwitterionic polymer brushes (ZwPB) are widely employed for surface modification due to their ability to mitigate non-specific biomolecular interactions (biofouling) and their potential for further functionalization. These properties make them highly effective in label-free biosensing applications, where specific binding of target molecules is crucial, since the primary objective is the detection of analytes in complex biofluids. However, despite their benefits, no existing coatings can fully prevent biofouling. To enhance the performance of these coatings, a deeper understanding of the molecular mechanisms underlying biofouling is essential.

In this study, we investigate the interactions between various ZwPB and proteins from crude human blood plasma using a combination of surface plasmon resonance (SPR), mass spectrometry (MS), and molecular dynamics simulations (MDS). Additionally, we address the limitations inherent to each of these methods in this context. SPR provides quantitative insights into the extent of fouling, while MS allows for the qualitative identification of fouled proteins. Furthermore, MDS elucidates the specific interactions between individual proteins and different types of ZwPB, offering deeper insights into the biofouling process.

Our findings contribute to the understanding of biofouling on ZwPBs and can potentially contribute to the future design and development of nano-coatings across a range of applications.

Hydrolytically Degradable and Biocompatible Highly-entangled Hydrogels

Alex I. Sunday[a], and Benjamin R. Freedman[b]

[a]Harvard College, Cambridge, Massachusetts, United States
[b]Harvard Medical School, Cambridge, Massachusetts, United States

Abstract:
Highly entangled (HE) hydrogels, utilizing long acrylamide chains with minimal crosslinking, hold potential as orthopedic adhesives and drug-delivery devices due to heightened stiffness compared to traditional hydrogels, often embrittled by higher crosslinking ratios. However, two critical factors for *in-vivo* applications—biocompatibility and degradation in biological liquids— are poorly understood for HE hydrogels. Therefore, this study aims to assess cell viability and develop a hydrolytically-degradable variant compatible with high-water-content biofluids. We hypothesize that acrylamide polymerization during hydrogel formulation promotes cell viability. Additionally, we speculate that low ratios of hydrolytically-degradable crosslinks would result in slow degradation while maintaining similar mechanical properties due to higher degrees of entanglements. 3T3 fibroblasts were exposed to conditioned media from HE hydrogels with nondegradable N, N'-Methylenebisacrylamide crosslinks (MBAA-HE) using a WST-1 assay to evaluate cell viability. The degradation of HE hydrogels with polyethylene glycol diacrylate crosslinks (PEGDA-HE) was tracked through dry weight measurements following lyophilization at 0, 7, 17, and 27 days. Mechanical properties were assessed with tensile testing at 1, 2, and 7 days. WST-1 analysis at 480 and 485 nm wavelengths revealed no cytotoxicity for MBAA-HE hydrogels. Initial findings indicated that PEGDA-HE hydrogels were slowly degrading. However, over 7 days, PEGDA-HE hydrogels exhibited elevated toughness and elasticity. These results suggested that higher degrees of polymer entanglements may impede degradation, improving toughness for longer deformation periods without fracture but decrease stiffness. Continued investigation into a PEGDA-HE hydrogel formulation balancing toughness and stiffness is needed, as toughness is relevant in mitigating continual mechanical loading and stress for orthopedic adhesives.

Symposium II: Materials for Electronics, Optics and Photonics

Session 1: Advances in Optoelectronics

Perovskite Photodetectors

Liang Li

Soochow University, Suzhou, Jiangsu, China

Abstract:
Perovskite, as a flexible and versatile semiconductor material, possesses a series of excellent optoelectronic properties, such as high light absorption coefficient, micrometer level carrier diffusion length, high mobility, and defect tolerance characteristics. These excellent semiconductor properties make perovskite materials no longer limited to traditional photovoltaic applications. My research group has been carrying out material preparation, physical properties, device structure, and functional system integration related to light-sensing application scenarios.

In this talk, I will report my group research progress on the preparation of perovskite thin films towards high-performance photodetectors with high detectivity and fast response time, which are used as basic functional units for micro spectrometers, multimodal hyperspectral imaging, and anti-noise spatially coupled optical communication, etc.

Photonic Metasurfaces Enhanced with 2D Materials for Nonlinear Applications and Optoelectronics

Odysseas Tsilipakos

Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation, 11635 Athens, Greece

Abstract:
Electromagnetic metasurfaces (MSs), ultrathin artificial materials composed of a periodic arrangement of resonant meta-atoms on a plane, have provided a platform for observing a broad range of linear (e.g., perfect absorption, wavefront manipulation, polarization control) and nonlinear (e.g., saturable absorption, frequency generation) phenomena at frequencies ranging from microwaves to the visible. To enable advanced functionalities, enhanced nonlinearity, and reconfigurability, two-dimensional (2D) photonic materials (e.g., graphene, transition metal dichalcogenides, black phosphorus, MXenes, etc.) are recently being incorporated in MS structures. In this work, we study two cases of 2D-material-enhanced metasurfaces, with important practical application: (i) a multiresonant graphene-based MS that supports tightly-confined graphene surface plasmon (GSP) resonances and can be utilized for third-harmonic generation at THz frequencies and (ii) a strongly-resonant dielectric metasurface overlaid with a transition metal dichalcogenide (TMD) layer, which can emit light at optical frequencies. In order to analyze and design such multiresonant resonant free-space structures, we develop a theoretical framework based on the concept of quasinormal modes (QNMs), i.e., the natural modes supported by non-Hermitian (leaky and/or lossy) systems. Both the linear and nonlinear spectral response can be retrieved and both specular reflection/transmission and higher diffraction orders can be accommodated by the framework. Full wave finite element method simulations are used to verify the validity of the obtained results. We find the framework to be very efficient and accurate. In addition, probing the resonant structure of the system under study provides important physical insight into the design process.

Tin Halide Perovskites for Photonics and Optoelectronics

Juan P. Martínez-Pastor

Instituto de Ciencia de Materiales de la Universidad de Valencia (ICMUV), Catedrático José Beltrán 2, 46980 Paterna, Spain

Abstract:

Metal halide ABX3 perovskites are a good solution for optoelectronic and photonic devices, being Sn-based ones the most promising non-toxic alternative. However, the use of Sn-perovskites still suffers from very low stability that can be increased by using antioxidative synthetic routes. Particularly, we have demonstrated efficient amplification of the spontaneous emission (ASE), which is achieved under relatively low excitation fluence threshold ($\approx$ 2 and $\approx$ 25 microJ/cm2 for 15 and 300 K, respectively) in backscattering and waveguiding geometries using rigid (Si/SiO2/FASnI3/PMMA) and flexible (PET/FASnI3/PMMA) substrates. Above the ASE threshold we simultaneously observed spectrally reproducible random lasing (RL) effect, which is characterized by a high mode stability and very high-quality factor that can be due to the high efficiency of light scattering by grains of the film. Further advances have been also achieved recently in FASnI3 films integrated in DBR-based vertical microcavities. Photodetectors based on inkjet-printed films of FASnI3 on ITO-prepatterned interdigitated electrodes on glass and PET substrates have been also successfully demonstrated with responsivies higher than 20 A/W in the best devices with areas as large as 3 mm2 and operational at > 100 kHz. The stability of these photodetectors under ambient conditions is not good, but operation in air is possible for several months with a transparent epoxy encapsulation. Higher stability can be obtained with 2D tin-perovskites, which also exhibit strong nonlinear optical properties. Another stable tin-perovskite is the Cs2SnI6 compound, which in the form of nanoparticles, is leading to a giant beam defocusing effect.

Fabricating Air-stable Copper Films with Exceptional Electrical Conductivity without Conventional Sintering

H. Jessica Pereira[a*], C. Elizabeth Killalea[b], David B. Amabilino[c], and Graham N. Newton[a]

[a]The GSK Carbon Neutral Laboratories for Sustainable Chemistry, School of Chemistry, University of Nottingham, Nottingham, NG7 2TU, United Kingdom.
[b]University Libre de Bruxelles, Avenue Franklin Roosevelt 50, B-1050, Bruxelles, Belgium
[c]Institut de Ciència de Materials de Barcelona, Consejo Superior de Investigaciones Científicas, Campus UAB, 08193 Bellaterra, Catalunya, Spain

Abstract:

Copper is an interesting metal, widely used in a myriad of fields including catalysis, additives, electronics, conductive inks and antimicrobial applications. Most of these applications are highly dependent on preserving the metallic nature of copper particles as oxidation alters the chemical, optical and electronic properties of copper limiting its use in these application spaces. Over the years, several methodologies have been adopted to mitigate oxidation of copper such as formation of bimetallic or alloyed particles with more stable metal/transition oxide shells protecting the core copper, fabrication of composites with other conductive material such as graphene and conducting polymers, partially embedding in substrates and use of ligands as capping agents. The use of ligands has proven to be very effective as small molecule ligands can provide sufficient protection to copper without disrupting flow of electrons between adjacent particles and therefore, particularly important for conductive applications. This talk will focus on novel, green approaches to synthesising ligand-capped metallic copper particles under ambient atmospheric conditions. The resulting metallic particles exhibit technologically important properties including, excellent oxidative stability, thermal stability, conductivity, catalytic activity and low temperature sintering capability. The latter is particularly beneficial for flexible electronics, as most of the substrates have low glass transition temperatures making them unsuitable for conventional high temperature processing. The benign nature of all chemicals and solvents used, together with the low temperature processing conditions, makes these copper particles a suitable material for diverse applications.

Long-range Supramolecular Assembly of a Pyrene-derivatized Polythiophene/MWCNTs Hybrid for Resilient Flexible Electrochromic Displays

Laura Maggini

Institute of Organic Chemistry, University of Vienna, Währinger Straße 38, 1090 Vienna, Austria

Abstract:
Organic electrochromic polymers hold great potential for integration into low-power flexible electrochromic displays due to their wide range of colors and simple processing. However, challenges such as inefficient charge transfer and degradation upon device integration hinder their practical applications. Herein, we report an innovative approach that utilizes template-induced supramolecular nanostructuring to engineer nanostructured electrochromic films with enhanced performance and durability. We designed a derivative of ECP Orange bearing a pyrene appendage capable of undergoing large-scale assembly in the presence of multi-walled carbon nanotubes, resulting in a compact, reproducible lamellar morphology when deposited onto conductive PET-ITO electrodes via spray-casting, a scalable and industrially compatible process for F-ECD manufacturing. Thanks to this nanostructuring, the flexible displays based on these hybrids exhibited enhanced electrochromic efficiency (t_{90}^{OX} = 3.6 s, t_{90}^{RED} = 0.3 s) and durability (ΔE_{50} 18k cycles) compared to those prepared with the pristine, unstructured polymer (t_{90}^{OX} = 53.2 s, t_{90}^{RED} = 2.5 s; ΔE_{50} 300 cycles). These performances were also maintained in larger-scale devices (20 cm^2), which still exhibited fast electrochromic switching (t_{90}^{OX} = 0.8 s, t_{90}^{RED} = 0.9 s). Importantly, in this work ECP Orange was employed as model compound to test our methodology, but this strategy could be virtually applicable to any polythiophene-based polymer, opens up a wide range of possibilities for colorful electrochromic displays in IoT applications. This work highlights the pivotal role of supramolecular nanostructuring in delivering high-performance functional organic materials suitable for real-world device applications.

Controllable Circular Polarization Lasing via Chiral Metamaterials

I. Katsantonisa,b, A. Tasolamproua,c, Th. Koschnyd, and M. Kafesakia,b,*

[a]*Institute of Electronic Structure and Laser, Foundation for Research and Technology Hellas (FORTH), Heraklion, Crete, Greece*
[b]*Dept. of Materials Science and Technology, Univ. of Crete, Greece.*
[c]*Dept. of Physics, National and Kapodistrian University of Athens, Athens, Greece*
[d]*Ames Lab and Dept. of Physics and Astronomy, Iowa State University, Ames, Iowa, USA*

Abstract:
We discuss and demonstrate numerically an ultracompact metasurface structure able to provide lasing of dynamically controllable polarization, ranging from linear to circular and from left-handed to right-handed circular. The metasurface is composed of metallic chiral scatterers properly embedded in a gain material comprising of dye molecules. A detailed coupled quantum-classical simulation model allows self-consistent simulations of the gain-metamaterial interplay, demonstrating the lasing emission is a pump-probe simulation approach.

Integration of Polyoxometalates into Redox-based Memory Applications: Challenges and Progress

Kirill Yu. Monakhova

Leibniz Institute of Surface Engineering (IOM), Leipzig, Germany

Abstract:
The talk will highlight recent advances in the study of polyoxometalates (POMs) as molecular capacitors and memristors (https://doi.org/10.1021/acsaelm.3c01751) for oxovanadium-based electronics (https://doi.org/10.1039/D3MH01926H). For example, the creation of a chemically programmed nano-

environment and multi-state switching of the "Au(111)–DNA-origami–POM" material obtained by assembling biocompatible precursors in solution will be discussed (https://doi.org/10.1021/acs.chemmater.3c00776). The designed biohybrid heterostructure exhibits synaptic-like behavior at room temperature. Its multi-logic function was investigated using scanning tunneling microscopy and spectroscopy. A study of switchable POM structures equipped with lanthanide-doped phthalocyanine macrocycles , which can be lithographically processed in the form of monolayers on graphite by the tip of a scanning tunnelling microscope (STM) to machine patterns with diameters ranging from 30 to 150 nm2, will also be presented (https://doi.org/10.1039/D3NH00345K).

Experimental and Theoretical Study of Spontaneous Light Emission Enhancement in ZnO Nanowires Gratings

E. Centeno[a]*, A. Martin[b,c], A. Potdevin[c], F; Réveret[c], R. Smaali[a], J. A. Capo Chichi[a], V. Kalta, E. Kachan[d], Y. Jourlin[d], M. Langlet[b], and G. Chadeyron[c]

[a]Université Clermont Auvergne, CNRS, Clermont Auvergne INP, Institut Pascal, F-63000 Clermont-Ferrand, France
[b]Université Grenoble Alpes, CNRS, Grenoble INP, LMGP, 38000 Grenoble, France
[c]Université Clermont Auvergne, CNRS, Clermont Auvergne INP, ICCF, F-63000 Clermont–Ferrand, France
[d]Laboratoire Hubert Curien, Université Jean-Monnet, Université de Lyon, IOGS, UMR CNRS 5516, 42000 Saint-Etienne, France

Abstract:
We theoretically and experimentally investigate the spontaneous light emission of ZnO nanowires arranged in grating structures. Through systematic calculations of light extraction and absorption efficiencies, along with the Purcell factor, we elucidate the influence of disorder on these optical processes. This analysis reveals the role of optical resonances in achieving directional light extraction and enhancing spontaneous emission. We demonstrate that the periodic structuring of ZnO nanowires at the micron scale is a robust and efficient solution to increase spontaneous emission efficiency.

Session 2: Detection Frontiers

Synthetic Methodologies for the Preparation of Plasmonic Nanoparticles with Chiral Morphology at the Single-particle Level

Jesús Mosquera[a]*, Sandra Baúlde[a], Alejandro Criado[a], Sara Bals[b], and Luis M. Liz-Marzán[c]

[a]Universidade da Coruña, Centro Interdisciplinar de química e bioloxía (CICA), Rúa As Carballeiras, 15071, A Coruña, Spain
[b]Electron Microscopy for Materials Science (EMAT), Universityof Antwerp, 2020 Antwerp, Belgium
[c]CICbiomaGUNE, Basque Research and Technology Alliance (BRTA) and CIBER-BBN, 20014 Donostia-San Sebastián, Spain; Ikerbasque, Basque Foundation for Science, 48013 Bilbao, Spain; Cinbio, Universidadede Vigo, 36310 Vigo, Spain

Abstract:
The field of chiral plasmonic nanoparticles (NPs) has recently experienced a significant breakthrough with the development of synthetic technologies that allows for the creation of NPs exhibiting chiral morphology at the single-particle level. A key factor driving this advancement is the utilization of chiral inducers—chiral organic molecules that, by interacting with the gold surface, effectively direct the growth of nanoparticles towards chiral morphologies.

Our research group has played an active role in designing chiral inducers and employing them to attain distinctive NPs morphologies. For example, by utilizing Au nanorods as seeds, we recently synthesized two types of anisotropic chiral Au NPs. The first type comprises a dense array of quasi-helical wrinkles surrounding the central gold nanorods, achieved using a molecule with axial chirality as chiral inducer. The second type consists of twisted

Au nanorods obtained with derivatives of the amino acid cysteine. These methodologies have yielded nanoparticles with significantly high g-factor values, reaching up to 0.2.

Exploring Anisotropic Ultra-high Frequency Thermal and Electromagnetic Properties of Structured Carbon Metastructures with Thermoelastic Optical Indicator Microscope

Arsen Babajanyan[a]*, Billi Minasyan[a], Hasmik Manukyan[a], Artyom Movsisyan[a], and Kiejin Lee[b]

[a]*Institute of Physics, Yerevan State University, Yerevan, Armenia*
[b]*Department of Physics, Sogang University, Seoul, Korea*

Abstract:
Through ultra-high frequency microwave exposure, we conducted a thorough investigation into the anisotropic thermal and electromagnetic (EM) characteristics of a structured carbon fiber/polyether ether ketone (PEEK) composite material. By using a thermo-elastic optical indicator microscope (TEOIM) alongside COMSOL Multiphysics simulations, we visualized the thermal and EM distribution within the carbon/PEEK lamina under direct heating. Our study reveals a strong correlation between the microwave heating mechanism, EM near-field distribution, and the relative orientation of EM polarization and carbon fiber direction. We estimated the thermal electrical conductivity of the composite material along the carbon fibers and their perpendicular direction to be approximately 4.5W/(m·K):0.67W/(m·K) and 39KS/m:7.7S/m, respectively. Furthermore, we identified distinct loss mechanisms for microwave power, providing valuable insights into heat mapping, which holds promise for material defect characterization and exploration. Our findings underscore the significance of carbon composite materials for engineers and developers, emphasizing their pronounced anisotropic properties at microwave frequencies.

Towards High-performance Photoactivated Organic Materials for Spin-based Quantum Sensors

Max Attwood[a]*, Felix Xu[a], Michael Newns[a], Louis Chen[a], Zhu Meng[b], Rebecca Ingle[c], Mark Oxborrow[a], Emma Bryan[a], Sandrine Heutz[a], Adrian Mena[d], Sarah K. Mann[d], Angus Cowley-Semple[d], and Sam Bayliss[d]

[a]*Department of Materials, Imperial College London, London, SW7 2AZ, United Kingdom*
[b]*Molecular Sciences Research Hub, Imperial College London, London, W12 0BZ, United Kingdom*
[c]*Department of Chemistry, University College London, London, WC1H 0AJ, United Kingdom*
[d]*James Watt School of Engineering, University of Glasgow, Glasgow, G12 8QQ, United Kingdom*

Abstract:
Organic molecules are emerging as promising candidates for a range of photoactivated quantum sensing devices such as masers and spin-ensemble magnetic field detectors. These devices rely on the photogeneration of electron spin-polarized triplet states in organic crystals of acene-doped-p-terphenyl or nitrogen-vacancy (NV) diamond. Sensing can be performed either by monitoring the spin coherence of these paramagnetic states or through their stimulated collapse by injection microwaves. However, due to inefficient electronic processes and triplet spin dynamics, the materials underpinning these technologies are hindered by either limited sensitivity or the prerequisite of a required strong light source to overcome the maser threshold. For these molecular quantum sensors to be widely applied, we must develop new materials with enhanced spin dynamics that simplify their operation and improve sensitivity.

To tackle these issues, we have designed novel approaches to tune the properties of candidate molecular systems and[2,3] synthesized several new triplet and radical-based materials capable of producing strong and long-lived electron spin polarisation. We have employed transient photoluminescence and absorption spectroscopy alongside optically detected or electron paramagnetic resonance to link their bulk electronic behaviour with their spin dynamics and, ultimately, their merit as quantum sensors. Our new materials demonstrate the capacity to operate at various resonant frequencies and can be photoexcited at more easily generated wavelengths. These results pave the way for the synthesis of more efficient and applicable molecule-enabled quantum technologies.

Design Rules for Structural Colors in All-dielectric Metasurfaces: From Individual Resonators to Collective Resonances and Color Multiplexing

Kévin Vilayphone, Mohamed Amara, Régis Orobtchouk, Fabien Mandorlo, Serge Mazauric, Xavier Letartre, Sébastien Cueff, Hai Son Nguyen, and Thomas Wood*

INSA Lyon, Ecole Centrale de Lyon, CNRS, Université Claude Bernard Lyon 1, CPE Lyon, INL, UMR5270, 69100 Villeurbanne, France

Abstract:
Obtaining vivid colours in reflectance from passive metasurfaces is of exceptional interest for large-scale display applications. Through the so-called 'colour printing' technique, exploiting resonators formed of transparent materials deployed in sub-wavelength arrays known as photonic crystal waveguides, we show that spectrally pure colours may be obtained by exploiting collective resonance effects. The materials considered are high-throughput and may be easily processed using nano-imprint techniques for high surface area coverage. Furthermore, we present an innovative design method using arrays with asymmetric lattices in order to obtain colours that are: (i) largely insensitive to the observation angle, opening up a wide range of display applications; and (ii) polarisation selective, giving rise to their use in the field of optical cryptography.

Assessment of Surface Preparation Methods for Mercury (Hg) Probe Schottky CapacitanceVoltage (MCV) on Epitaxial Silicon

Cristina Sanna[a,*], Patrick Taylor[a], Robert Hillard[b], Samuel Frey[b], Dan McDonald[b], Jonny Hoglund[b], Gyula Zsakai[c], Attila Marton[c], and Peter Horvath[c]

[a]GlobalWafers Co. Ltd, 28100 Novara, Italy
[b]Semilab USA, Billerica, Massachusetts, United States of America
[c]Semilab, H-117 Budapest, Hungary

Abstract:
Mercury probe (Hg-probe) Schottky capacitance-voltage (CV) is widely used for carrier density and resistivity profiling in silicon epitaxial layers. Preparation of the silicon surface is crucial for obtaining high-quality CV measurements. There are a variety of methods currently being used to treat bare silicon epitaxial and polished bulk surfaces in preparation for Hg-Schottky CV measurements. The treatments include wet chemical and dry treatments. Usually, the treatment can be the limiting factor for both the measurement time and quality. In this evaluation, a number of typical treatments are evaluated for P-Type Epitaxial silicon surfaces. A novel concept for treating surfaces has also been investigated, which involves placing a silicon wafer in a chamber where it is exposed to a thermal and optimized ambient. This pretreatment chamber is referred to as PTC. A physics-based assessment of the typical P-type silicon surface treatments is made and presented.

Triboelectric Sensors for a Comprehensive Normal-shear Stress Perception

Songtao Hu[a]*, Haoran Li[a], Wenhui Lu[a], Tianyu Han[a], Youzhong Xu[a], Xi Shi[a], Zhike Peng[a,b], and Xiaobao Cao[c]*

[a]Shanghai Jiao Tong University, Shanghai, China
[b]Ningxia University, Yinchuan, Ningxia, China
[c]Guangzhou Laboratory, Guangzhou, Guangdong, China

Abstract:
As an important branch of flexible electronics, flexible tactile sensors have demonstrated outstanding potential in fields like robotics, sports science and medical research. Specifically, multidimensional tactile sensors are highly desired for a comprehensive sensing of normal and shear stress. However, the constraints of the external

power supply have impeded the miniaturization, portability and continuity of tactile sensors. Triboelectric nanogenerator (TENG), an emerging technique for mechanical-to-electrical energy conversion, opens a new avenue for self-power sensing.

We reported a soft tactile sensor with a PDMS/MXene composite film as the functional layer. Inspired by the spinosum layer in the human skin, the sensor consists of four TENG units with single-electrode-mode triboelectrification to generate asymmetry electric outputs among them, which enables the decoupling of multidimensional loads. The sensitivity reached 10.15 mv N−1 with the resultant load ranging from 0 N to 8 N and the angle ranging from 0° to 30°. As a biological laboratory automation application, our sensor was installed on a robot manipulator to realize an automatic pipetting operation based on force feedback, solving the problem of droplet residue. Further, a self-powered sensing insole with a TENG sensing array was developed for the mapping of normal and shear plantar stress. The insole can dynamically capture plantar stress variations to distinguish between different states during a standing long jump, thereby enabling sports performance evaluation and rectification. Moreover, with the assistance of artificial intelligence in signal processing, our insole can precisely identify different abnormal gaits, highlighting its potential for disease diagnosis and rehabilitation.

Measurement of Emissivity with a New IR Thermal Sensor Dubbed TMOS and a New Approach

Yael Nemirovsky[a,b]*, Moshe Avraham[a], and Jonathan Nemirovsky[a]

[a]Electrical and Computer Engineering Faculty, Technion—Israel Institute of Technology, Haifa 32000, Israel
[b]TODOS Technologies, Airport city, Israel

Abstract:
The concept of emissivity has been with the scientific and engineering world since Planck formulated his blackbody radiation law more than a century ago. Nevertheless, emissivity is an elusive concept even for experts. It is a vague and fuzzy concept for the wider community of engineers. The importance of remote sensing of temperature by measuring IR radiation has been recognized in a wide range of industrial, medical, and environmental uses. One of the major sources of errors in IR radiometry is the emissivity of the surface being measured. In real experiments, emissivity may be influenced by many factors: surface texture, spectral properties, oxidation, and aging of surfaces. While commercial blackbodies are prevalent, the much-needed grey bodies with a known emissivity, are unavailable. This study describes how to achieve a calibrated and stable emissivity with a blackbody, a perforated screen, and a reliable and linear novel IR thermal sensor, dubbed TMOS. The Digital TMOS is now a low-cost commercial product, it requires low power, and it has a small form factor. The methodology is based on two-color measurements, with two different optical filters, with selected wavelengths conforming to the grey body definition of the use case under study. With a photochemically etched perforated screen, the effective emissivity of the screen is simply the hole density area of the surface area that emits according to the blackbody temperature radiation. Measured results are reported.

Session 3: Heterostructures in Electronics

Switching of Perpendicular Magnetization by Magnon Torque in All Oxide Heterostructures

Dongxing Zheng, Chen Liu, Yan Li, Aitian Chen, and Xixiang Zhang*

Physical Science and Engineering, King Abdullah University of Science & Technology, Saudi Arabia

Abstract:
The search for efficient approaches to realize local switching of magnetic moments in spintronic devices has attracted intense interests. Magnetization switching driven by magnons is a promising technology that can significantly reduce energy dissipation and potential damage to spintronic devices. We have successfully demonstrated switching of perpendicular magnetization through magnon torque in specially designed all-oxide heterostructures, namely, $SrRuO_3/NiO/SrIrO_3$ and $SrRuO_3/LaMnO_3/SrIrO_3$. Notably, field-free switching of

magnetization was realized in $SrRuO_3/LaMnO_3/SrIrO_3$ heterostructures in which a ferromagnetic $LaMnO_3/SrIrO_3$ interface was created by charge reconstruction. This ferromagnetic interface generates a spin current with out-of-plane spin polarization that breaks the mirror symmetry, consequently, facilitates the deterministic switching of magnetization through SOT of magnons. Importantly, the threshold current density needed to manipulate the magnetization is significantly lower than that in conventional metallic systems. These findings suggest a promising pathway towards the development of highly efficient, all-oxide spintronic devices based on magnons.

Manipulation of the Polarization of THz Waves by Woven Metal Mesh Structures

Tigran Abrahamyan*, Henrik Parsamyan, Davit Manukyan, Arsen Babajanyan, and Khachatur Nerkararyan

Institute of Physics, Yerevan State University, Yerevan, Armenia

Abstract:
This work experimentally investigated the rotation of the polarization of electromagnetic waves at THz frequencies by a woven mesh structure. We show that a careful choice of the woven mesh orientations concerning the propagation and polarization directions of the THz signal enables efficient resonant control over the polarization originating from the coupling of dipoles excited parallel and perpendicular to the incident field polarization. Our results can provide new insights into all-metallic free-standing THz components for polarization control, filtering, and sensing.

Ultra-high Efficiency of SOT-MRAMs Using MTJs with Strain-induced Magnetic Anisotropy

Hiroaki Yoda*, Satoru Araki, Taisuke Yoda, Yuichi Ohsawa, Yuichi Yamazaki, and Tomomi Yoda

YODA-S, Inc., Tsukuba, Ibaraki, Japan

Abstract:
To break through the limits of conventional MRAMs, MTJs with strain-induced magnetic anisotropy (SIMA-MTJs) were intensively tested as SOT-MRAM cells. Small critical switching-current of 10-25 µA and switching-voltage of about 0.06V, and almost no retention energy dependence of them were predicted and confirmed by experiments. High write efficiency of 1750 $k_B \cdot T$ /V (4.1 $k_B \cdot T/\mu A$) and high write-power efficiency of 100 ($k_B \cdot T$ /(µA·V) were obtained. The efficiency is much higher than those of conventional STT-MRAM with perpendicular magnetic anisotropy.

Furthermore, temperature dependence of retention energy of SIMA-MTJs were estimated by performing repeated measurements on the coercivity of the storage-layer and fitting the switching probability data obtained from them with Sharrock's formula. The retention energy of SIMA-MTJs at 85°C increased by 14% compared with that at room temperature on average. Also, over 300% of tunnel magnetoresistance (TMR) was demonstrated with 1.9nm thick storage-layer. Further, it was estimated that the switching current for 1.9nm thick storage-layer can be lowered to the level of 20µA with retention energy of $80k_B T$ by practically available values of interface magnetic anisotropy, Ks=1.6 erg/cm², and spin-Hall angle of 0.3.

Nanodevices Based on Carbon Nanotubes

Taher Ghomian[a,b]

[a]Department of Electrical & Computer Engineering, University of Maine, Orono, ME 04469, USA
[b]Frontier Institute for Research in Sensor Technology, University of Maine, Orono, ME 04469, USA

Abstract:
The development of high-performance devices for potential technological applications, such as portable and

implantable electronics capable of parallel monitoring and detection of several parameters has emerged as one of the ultimate goals of science and technology for next-generation electronics. During the last few decades, the use of nanomaterials has enabled the continued decrease in the size of electronics and has substantially improved their functionalities. Among a variety of nanomaterials, carbon nanotubes (CNTs) are probably the most important materials owing to their unique physical, chemical, and electronic properties. All these are coupled with 1D transport behavior, encouraging many potential applications for nanoscale devices working at room temperature. However, despite these remarkable properties and extensive studies, CNTs have yet to be used in technological applications. This is because the interaction of CNTs with the environment may not be accurately under control in a high throughput fabrication process and predicting electronic properties as different components are integrated is difficult. As such, in most conventional devices made of CNT, a large number of nanotubes are deposited on the substrate to alleviate the undesirable surrounding effect. However, to take advantage of the low dimensionality properties such as higher sensitivity, higher integration density, and low power consumption the device should be composed of a single or a few CNTs. This talk will focus on enabling reliable and high throughput fabrication of devices based on a few CNTs.

Young Researchers Presentations

Impedance Characteristics of Polycrystalline $ZnGa_2O_4$ Thin Films Under Solar Blind UV Irradiation

Reiya Kase[a]*, Ryunosuke Maeda[a], Yuya Oguma[a], Kazunuki Yamamoto[b], and Satoshi Ishii[a]

[a]Tokyo Denki University, Hiki-gun, Saitama, Japan
[b]Chiba University, Chiba-shi, Chiba, Japan

Abstract:
$ZnGa_2O_4$ (ZGO) has a wide bandgap above 4.8 eV and has potential applications in optical devices targeting solar blind (SB) light (250-280 nm). In our previous work, we found that annealing during thin film formation reduced the photocurrent in polycrystalline ZGO thin films prepared from hydrothermally synthesized nanoparticles. In this study, the impedance characteristics of polycrystalline ZGO thin films were evaluated to investigate the effect of annealing-induced grain boundary changes on the electrical properties. In the experiment, ZGO nanoparticles were first hydrothermally synthesized, then mixed with a binder and spin-coated onto the surface of a quartz substrate. Then, ZGO thin films with a thickness of 5 ⊠m were prepared by annealing the substrate for one hour in air (500-800 °C). The crystal structure of the thin films was characterized by X-ray diffraction (XRD), and the impedance was measured with SB light (254 nm) irradiation at an amplitude of 5.0 V and a frequency range of 1.0 to 5.5 MHz using comb-shaped Au electrodes on the thin film surface. The XRD spectrum showed minimal changes, with only a slight reduction in line width observed with increasing annealing temperature. However, the complex impedance plots demonstrated that the radius of the arcs corresponding to the grain boundaries increased with increasing annealing temperature, indicating an increase in grain boundary resistance. Collapse was also observed on the low frequency side of the arc. These results suggest that annealing formed a different structure near the grain boundary and increased the electrical resistance of the thin films.

Fiber-integrated Non-volatile Optical Modulator Based on $Ge_2Sb_2Te_5$

Xiang Li*, Zhihai Liu, and Yu Zhang

Key Lab of In-fiber Integrated Optics, Ministry Education of China, Harbin Engineering University, P. R. China

Abstract:
Optical modulators are vital for many applications, including telecommunication, data communication, optical computing, and microwave photonic networks. However, traditional optical modulators required optical Kerr effect and Pockels effect to operate, these devices suffered due to the low index contrasts of semiconductor materials and high-power consumption. Here, we demonstrate an all-optical non-volatile optical modulator,

based on fiber Michelson interferometer, by integrating the phase-change material Ge2Sb2Te5 (GST) with fiber. By adjusting the pulse laser to switch the phase state of phase change material, then converting optically induced reflectivity modulation in the GST-coatted arm of the interferometer into the intensity modulation at the output of the Michelson interferometer. In this Letter, the proposed fiber integrated optical modulator can realize bidirectional modulation of the intensity of output light. Experimentally, the maximum extinction ratio was ～13 dB. Moreover, a demonstration of optical multiplier and logic device is performed to prove the practical potential of the proposed optical modulator in the photonic networks. Hopefully, this study can lay some experimental basis for all-optical fiber non-volatile data transmission and optical computing in real applications.

Symposium III: Future Materials for Energy, Environment and Sustainability

Session 1: Materials for Environmental Sustainability

Nanoplastics Retention and Transport in Filtration Systems

Serge STOLL[a]*, Gabriela HUL[a], Hande OKUTAN[b,d], Philippe LE COUSTUMER[b,c], and Wei LIU[a]

[a]Department F.-A. Forel for Environmental and Aquatic Sciences, Institute for Environmental Sciences, University of Geneva, 1205, Geneva, Switzerland
[b]Université de Bordeaux Montaigne, Ecole doctorale, Pessac, France
[c]Université de Bordeaux, Bordeaux Imaging Center CBRS – INRAE- INSERM
[e]University of Mugla Sitki Kocman, Department of Geological Engineering, Mugla, Turkiye

Abstract:
Information about influence of surface charges on nanoplastics (NPLs) transport in porous media, influence of NPLs concentrations on porous media retention capacities and changes in porous media adsorption capacities in the presence of natural water components are still scarce. In this study, laboratory column experiments are conducted to investigate transport behavior of positively charged amidine polystyrene (PS) latex NPLs and negatively charged sulfate PS latex NPLs in quartz sand columns saturated with ultrapure water and Geneva Lake water (natural conditions) respectively. Results obtained for ultrapure water show that amidine PS latex NPLs have more affinity to negatively charged sand surface than sulfate PS latex NPLs because of the presence of attractive electrical forces. As for the Geneva Lake water, under natural conditions, both NPLs types and sand are negatively charged. Therefore, the presence of repulsion forces reduces NPLs affinity to sand surfaces. The calculated adsorption capacities of sand grains for the removal of both types of NPLs for both types of water are oscillating around 0.008 and 0.004 mg/ g for NPLs concentration of 100 and 500 mg L^{-1}. SEM micrography shows individual NPLs or aggregates attached to the sand and confirms the limited role of adsorption process in NPLs retention. The important NPLs retention, especially in the case of negatively charged NPLs, in Geneva Lake water saturated columns is related to heteroaggregates formation and their further straining inside narrow pores. The presence of dissolved organic matter and metal cations are then crucial to trigger aggregation process and NPLs retention.

Selenium Nanoparticle Impacts on Microorganisms: Effect of Coating, Dissolution and Aggregation

Wei Liu[a]*, Yuying Chen[b], Xiaojing Leng[b], and Serge Stoll[a]

[a]Department F.-A. Forel for Environmental and Aquatic Sciences, University of Geneva, Carl-Vogt 66, CH-1211 Geneva, Switzerland
[b]Key Laboratory of Functional Dairy, College of Food Science and Nutritional Engineering, China Agricultural University, Beijing 100083, China

Abstract:
Understanding the impact of selenium nanoparticles (SeNPs) in aquatic systems by considering SeNPs physicochemical properties and environmental media characteristics is a concern of high importance for the evaluation and prediction of risk assessment. In this study, chitosan (CS) and sodium carboxymethyl cellulose (CMC) coated SeNPs were first used as stability agents to prepare coated CS-SeNPs and CMC-SeNPs. Then, the aggregation behavior, surface charge modifications in presence of natural organic matter and ions, dissolution, and algae toxicity of CMC-SeNPs and CS-SeNPs were investigated to gain insight into the effect of different surface coatings, dissolution, and aggregation of SeNPs on algae toxicity in a natural water environment (Lake Geneva water) and a culture medium of *Poterioochromonas malhamensis*, a widespread mixotrophic flagellate. It was found that SeNPs are 5–10 times more toxic in Lake Geneva water compared to the culture medium, indicating that traditional algal tests currently conducted in Waris-H medium underestimate the toxicity of NPs in natural aquatic environments. Despite significant dissolution, results reveal that the SeNPs themselves are the main toxicity driver but not the released ions. Regarding the nature of the coating, CS-SeNPs exhibit higher toxicity in

Lake Geneva water and cell culture medium to algae cells than CMC-SeNPs. Surface coating is found the most influential toxicity factor of SeNPs in both media whereas SeNPs diameters are found a minor factor in toxicity. These results highlight the importance of considering in detail both NPs intrinsic and media properties in the evaluation of NPs biological effects.

Utilizing Reticular Chemistry: Designing Functional Materials for Environmental Solutions

Giasemi K. Angeli

Theoretical and Physical Chemistry Institute/ National Hellenic Research Foundation, Athens 11635, Greece

Abstract:
Reticular Chemistry has emerged as a powerful approach for designing tailor-made materials with specific structural and physicochemical characteristics[1]. Among these materials, Metal-Organic Frameworks (MOFs) stand out as prime examples of successful application of Reticular Chemistry principles[2]. MOFs are constructed by strategically combining organic and inorganic building units. These are usually organic carboxylate linkers presenting diverse geometry and connectivity numbers, while the inorganic building blocks (described as the secondary building unit) can either be discrete polynuclear oxo-metal clusters or one-dimensional chains[3]. The judicious selection of these building blocks according to Reticular chemistry enables precise control over the resulting framework topology, granting significant control over the pore shape, size, and functionality of MOFs[4]. Consequently, Reticular Chemistry has greatly contributed to the exponential growth of this unique family of porous materials, which continually provides us with tailor made materials for a plethora of applications, emphasizing on the fields of energy and the environment.

Herein we will present and discuss selected examples of MOFs synthesized using Reticular Chemistry principles, highlighting the significance of each building block's structural characteristics (shape, size, nuclearity and functionality) in framework formation. Diverse examples of MOFs based on multitopic carboxylate linkers and high valence metals (e.g., Zr (IV), Ce (IV) and Rare Earths (III)) will be presented in detail. Additionally, the synthetic methodologies will be analyzed alongside the materials' physicochemical characterization and performance evaluation regarding various environmental and energy-related applications.

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Nanocarbons for Sustainability Solutions and CO2 Capture

Wala Algozeeb*, and Noha Alshihri

Research and Analytical Services Department, Saudi Aramco, Dhahran, Saudi Arabia

Abstract:
The economic production of advanced materials such as nanocarbons has long been a challenge delaying their commercial deployment in various large-scale applications. In this work, production of various nanocarbons, including nonporous carbon and graphene, from low-value petroleum feeds is presented. Several petroleum feeds were studied to understand the effect of their composition on the produced nanocarbon's properties. The results showed that the properties of the produced nonporous carbon can be tuned by changing the feed and reaction parameters. Furthermore, sulfur doped carbon was produced from low value sulfur containing petroleum feeds. The utility of the porous carbon was demonstrated as a material for CO2 capture with up to 18 wt% uptake from flue gas. In addition to water harvesting from air. This work contributes to the development of sustainable freshwater resources but also addresses the challenge of valorizing petroleum waste streams, offering a dual benefit for both environmental and economic sustainability.

Transforming Waste into Sustainable Construction Materials: Durable Geopolymers from Recycled Sources

Ielo I[a], Cigala MR[a], Tripodo A[b], Sabatino G[b,c], Papanikolaou G[a], Lanzafame P[a], and De Luca G[a]

[a]Department of Chemical, Biological, Pharmaceutical and Environmental Sciences, University of Messina, Viale F. Stagno d'Alcontres, 31 – 98166 Messina, Italy
[b]Department of Mathematical and Computer Sciences, Physical Sciences and Earth Sciences, University of Messina, Viale F. Stagno d'Alcontres, 31 – 98166 Messina, Italy
[c]National Institute of Oceanography and experimental Geophysics, Via dei Mille 28 – 98057, Milazzo, Italy

Abstract:
The construction industry faces a growing challenge in managing waste materials, making the development of sustainable alternatives critical. This study investigates the preparation of geopolymers using construction and demolition waste materials, such as cement and brick waste, along with glass waste. Specifically, crushed glass was used to produce sodium silicate, a key source of silicate ions and alkali necessary in geopolymerization processes. The performance of this in-house activator was compared to that of the commercial counterpart.

Eight geopolymer formulations were prepared and characterized using SEM-EDX, IR, and XRD techniques. Durability against harsh environments was assessed through immersion in water, hydrochloric acid (pH $\sim$ 1), and sodium hydroxide (pH $\sim$ 13) solutions for seven days. The samples were then dried and weighed to determine mass loss, revealing promising resistance in certain formulations.

Our study emphasizes the potential of transforming waste materials into high-performance, durable geopolymers as construction materials. By optimizing waste-derived geopolymers, we can achieve significant environmental benefits through waste recycling and contribute to the advancement of sustainable construction technology.

Ligno-cellulosic Fiber Mediated Columnar-structure in Matrix Composite

Séverine A.E. BOYER*

CEMEF-CNRS 7635, MINES Paris PSL, SOPHIA ANTIPOLIS, France

Abstract:
Lignocellulosic fibers have countless beneficial features such as biodegradability, renewability and diversity. Further attempts are then required (virgin, recycled or selectively modified raw ligno-cellulosic fiber; quality, size or amount, etc.) to promote them as sustainable materials[1,2]. This work refines chemo-physical effect in solidification transformation. The columnar-structure induced by the ligno-cellulosic fiber types of the matrix composite is used as an indicator. Among key things, is the dependence of nature of the fiber and the number of germs activated at the interface fiber/matrix.

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Integrating Numerical Assessment and Experimental Disassembly for Sustainable Evaluation of Bonded CFRP Structures: A Life Cycle Analysis Approach

Janko Kreikemeier

German Aerospace Center, Lilienthalplatz 7, 38108, Braunschweig, Germany

Abstract:

Bonded CFRP structures offer numerous advantages over riveted CFRP structures, including faster processing speed, greater pre-assembly potential, enhanced repair and maintenance capabilities, as well as improved disassembly and rejoining capabilities. One of the key benefits of bonded CFRP structures lies in their inherent reusability, as they can undergo non-destructive disassembly and be reused in a subsequent joining process. This potential for sustainable reuse holds promise for minimizing the CO2 footprint associated with manufacturing processes, thereby contributing significantly to the global effort to combat climate change.

In this presentation, we introduce initial strategies for the structural disassembly of CFRP structures, with a primary emphasis on preserving the integrity of the initial structures for potential reuse in subsequent processes. We delve into the concept of disassembly, outlining its principles and discussing the merits and drawbacks of the proposed approach.

Moreover, we present an analytical approach aimed at describing the force effects experienced during the disassembly process. This analytical method is complemented by numerical simulations, allowing for a comparative analysis that underscores the strengths and weaknesses of each approach. Our comparison highlights the accuracy and reliability of the analytical approach, as well as the ability of the numerical approach to realistically depict failure behavior during disassembly. By integrating both analytical and numerical methodologies, we aim to develop a comprehensive framework for optimizing the disassembly process of bonded CFRP structures, thereby advancing their sustainability and contributing to broader environmental conservation efforts.

Session 2: Energy Production

Selective Absorber Coatings for Solar-thermal Energy Conversion

J.C. Sánchez-López[a]*, T.C. Rojas[a], and R. Escobar-Galindo[b]

[a]*Instituto de Ciencia de Materiales de Sevilla (ICMS), CSIC-Universidad de Sevilla, Sevilla, Spain*
[b]*Escuela Politécnica Superior, Universidad de Sevilla, Sevilla, Spain*

Abstract:
The search for new materials with improved performance for use in renewables energies has become a crucial issue due to the depletion of fossil fuels, increasing concentration of greenhouse gases and climate changes. In photothermal applications, the development of thermally stable solar selective absorber materials is a key feature for improved solar-to-heat conversion efficiency and durability. Increasing the working temperature of the absorber material conveys a more cost-efficient and high-performance solar conversion process. Spectral selectivity means a surface with a high absorptance in the solar wavelengths (0.3 to 2.5 μm) and low emittance in the infrared thermal radiation wavelengths (2.5 to 25 μm). Intrinsic absorber materials are generally non-selective, and therefore, material design is employed to achieve the adequate optical behavior. In this talk, the use of solar selective absorber coatings based on multilayered architecture is presented for solar harvesting and thermal conversion applications. In particular, our recent results based on transition metal nitride (CrAlN) layers with different stoichiometries topped with an anti-reflective alumina layer are presented [1-3]. The adequate combination of these multiple ceramic layers in optimized thicknesses enables good spectral selectivity, along with enhanced oxidation and thermal resistance. The presentation will encompass the entire process, starting from the design and fabrication using magnetron sputtering technology, through the assessment of chemical and optical characteristics, to the final testing under high radiation conditions.
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Solid Polymer Electrolytes Based on Nitrogen Groups as a New Generation of Electrolytes for Ca-multivalent Secondary Batteries

Antonio Peñas-Sanjuán*, Miguel Ángel González-Lara, Belén Martínez-Moral, Rubén CruzSánchez, and Manuel Melguizo

University of Jaén, Jaén, Spain

Abstract:

Lithium-ion batteries have dominated the energy storage sector since the 1990s, but a recent global trend has brought about the need to develop transition-metal-free energy storage systems. Calcium metal based rechargeable batteries have recently gained a great deal of attention, however, although Ca batteries are expected to provide efficient, safe and costeffective battery solutions, a key challenge in their practical implementation is the lack of electrolyte materials with high ionic conductivity, high interphase stability and highly reversible plating and stripping processes. Extensive investigations have been performed regarding liquid electrolytes, which showed low efficiencies due to Ca reactivity and the formation of blocking electrolyte/electrode interfaces, as well as solid polymer electrolytes, which rendered low ionic conductivities (7.0×10^{-6} - 1×10^{-3} S cm-1) and difficulty with achieving high redox rates. Herein, we show a series of new innovative polymeric solid electrolytes based on polyamines, particularly triazoles and aliphatic amines, with high Ca-ion conductivity (>1mS cm-1), wide electrochemical window, as well as excellent thermal, electrochemical and mechanical stability. Solid-state electrolytes were developed and optimized using different type and concentration of salts. The electrolytes were integrated with porous battery electrodes and tested in real devices, employing half-cell formats.

Towards Tailored Radiative Properties for High-temperature Materials via Multi-scale Geometry Engineering

Charles-Alexis Asselineau[a,b]

[a]Universidad Politecnica de Madrid (UPM), Escuela Tecnica Superior de Ingenieros Industriales (ETSII), Madrid, Comunidad de Madrid, Spain
[b]Australian National University (ANU), School of Enineering (SoE), Canberra, Australian capital, Territory, Australia

Abstract:

The decarbonisation of high-temperature and energy intensive processes (cement, steelmaking, chemical commodities) is a significant industrial challenge. In this effort, many high-temperature processes are likely to progressively switch from combustion to electrically fueled emissive heating which strongly depends on the optical properties of materials. Such optical properties are very challenging to reliably and economically alter with conventional techniques as high-temperatures and oxidizing atmospheres are damaging to conventional coatings and depositions.

The alternative approach proposed in the MSCA HEASeRS project consists in multi-scale geometry alteration of bulk materials to obtain desirable optical properties. At the micro-scale the surface roughness of material can be altered, at the meso-scale, sub-mm to cm-sized surface features can be added and at the macro-scale, the overall geometrical design of a radiant device can be optimized for desired optical functions.

In this work, we present the efforts deployed in the MSCA HEASeRS project to understand more accurately the drivers behind the optical properties of high-temperature materials and some progress on surface and shape modification.

Design of Electrode Materials for Na-S Batteries

Yan Yu

University of Science and Technology of China, HeFei, Anhui, China

Abstract:

Room temperature sodium-sulfur (Na-S) battery is considered as one of the most promising energy storage devices because of its high energy density and abundant resources of Na and S. However, several challenges including low electronic conductivity of S, shuttle effect and slow conversion of polysulfides, and dendrite growth of Na anode lead to low reversible capacity, short cycle life and potential safety hazards of Na-S batteries. Rational design and construction of catalysts is the key to achieve advanced Na-S batteries. Based on this consideration, we select and synthesize efficient catalytic materials by theoretical calculation and experimental optimization, which effectively reduce conversion reaction barrier of sulfur and enhance utilization and reaction kinetics of S cathode. Besides, we propose the protection strategies for Na anode associated with constructing conductive skeleton and artificial interface protection layer, which effectively induce uniform deposition of Na, suppress Na dendrites growth and buffer volume expansion of Na anode. In addition, we reveal electrochemical reaction mechanism of Na-S batteries by systematic *in situ* characterization technologies, which provide important scientific guidance for developing novel high-performance Na-S batteries.

Electrochemical Hydrogen Pump/compressor - Gas Diffusion Electrodes, Membrane Electrode Assembly and Possibility for Two Stage Compression

Galin Borisov*, Nevelin Borisov, and Evelina Slavcheva

Institute of electrochemistry and energy systems Acad. Evgeni Budevski – Bulgarian Academy of Science, Sofia, Bulgaria

Abstract:

The electrochemical hydrogen pump/compressor (EHP/EHC) offers numerous advantages over mechanical compressors, such as superior energy efficiency, stationary mechanical components, and the ability to operate at high pressures without pre-treatment of the supplied reactant. However, a key challenge lies in the membrane electrode assembly (MEA), which determines the electrochemical conversion rates and the differential pressure between gas diffusion electrodes, impacting overall energy efficiency. Experimental findings in this study reveal the effects encountered when scaling up the MEA with commercial Pt-based gas diffusion electrodes and Nafion 117, alongside the device's ability to function in two-stage compression mode. Scaling up the electrode surface results in approximately a 6 mV.cm-2 increase in cell voltage in single-cell mode, with current densities ranging from 0.06-0.6 A cm-2. Galvanostatic tests were conducted to evaluate EHP/EHC efficiency at a 16-bar differential pressure, showcasing its adaptability to various electrical configurations. These results underscore the potential of EHP/EHC technology for hydrogen purification and compression, albeit with challenges surrounding MEA scaling and optimization for enhanced energy efficiency.

What are the Challenges and Opportunities of ZnFe2 O4 Photoanodes for PEC Water Splitting Applications?

Xiaodi Zhu[a]*, Zhiyong Jiang[a], Néstor Guijarro[b], Kevin Sivula[c], and Jun Bao[a]

[a]*National Synchrotron Radiation Laboratory University of Science and Technology of China, Hefei, Anhui, China*
[b]*Institute of Electrochemistry, Universidad de Alicante, Alacant, Spain*
[c]*Laboratory for Molecular Engineering of Optoelectronic Nanomaterials, École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland*

Abstract:

Photoelectrochemical (PEC) water splitting is a promising route for the scalable and cost-effective storage of solar energy and chemical fuel production, which are critical for a sustainable, carbon-neutral, and global energy economy. While impressive solar-to-hydrogen conversion efficiency using PEC devices has been demonstrated, the development of low-cost and robust photoelectrode materials that deliver high-performance while also

tolerating the harsh PEC operating conditions is still required. Among various metal oxides, zinc ferrite ($ZnFe_2O_4$) shows great potential as photoanode for PEC water splitting by converting solar energy into hydrogen owing to its suitable band structure, excellent visible light capture ability, photochemical stability as well as flexible structural adjustments. In this talk, a series of our progress on improving the PEC performance of $ZnFe_2O_4$ photoandes will be presented, including the physiochemical mechanism of spinel inversion degree, dual metal active sites, non-metal modulation on its PEC performance. We will use these examples to illustrate challenges and opportunities for its applications in PEC water splitting.

Metal-organic Frameworks in Hydrogen Technologies: Proton Exchange Membrane Fuel Cells and Green Hydrogen Generation

S. Carrasco*, J. Ferrando, P. Salcedo-Abraira, C. Biglione, and P. Horcajada

Advanced Porous Materials Unit. IMDEA Energy, Avda. Ramón de la Sagra 3, 28935 Móstoles, Madrid, Spain

Abstract:

Metal-Organic Frameworks (MOFs) are porous coordination polymers composed of inorganic units linked by organic polycomplexant ligands, exhibiting exceptional porosity and well-defined structures that can be easily tuned in terms of composition and structure, allowing for adjustments based on specific applications[1]. MOFs emerge as promising materials in hydrogen technologies because of the fast hydrogen adsorption/desorption kinetics, the ability to reversibly uptake hydrogen, the storage capacity at low temperatures and their (photo/electro)activity as catalysts to efficiently split the water molecule into hydrogen and oxygen[2]. In this presentation, we show different MOF-based platforms developed in our unit for:

A) developing proton exchange membrane fuel cells (PEMFCs) devices, upon integrating IEF-7 (bismuth pyrene tetraphosphonate) and UPG-1 (zirconium triazine triphosphonate) in polymeric matrices. Different strategies were tested to improve the conductivity: (i) the synthesis of intrinsically conductive MOFs based on organic ligands with labile protons[3], (ii) the insertion of a proton carrier within the porosity of the MOF[4], and (iii) cation exchange of the labile protons within the framework[5].

B) producing green hydrogen through the photocatalytic overall water splitting reaction (OWS), using IEF-11 (titanium squarate)[6]. This material showed exceptional (photo)chemical properties (solar light absorption, low electron-hole recombination rates, high stability and robustness) ascribed to the uniqueness of the Ti structural arrangement, resulting in the highest rates of H_2 production in OWS to date in isolated MOFs. More importantly, the crystal structure remained intact even after 10 consecutive catalytic runs.

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Discovering Ion-electron Interactions at V_2O_5/LiPON Electrochemical Interfaces Using Depthresolved Cathodoluminescence Spectroscopy

Leonard J. Brillson[a]*, David M. Stewart[b], Angelique Jarry[b], and Gary Rubloff[b]

[a]Departments of Physics and Electrical & Computer Engineering, The Ohio State University, Columbus, Ohio 43210, USA
[b]Department of Materials Science and Engineering, Institute for Systems Research, University of Maryland, College Park, Maryland 20742, USA

Abstract:
Vanadium pentoxide (V_2O_5) is a well-known solid-state electrochemical cathode material that has attracted considerable interest for its potential use in solid-state lithium-ion batteries. We pioneer the use of depth-resolved cathodoluminescence spectroscopy (DRCLS) to monitor the changes in the electronic structure of lithiated V_2O_5 from the free surface to the thin film bulk several hundred nm below as a function of lithiation. A combination of DRCLS and X-ray photoemission depth profiling (XPS) measured the pronounced changes in both the electronic density of states and lithium composition near the nanoscale, buried $Li_xV_2O_5$/LiPON interface. DRCLS studies of electrochemically lithiated bare V_2O_5 and the sputter-deposited V_2O_5 plus LiPON overlayer electrochemically lithiated in stages both showed that in the bulk the luminescence intensity of the "split-off" hybridized bonding density of states was anticorrelated with XPS-measured Li content, decreasing as the Li content increased. However, the LiPON overlayer was found to modify the band structure of the underlying $Li_xV_2O_5$ (LVO) to a depth of at least 30 nm beneath the V_2O_5 interface. While DRCLS near the electrochemically lithiated LiPON/LVO interface indicated a low Li content, XPS depth profiling revealed strong Li changes from the intimate interface to a minimum tens of nm below, demonstrating a strong interaction between band structure and Li electrochemical potential near this heterojunction. These results provide evidence for substantial effects on the local band structure near an electrolyte/cathode interface, how interfaces can dominate the movement of charge, as well as insights into the electrochemical interface behavior of solid-state batteries in general.

Recent Developments in Narrow Energy Gap Photoactive Absorbers for Wavelength-selective Transparent Photovoltaic Devices

Terence Wong

Nanyang Technological University, Singapore, Singapore

Abstract:
Recent developments in narrow energy gap, infra-red selective absorbers for transparent photovoltaics (TPV) is presented. The TPVs are niche devices important for reducing the carbon footprint of buildings and enables windows to become both a power source and medium for daylight. Unlike the more common semitransparent TPVs, the photoactive absorber of wavelength selective (WS) TPVs does not absorb visible light photons and thus appear visibly transparent. Both organic and inorganic absorbers with an energy gap below 1.65 eV will be discussed in this talk. The organic absorbers are typically bulk heterojunction blends of a narrow gap conjugated polymer and non-fullerene acceptor with champion devices demonstrating a power conversion efficiency of 5.74% and average visible transmittance of >60%. The main observation is that despite the rapidly increasing number of synthesized NFAs, suitable donor-acceptor combinations for WS-TPV is still very limited. This is due to the encroachment of the dual peak absorption spectrum of both donor and acceptor into the visible spectral region. A new metric called spectral range ratio is proposed to classify absorbers for WS-TPV applications. A molecular design strategy to increase the SRR based on the frontier molecular orbital theory will be presented. The final part of this talk will focus on the density of states limitation of colloidal chalcogenide quantum dot (PbS, PbSe) solar cells. For WS-TPV, long term research effort should be on organic TPV devices.

Stable Photoelectrochemical Oxidation Followed by Li⁺-deintercalation at Solid/solid Interfaces Toward Solar Energy and Conversion

Kenta Watanabe

Department of Chemical Science and Engineering, School of Materials and Chemical Technology, Tokyo Institute of Technology, Yokohama 226-8501, Japan

Abstract:

Electorchemistry focuses on interactions between electrons and materials. Photoelectrochemistry includes interactions between photons and electrons in addition to interactions between electrons and materials, leading to conversion of photo-to-electrical and electrial-to-chemical energies. Electrochemistry has been expanded from reactions at solid/liquid interfaces to those at solid/solid interfaces by development of solid electrolytes. However, photoelectrochemistry has been hardly conducted at solid/solid interfaces. Therefore, photoelectrochemistry is expected to be applied into solid/solid interfaces, for solar energy conversion and storage.

We have successfully demonstrated the stable photoelectrochemical oxidation followed by Li⁺-deintercalation at the semiconductor/solid-electrolyte (solid/solid) interface by using the thin-film type all-solid-state cell comprising anatase TiO_2 doped with Nb (a-TiO_2:Nb) as a photoelectrode, amorphous Li_3PO_4 (LPO) as a solid-electrolyte, and metallic Li as a counter electrode (a-TiO_2:Nb/LPO/Li). The photoelectrochemical oxidation proceeded when a-TiO_2:Nb was located at more positive potentials than its flat band potential. This is due to the band bending toward negative potentials. These results indicate that the photoelectrochemical oxidation proceeds at semiconductor/solid-electrolyte interfaces with based on the same principle as those at semiconductor/liquid-electrolyte interfaces. This finding extended photoelectrochemistry from solid/liquid to solid/solid interfaces. The author belives that photoelectrochemistry at solid/solid interfaces would contribute to solar energy conversion and storage.

Dissecting the Core-shell Interface Effect on the Thermal Stability of Microencapsulated Phase Change Materials for Efficient Thermal Energy Storage Application

Melbert Jeem[a]*, Kaixin Dong[a], Joshua Chidiebere Mba[a], Takahiro Kawaguchi[b], Yuto Shimizu[b], Tomokazu Nakamura[a], and Takahiro Nomura[a]

[a]Faculty of Engineering, Hokkaido University, Sapporo, Hokkaido, Japan
[b]Graduate School of Engineering, Hokkaido University, Sapporo, Hokkaido, Japan

Abstract:

Microencapsulated phase change materials (MEPCM) stand at the frontier of enhancing thermal energy storage, leveraging the core-shell interface to address the challenges of leakage and volumetric changes typical of PCM. This presentation will detail our recent progress in the intricacies of metal alloys-based MEPCMs, spotlighting the role of immiscible α-Al_2O_3 nanoparticles and Sn microparticles' in their successful fabrication of MEPCMs. Beyond their fundamental thermal properties, such as latent heat capacities, our atomic-scale investigations have uncovered the formation of SnO and SnO_2 nanoparticles within the α-Al_2O_3 matrix. This discovery is key to enhancing the thermal stability of MEPCMs during extended cycles of endothermic and exothermic reactions. Notably, this process significantly reduces supercooling, leading to an increased rate of Sn nucleation during the solidification phase, thereby enhancing the material's thermal efficiency. Employing first-principles calculations, we explored the atomically resolved SnO2/α-Al_2O_3 interface, revealing how these interactions contribute to a lower energy barrier for nucleation. The observed hybridization of Sn 3*p* and Al 3*p* electron states at this interface highlights the complex interplay at the atomic level that results in improved MEPCM's performance. This is showcased in exceptional thermal durability of the MEPCMs in composite form, as well as its durability under extreme thermal cyclic test. We offer a nuanced perspective on how atomic-scale imperfections within the crystal lattice can impact energy storage capabilities, setting the stage for development of more efficient thermal energy storage solutions.

Solid-state Lithium Batteries: Market Trends and Innovations

Chad Lindner

American Elements, Los Angeles, CA, United States

Abstract:
Considering the increasing demand for energy storage solutions, this speech addresses pivotal market trends in lithium and explores innovative strategies to address supply and environmental concerns. This speech will highlight the innovative contributions of American Elements in the production of Mxenes and other cutting-edge materials, focusing on their applications in enhancing solid-state Lithium batteries. Attendees will gain insights into the current trends, challenges, and opportunities in the field, enriching their understanding of how emerging materials are shaping the future of energy storage technologies.

Scanning Electrochemical Microscopy for Characterizing Electrode/electrolyte Interfacial Processes of Lithium-ion Batteries

Rong He[a,b]*, Meng Zhou[b], Hongmei Luo[b], and Robert Tenent[a]

[a]National Renewable Energy Laboratory, Golden, CO 80401, USA
[b]Department of Chemical and Materials Engineering, New Mexico State University, New Mexico 88003, USA

Abstract:
Lithium-ion batteries (LIBs) are widely employed in portable electronics and new energy vehicles and other devices, owing to the high energy density and rechargeable features. The electrode/electrolyte interface (EEI) plays an essential role in battery electrochemical performance and durability. Scanning electrochemical microscopy (SECM) is an *in situ* scanning probe technique that can directly monitor electrochemical processes at different interfaces. This technique has been used as an analytical tool for LIB studies and enables the direct characterization of the electrochemical reactivities of active species in LIBs during cycling. This presentation will cover the basics of SECM including its working mechanism and operating modes, and the applications in characterizing electrode/electrolyte interfacial processes of LIBs. SECM offers the opportunities to better understand the LIB working and degradation mechanisms, providing guidance for future rational design of stable electrode/electrolyte interfaces of next-generation LIBs.

Session 3: Energy Harvesting

Advanced Materials for Near Ambient Temperature Energy Harvesting

O.J. Dura[a]*, C. M. Andreu[a], S. Merino[a], and E. Vazquez[a]

[a]Instituto Regional de Investigación Científica Aplicada (IRICA), Universidad de Castilla-La Mancha, Ciudad Real, E-13071, Spain

Abstract:
All machines from combustion engines to microprocessors or living systems generate heat, which mostly is considered waste-heat. Around 40% of the total waste heat is lost as low-grade heat below 140 ^{0}C and its efficient utilization represents a great challenge[1, 2]. The harvesting of the waste heat would improve the energy efficiency and it would reduce the overall emissions. Thermoelectric materials (TE) can supply power under a temperature gradient. The conventional thermoelectric materials are based on the Seebeck effect and the intrinsic behavior of electrons and holes in inorganic compounds. However, these materials consist mainly into rare and expensive elements, and most are suitable for high temperatures. An alternative to conventional TE are ionic thermoelectric materials (i-TE) that use ions as charge carriers through thermodifussion (Soret effect), or through the thermogalvanic effect by using ionic redox couples[3].

Here, we summarize the three effects on which thermoelectricity is based and we will review briefly the main advantages and disadvantages of i-TE versus conventional TE. Finally, we will discuss our latest results related to the improvement of thermoelectric efficiency by design thermogalvanic hydrogels.

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CO_2 Capture for Energy Harvesting: Atomistic Modelling of the Working Mechanism

Federico Raffone[a,*], Davide Molino[a], Pietro Zaccagnini[a,b], Alessandro Pedico[a,c], Simone Martellone[a,b], Giuseppe Ferraro[a,b], Sergio Bocchini[a,b], Giancarlo Cicero[a], and Andrea Lamberti[a,b]

[a]Politecnico di Torino, Dipartimento di Scienza Applicata e Tecnologia (DISAT), Corso Duca Degli Abruzzi, 24, 10129 Torino, Italy
[b]Istituto Italiano di Tecnologia, Center for Sustainable Future Technologies, Via Livorno 60, 10140 Torino, Italy
[c]Istituto Nazionale di Ricerca Metrologica, Str. delle Cacce, 91, 10135 Torino, Italy

Abstract:

It is well known that industrial process by-products pose a great threat for the environment. Among them, CO_2 is considered one of the most harmful. CO_2 release in the atmosphere can be avoided by exploiting carbon capture, the process of sequestration of CO_2 thanks to a chemical reaction with a more stable compound. The technologies so far employed for capturing CO_2 are limited to the only selective capture and release of harmful gas, so they do not involve any form of energy recovery. Our research group has recently developed a new device able to harvest energy while absorbing CO_2, exploiting a supercapacitor setup in which an ionic liquid (IL) is both the electrolyte and the capturing agent. CO_2 gas is fluxed through one of the two electrodes. The portion of the IL in proximity of the electrode captures the CO_2 while, on the other side of the device at the counter electrode, the IL remains unchanged. At the same time, a voltage rise is measured. Energy is, then, extracted by discharging the device. Because the CO_2 capture of the IL is a chemical process and not an electrochemical one, the reasons of the voltage increase are still unclear. By means of classical molecular dynamics simulations, it was possible to associate the potential variation to the effect of charge redistribution in the ion of the IL induced by the capture of CO_2 and to the difference in chemical potential between the two ends of the device.

Electrocatalytic Nitrate to Ammonia

Shuyan Gao

Hennan Normal University, Xinxiang, Henan, China

Abstract:

Electrocatalytic nitrate reduction to ammonia (NRA) is an emerging and green ammonia synthesis process that has received widespread attention. The rational design of electrocatalysts plays a key role in achieving efficient NRA. Transition metal copper (Cu) featuring d-orbital energy levels closely matching the lowest unoccupied molecular orbital levels of NO_3^-, exhibits excellent activation capability toward NO_3^-. However, Cu-based catalysts still demonstrate a relatively high overpotential in practical reactions, necessitating further optimization of the adsorption energy of NRA intermediates to achieve efficient ammonia production at lower overpotentials. In this work, we systematically investigate the structure-performance relationship of copper-based catalysts in NRA via constructing multi-principal-element alloys with multi-principal-element synergy and efficient active sites for the production of ·H. This work aims to enhance the adsorption energy of intermediates and facilitate the hydrogenation process. Combining experimental studies with density functional theory analysis, we delve into the reaction mechanism of NRA with the variation of active principal elements.

Electrification Phenomena on Biological Surfaces and Potential Uses

Fabian Meder

Lab for Surface Phenomena and Integrated Systems, The BioRobotics Institute, Sant'Anna School of Advanced Studies, Pisa, Italy

Abstract:
Formation of static charges through phenomena like contact or triboelectrification is typically associated with artificial polymers such as PTFE. Nonetheless, it also occurs in nature on biological surfaces, such as the nanostructured waxes found on most plant leaves. Contact with solids and liquids charges the waxes and the outer leaf surface. In my presentation I will address the charging phenomena as function of material's contact that cause it and I will highlight what happens in the leaf tissue. Moreover, the current generated when leaves move in the wind, along with artificial leaves designed to enhance the charging, can be directly used to power devices. A single leaf or just a few are sufficient to power LEDs, sensors, and wireless signal transmission. This offers a perspective on harvesting energy from natural surfaces and directly using them as micropower sources to facilitate, for example, environmental monitoring.

Giant Piezoelectricity in Nanoporous (Ba,Ca)(Ti,Zr)O₃

Yukana Terasawa[a,b]*, Toru Asahi[c,d], and Yusuke Yamauchie[f,g]

[a]*Faculty of Advanced Science and Technology, Kumamoto University, Japan*
[b]*Comprehensive Research Organization, Waseda University, Japan*
[c]*Faculty of Science and Engineering, Waseda University, Japan*
[d]*Research Organization for Nano & Life Innovation, Waseda University, Japan*
[e]*Department of Materials Process Engineering, Graduate School of Engineering, Nagoya University, Japan*
[f]*Australian Institute for Bioengineering and Nanotechnology (AIBN), The University of Queensland, Australia*
[g]*Department of Plant and Environmental New Resources, Kyung Hee University, South Korea*

Abstract:
The creation of porous structure in the dielectric materials has shown great improvement. Barium titanate ($BaTiO_3$; BTO) family is known as one of the environmentally friendly lead-free piezoelectric materials to replace lead zirconate and lead titanate, $Pb(Zr,Ti)O_3$ (PZT). Especially, $Ba_{0.85}Ca_{0.15}(Ti_{0.9}Zr_{0.1})O_3$ (BCZT) film has attracted attention as a promising piezoelectric material. However, the value of piezoelectric strain constant d_{33} and electromechanical coupling factor k_{33} in BTO is still far behind that of its commercially available Pb-based counterparts[1]. In our study, we have succeeded in synthesizing nanoporous BCZT film using sol-gel spin-coating method. The piezoelectric charge constant d_{33}, which represent piezoelectricity showed about 7500 pm V^{-1}. This value is more than an order of magnitude larger than that of PZT ceramics, a typical conventional lead-based piezoelectric material[2]. It is thought that the porous structure made the crystal lattice distort. As evidence, the strain field was about 30 % and was the primary contributor to higher piezoelectricity[3].

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[1] D. Berlincourt and H. Jaffe, *Phys. Rev.* **111**, 143–148, 1958
[2] L. Li et al., *J. Electron. Mater.*, **42**, 2564–2569, 2013
[3] M. Billah, Y. Terasawa et al., *Chem. Sci.*, **15**, 9147-9154, 2024

Young Researchers Presentations

Coarse-grained Ferritic Fe-10Al-4Cr-4Y₂O₃ Nanocomposite as a Top Material for the Green Energetics

Bártková Denisa[a,b]*, Svoboda Jiří[a], Gamanov Štěpán[a,c], and Dymáček Petr[a,b]

[a]*Institute of Physics of Materials CAS, Brno, Czech Republic*
[b]*Institute of Materials Science and Engineering, Brno University of Technology, Brno, Czech Republic*
[c]*Central European Institute of Technology, Brno University of Technology, Brno, Czech Republic*

Abstract:

In the current climate and geopolitical situation, the attention of scientists, politicians and the public is focused on greener and more economical energy sources. Hydrogen, fission, and fusion energy are areas with great potential. However, all these technologies place considerable demands on materials.

The overall efficiency of the power cycle is related to increasing the maximum operating temperature of the plant. This places higher and higher demands on the creep and thermal resistance of the material, high corrosion resistance and chemical compatibility with coolants and fuels. Price and ease of production are also important criteria.

A material that meets most of these requirements should be a) single crystalline or coarse-grained, b) contains stable precipitates resistant to coarsening, and c) forms a stable protective layer on the surface. Such properties can be very well met by oxide dispersion strengthened alloys (ODS) such as the coarse-grained Fe-10Al-4Cr-4Y$_2$O$_3$ ODS nanocomposite (denoted as FeAlOY) developed by the authors. Its excellent creep properties at temperatures 1100 – 1300 °C are given by tenfold higher volume fraction of stable Y$_2$O$_3$ nanodispersoid than in classical ODS alloys. Excellent oxidation resistance is guaranteed by high content of Al in the matrix.

The manufacturing process of the FeAlOY comprises of many variables as the type and quality of input components, production of powders by mechanical alloying, consolidation parameters and thermomechanical processing. Some important parameters are summarized in the lecture.

Effect of Cationic Impurities in Recycled Active Materials for Lithium-ion Batteries

Elie Fayad[a,b], Domitille Giaume[a], and Nadia Soulmi Chibani[b]

[a]*Chimie-ParisTech, PSL Research University, CNRS Institut de Recherche de Chimie-Paris (IRCP), 75005 Paris, France*
[b]*Ampere - Renault Group – Technocentre, 78280 Guyancourt, France*

Abstract:

Across the electric vehicle industry, using high-quality materials seems crucial for ensuring the reliability and reproducibility of battery performance. The use of "battery grade" precursors has been the established norm to prevent, for example, the introduction of certain impurities that have been shown to alter the morphology and electrochemical signatures of the produced active materials.[1,2] However, the impending arrival of European legislation[3] concerning the mandatory valorization of critical materials like cobalt, nickel, and lithium in recycling processes signals a shift.

This shift introduces recycled materials of a lower purity compared to battery-grade materials, raising questions about their impact and a potential re-evaluation of the battery grade standard. By exploring the effects of these impurities, whose amounts surpass the battery grade specifications, our research aims to provide insights into the efficacy of utilizing recycled materials in battery production processes. Our work was focused on NMC chemistry, a common cathode active material composed by a lithium nickel cobalt manganese oxide. By initially implementing a reproducible synthesis of the phase, the impact of Cu, Fe and Al impurities on the properties of the materials was studied, through computational, chemical, structural and morphological characterization techniques. Finally, we assessed the electrochemical performance of the synthesized materials.

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[2] Peng, C.; Lahtinen, K.; Medina, E.; Kauranen, P.; Karppinen, M.; Kallio, T.; Wilson, B. P.; Lundström, M. Journal of Power Sources 2020, 450, 227630.
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Composite Organic Ionic Plastic Crystal Membranes: The Effect of Etherfunctionalized Cations on Light-gas Separation Performance

Muhammad Shaharyar[a], Douglas R. MacFarlane[b], Mega Kar[a], Azra Sourjah[a], Killian S. Fraysse[a], Cara M. Doherty[c], Durga Achariya[c], Luke A. O'Dell[d], and Jennifer M. Pringle[a]

[a]Institute for Frontier Materials, Deakin University, Burwood, VIC 3125, Australia
[b]School of Chemistry, Monash University, Clayton, VIC 3800, Australia
[c]Commonwealth Scientific and Industrial Research Organisation (CSIRO), Manufacturing, Clayton, VIC 3168, Australia
[d]Institute for Frontier Materials, Deakin University, Geelong, VIC 3216, Australia

Abstract:
In light of increasing concerns about climate change, there is a growing need for innovative solutions to address CO_2 emissions. Addressing this urgency, this work presents a unique approach to CO_2 separation utilizing composite membranes of organic ionic plastic crystals (OIPCs) with ether-functionalized cations and poly(vinylidene fluoride-co-hexafluoropropylene) (PVDF-HFP). Here we report the gas separation performance of OIPC-based membranes of 3,3-dimethyloxazolidinium [C1moxa]+, 4-ethyl-4-methylmorpholinium [C2mmor]+ and 4-isopropyl-4-methylmorpholinium [Ci3mmor]+ cations paired with the bis(fluorosulfonyl)imide [FSI]-anion. These composites demonstrated very good gas separation properties, especially [C1moxa][FSI] which produced a permeability of 63 Barrers for CO_2 and an overall selectivity (CO_2/N_2) of 205, which is the highest amongst all the OIPCs reported so far. Additionally, a large change in separation performance was observed for the [Ci3mmor][FSI] membrane upon heating above the solid-solid phase transition (II - I) at 48 °C; the CO_2 permeability increased from 7 to 163 Barrers and an approximately 3-fold increase in selectivity was observed. These findings advance the design of composite membranes based on OIPCs towards increased selectivity and sustained effectiveness in the separation of light gases.

Exploration and Development of Repairable Sulfur-based Polymer Composites

Y. Athulya Wickramasingha[a], Justin M. Chalker[b], and Luke C. Henderson[a]

[a]Institute for Frontier Materials., Deakin University, Waurn ponds, Geelong, Victoria , 3216, Australia
[b]College of Science and Engineering, Flinders University, Adelaide, South Australia 5042, Australia

Abstract:
Sulfur-based polymers exhibit unique properties such as repairability, reshaping capability, high affinity for heavy metals, and resistance to harsh solvents and acidic conditions, making them promising for durable and sustainable applications. This study investigates sulfur-based polymers to address their inherent limitations, particularly in mechanical strength and electrical insulation, by incorporating carbon fibers, including reclaimed forms of carbon fiber. Introducing composites with reclaimed carbon fibers significantly enhances mechanical strength while retaining mechanical strength over 5 cycles of breaking and repairing (Figure 1).[1] This dual enhancement extends material lifespan and usability across various applications, aligning with sustainability objectives. Furthermore, optimization of the sulfur-dicyclopentadiene synthesis method reduced operating temperatures from 140°C to 120°C and minimized cure times down to 5 hours for adhesive applications *(accepted publication)* compared to the original synthesis. These improvements enhance safety, energy efficiency, and scalability in industrial settings, reducing environmental footprint. Overall, this body of work highlights the potential of sulfur-based polymer composites in advancing sustainable material solutions. By presenting repairable materials made using reclaimed carbon fibre products with good mechanical strength, and scalable synthesis methods, we aim to promote resilience and environmental responsibility in materials engineering while removing barriers to use these special sulfur-based polymers in a wider range of applications.
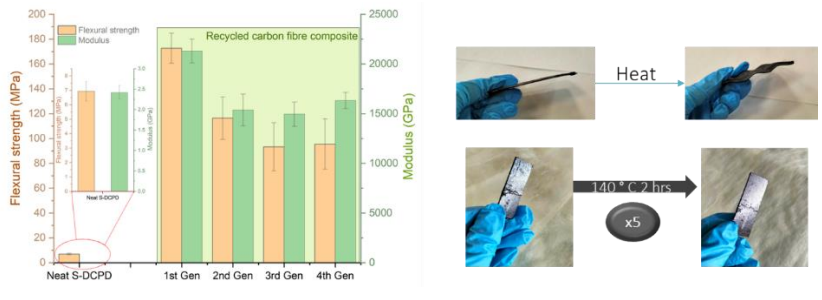
Figure 1. Flexural strength and modulus evolution of reclaimed carbon fiber composites that are tested to failure, repaired and retested over 5 cycles.

Symposium IV: Nanotechnology and Nanomaterials

Session 1: Synthesis and Manufacture I

Pulsed Laser Ablation Synthesis of Nanoparticles in Spectral Methods

Karel Novotný[a]*, Ivo Krempl[a], Lubomír Prokeš[a], Lukáš Pečinka[a,b], Petr Vaňhara[b,c], and Josef Havel[a]

[a]Dept. of Chemistry, Fac. of Science, Masaryk University, Brno, Czech Republic
[b]International Clinical Research Center, St. Anne's University Hospital Brno, Czech Republic
[c]Dept. of Histology and Embryology, Fac. of Medicine, Masaryk University, Brno, Czech Republic

Abstract:
This presentation aims to demonstrate the potential of pulsed laser ablation synthesis (PLA), the possibility of monitoring the ablation process by spectroscopic methods and, in the case of tellurium nanoparticles (NPs), also their use in mass spectrometry. An experimental setup enabling the synthesis of Te NPs in gas or liquid environments with lasers operating at different wavelengths was designed and tested. It was discovered that the optimal way of preparing Te NPs is by laser ablation synthesis in liquid, and acetone appears to be the ideal organic solvent. The prepared Te NPs were used for a pilot study of their use with the MALDI-MS technique. A significant effect was observed when Te NPs were used in a MALDI-MS analysis of macrocycles, which resulted in a decline in the formation of matrix adducts. Because the basic principle of the PLA is a material ejection after focusing a highly energetic laser pulse on a target immersed in liquid, the process is also accompanied by the emergence of laser-induced plasma (LIP). It will be demonstrated that spectroscopic analysis of LIP emission offers a powerful method for monitoring the processes taking place during the ablation generation of nanoparticles.

Roll-to-roll Dry Transfer of Large-scale Chemical Vapor Deposition Graphene

Wei Li*, Enrique Velasquez Morquecho, Christopher B. Martin, and Dongmei Chen

Walker Department of Mechanical Engineering, The University of Texas at Austin, Austin, Texas, USA

Abstract:
Since its discovery, graphene has been envisioned for a wide range of advanced applications, such as flexible displays, solar cells, sensors for wearable electronics, and gas separation membranes. A major challenge for graphene applications is the lack of mass production technology for high quality and large-scale graphene manufacturing. Large-scale graphene can be grown on metal substrates using chemical vapor deposition (CVD). After the growth, CVD graphene needs to be transferred to a target substrate, such as a polymer film, for device fabrication. Our work is focused on developing a roll-to-roll (R2R) dry transfer process for large-scale CVD graphene. The transfer process is fast, controllable, and environmentally benign. It avoids graphene contamination and allows the reuse of graphene growth substrate. The R2R dry transfer process will be presented, along with results from fabricating graphene-based field-effect transistors (GFETs) using the dry-transferred graphene. We show that these flexible GFETs have a near-zero doping level and a gate leakage current one to two orders of magnitude lower than those fabricated using wet-chemically etched graphene.

Tunable Covalent Micropatterning of Graphene by Emulsions

Marina Garrido*, Alicia Naranjo, Natalia Martín Sabanés, and Emilio M. Pérez

IMDEA Nanociencia, C/ Faraday 9, Ciudad Universitaria de Cantoblanco, Madrid, 28049, Spain

Abstract:
One of graphene's drawbacks is its zero band-gap. The lack of an off state in graphene devices hampers its use in electronic applications. This inconvenience can be addressed by the opening of graphene's band-gap using

covalent functionalization, since the disruption of its π skeleton causes significant changes in its electronic and band structures. This modification can be fine-tuned by the selective functionalization of the basal plane of graphene, obtaining a material where the properties of the pristine and functionalized graphene are simultaneously present. However, all graphene carbon atoms present identical reactivity, making this selective functionalization very challenging.

One methodology to overcome this disadvantage is the patterning of graphene, allowing its spatially controlled modification. Within this context, several approaches have been conceived successfully, such as the electron beam lithography, the laser writing and the use of Moiré patterns, among other. Nevertheless, these strategies employ specific and expensive equipment that works under very controlled conditions.

In this contribution, we present the versatility of an easy and scalable method for the spatially controlled covalent functionalization of graphene based on the employment of microemulsions.

Synthesis of Butterfly-like Shaped Gold Nanomaterial: Toward the Regulation of Liquid–Liquid Phase Separated Droplets as a Small Reaction Field

Tomohiro Nobeyama

Pure and Applied Physics, Tsukuba University, 1-1-1 tennodai, Tsukuba, Ibaraki 305-0006, Japan

Abstract:
Liquid-liquid phase separated (LLPS) droplets are attracting attention as fundamental reaction fields in a living cell. Droplets play some critical roles in regulating protein behaviors, including enzyme compartmentalization, stress response, and disease pathogenesis. The dynamic manipulation of LLPS droplet formation/deformation has become an important target in nanobiotechnology. Recently, we proposed a first nanomaterial-based device, butterfly-shaped gold nanomaterials (GNBs), which is a novel nanodevice for manipulating LLPS droplet dynamics. The growth process of GNBs is analyzed by time-lapse electroscopic imaging, time-lapse spectroscopy, and additive assays to analyze the kinds of weak interactions related to maturation of GNB shape. The concave surface of the GNBs interacts with the droplet precursors to facilitate LLPS droplet formation. Near-infrared laser irradiation of the GNBs allows on-demand deformation of the droplets through localized thermal effects of the GNBs as a type of anisotropic gold nanomaterial. The innovative design of GNBs represents a promising strategy for manipulating LLPS dynamics and offers exciting prospects for the future. In the invited talk, I would also like to share some recent achievements about the regulation of enzymatic activity in the GNB-protein droplets.

Mechanochemical Approach for the Fabrication of Carbon Based (nano)composites: From Environmental Remediation to Piezoresistive Devices

Antonio Turco

Institute of Nanotechnology National Research Council, Ecotekne Via Monteroni 1, 73100 Lecce, Italy

Abstract:
(Nano)carbon/polymeric 3D porous composites have been widely developed as innovative materials in different field of applied research such as environment, biomedicine and sensors. Functionalized nanocarbon is usually used to allow its adsorption on the surface of porous polymeric material. However, both the functionalization and the surface localized distribution of the nanomaterial can limit the (nano)carbon effect on conductivity, chemical and mechanical stability thus compromising the material performances. Novel mechanochemical strategies to prepare Nanocarbon 3D porous composite material is developed. The fabrication route does not require complex apparatus and CNTs chemical functionalization to allow their homogenous dispersion in the polymeric matrices. Moreover, foams of any shape and dimensions can be produced with neither complex machinery and procedures nor wastes production. The obtained material is characterized by the presence of well dispersed pristine (nano)carbon on both surface and bulk of the polymeric matrix. The composites exhibited superhydrophobicity

and superoleophilicity, being able to separate high volume of oils from water with high efficiency. Moreover, the composites can be squeezed to recover the adsorbed oil and recycled for a new cycle of oil absorption. The material evidenced high conductivity and improved piezoresistive properties with excellent compressive stress (>150 kPa), sensitivity at low displacement (29 kPa−1) and limit of detection for both pressure (2 Pa) and extension (130 nm). These excellent features could allow the use of the as prepared nanocomposite in different applications ranging from wearable devices to robotic or infrastructure monitoring with outstanding flexibility.

Multifunctional PEO Coatings

Paweł Głuchowski[a,b] *, Dominka Czekanowska[a,b], Daniela Kujawa[a,b], Katarzyna Hałubek-Głuchowska[a,b], Anna Łukowiak[b], Agata Musiałek[a,b], Konrad Szustakiewicz[c], Kristina Mojsilovic[d], Rastko Vasilic[d], Ting Wu[e], Qianqian Chen[e], Maxim Starikevich[e], Carsten Blawert[e], and Maria Serdechnova[e]

[a]Graphene Energy Ltd, PL-50422, Wroclaw, Poland
[b]Institute of Low Temperature and Structural Research, Polish Academy of Sciences, Wrocław, 50-422, Poland
[c]Faculty of Chemistry, Wroclaw University of Science and Technology, PL-50370 Wroclaw, Poland
[d]Faculty of Physics, University of Belgrade, RS-11000 Belgrade, Serbia
[e]Institute of Surface Science, Helmholtz-Zentrum Hereon, 21502 Geesthacht, Germany

Abstract:
Plasma Electrolytic Oxidation (PEO) is a surface treatment process extensively studied in recent years for its ability to produce thick, dense metal oxide coatings. This process is especially effective on light metals, primarily enhancing their wear and corrosion resistance. Recently, the PEO process has also been used to produce composite coatings by adding functional nanoparticles to the electrolyte.

This work presents the multifunctional properties of PEO coatings on light metal alloys with various particle additions. To increase the functionality of these coatings, various phosphors were incorporated, thereby enhancing their functional capabilities. The coatings' structure and morphology were characterized using X-ray Diffraction (XRD) and Scanning Electron Microscopy (SEM), both on the surface and in cross-section. Additionally, the chemical composition of the layers was analyzed using Glow Discharge Optical Emission Spectroscopy (GDOES) and Energy Dispersive Spectroscopy (EDS) on both the surface and cross-sections. The photocatalytic properties of the coatings were evaluated on samples containing graphene@TiO_2 particles by monitoring the photodegradation of bisphenol A using UV-Vis absorption spectroscopy. For temperature sensing properties, $Er_{0.02}Yb_{0.4}Y_{1.58}O_3$ additives were tested. Contactless temperature measurements were conducted across a broad temperature range to determine the most effective range for practical use. Furthermore, SiO-CaO glasses doped with Yb^{3+}/Er^{3+} ions were utilized to prepare coatings on alloys intended for implant applications.

Opening the Bandgap of Graphene

Bin Chen[a,b,c]*, Mingzhi Yuan[b,c], Feng Ke[d], Lingkong Zhang[c], Yi Yang[b,c], Yabin Chen[e], and Jialin Lei[f]

[a]Shanghai Advanced Research in Physical Science, Pudong, Shanghai 201203, China
[b]School of Science, Harbin Institute of Technology, Shenzhen 518055, China
[c]Center for High Pressure Science and Technology Advanced Research, Pudong, Shanghai 201203, China
[d]State Key Laboratory of Metastable Materials Science and Technology, Yanshan University, Qinhuangdao, Hebei 066000, China
[e]School of Aerospace Engineering, Beijing Institute of Technology, Beijing 100081, China
[f]Department of Chemistry, Louisiana State University of Alexandria, Alexandria, Louisiana, LA 71302, USA

Abstract:
Graphene-based nano-devices developed rapidly since the first successful fabrication of atomthin graphene in 2004. Graphene is considered as an important candidate material for postsilicon electronics. However, one of the big obstacles for semiconductor applications is the lack of sizable bandgap in graphene. The largest bandgap of

~0.3 eV was previously achieved in bilayer graphene by various means, but still far below a workable value for practical applications. Here we report our efforts to achieve an intrinsic bandgap of ~2.5 eV in trilayer graphene, which has been confirmed with both *in situ* high-pressure electrical transport and optical absorption measurements. The wide bandgap induced by compression can be quenched to near ambient conditions, hinting a rosy future for graphene-based electronic devices.

Design of MOF/Gelatin Hydrogel Composites Mediated by Coacervation Process for the Capture of Volatile Organic Compounds

N. Steunou* and S. Biswas

Institut Lavoisier de Versailles, Université Paris-Saclay, UVSQ, 78035 Versailles cedex, France

Abstract:
Metal-Organic Frameworks (MOFs), a class of porous and hybrid materials, have sparked tremendous research interests due to their highly ordered pore structure, high internal surface areas and chemical functionality. These unique properties make this class of materials very promising for a wide range of applications including gas separation, sensing, catalysis, biomedicine etc. However, typical MOF syntheses generally produced powdered materials. The intrinsic fragility of MOF powders and their notoriously poor processability and handling strongly hampers the potential of developing applications by using MOFs.

Here, we report a novel and easy-handle strategy for the synthesis of hydrogel composites combining gelatin and a series of Zr^{4+} MOFs bearing different functional organic linkers.[1] Gelatin is one of the most commonly used biopolymer in industry for drugs and cosmetics microencapsulation due to its low cost, biodegradability and nontoxicity. Herein, we showed that the thermo-reversible character of gelatin associated to a liquid-liquid phase separation process, i.e. coacervation, could be exploited to prepare a series of gelatin/MOF composites that combine attractive features such as high MOF loading (> 80 wt%), large porosity, homogeneous MOF distribution in the host matrix.[1] These MOF-gelatin composites could be shaped as films or monoliths on large scale and remarkably they showed high performance for the selective capture of acetic acid under humid ambient conditions.[1] They can thus be considered as a novel type of highly efficient adsorbents in cultural heritage preservation.

Reference: [1] Biswas, S *et al*, Chem. Mater., **2022**, 34, 9760-9774.

Session 2: Synthesis and Manufacture II

Scaling Up Excellence: Advanced Exfoliation Techniques for Industrial Nanomaterial Production

Antonio Esau Del Rio Castillo

BeDimensional s.p.a., Genoa, Italy

Abstract:
The scalable production of high-quality, exfoliated nanosheets from layered materials is pivotal for advancing applications in nanotechnology and materials science. This study focuses on the liquid phase exfoliation of graphite, hexagonal boron nitride (h-BN), transition metal dichalcogenides (TMDs), mica, and black phosphorus using wet-jet milling, a method distinguished by its scalability and repeatability.

Wet-jet milling applies high shear forces and pressure to effectively delaminate bulk materials into few-layer nanosheets without significantly compromising their intrinsic properties. Our investigation demonstrates that this technique consistently produces nanosheets with controlled thickness and lateral dimensions, essential for various industrial applications. Detailed characterization of the exfoliated materials was performed using

techniques such as atomic force microscopy (AFM), transmission electron microscopy (TEM), and Raman spectroscopy, confirming the high quality and uniformity of the nanosheets.

Key results include achieving an exfoliation efficiency of up to 90% for graphite and h-BN, with similar success rates observed for TMDs, mica, and black phosphorus. Moreover, the process parameters were optimized to enhance yield and minimize defects. We also explored the functional integration of these nanosheets in electronic, optoelectronic, and energy storage devices, demonstrating significant improvements in performance metrics.

This study underscores the potential of wet jet milling for the large-scale, repeatable production of exfoliated materials, providing a reliable pathway to meet the growing industrial demand. The implications of these findings for the future of materials science and nanotechnology will be discussed, highlighting the method's versatility and its role in fostering innovation.

Vanadium-sulfide Layers Prepared with Atomic Layer Deposition

Zsofia Baji*, Zsolt Fogarassy, Attila Sulyok, and Zoltan Szabo

HUN-REN Centre for Energy Research, Budapest, Hungary

Abstract:
After the success of graphene, the interest turned towards different 2D materials, which have new properties different from their bulk versions, such as thickness-dependent or crystalline structure depending band structures. Transition metal dichalcogenides (TMD) have a structure of MX2, where X can either be S or Se, which are covalently bonded to the transition metals. These are Van der Waals materials with 2D-like layers of a sheet of transition metals sandwitched between two sheets of chalcogen atoms, and these three-atom thick planes are bonded by week van der Waals forces.

The preparation of TMDs has so far faced some difficulties, but Atomic layer deposition offers an optimal solution to this problem. The search for chemically feasible processes for the deposition of sulphide materials is currently active.

Vanadium-sulphide is a less researched TMD material, which is in the focus of much research effort, as it promises to be versatile in the energy field, as an electrode material. It has a layered structure with 5.76 Å between the hexagonal VS2 layers. Its electron structure has been extensively studied with theoretical calculations, and a band gap of around 1 eV was predicted.

The present work reports on the deposition of vanadium-sulphide layers from tetrakis(ethylmethylamino)vanadium and H_2S. The use of this precursor combination has so far not been reported.

Influence of Sintering Modes During Hot Pressing of Partially Stabilized ZrO_2 Nano Powders on Reproducibility of Mechanical Properties

Edvin Hevorkian[a]*, Miroslaw Rucki[b], Waldemar Samociuk[a], and Vladymir Chishkala[c]

[a]*Faculty of Production Engineering, University of Life Sciences in, Lublin, Poland*
[b]*Kazimierz Pulaski University of Technology and Humanities in Radom, Radom, Poland*
[c]*Physics faculty Karazin Kharkiv National University, Kharkiv, Ukraine*

Abstract:
Ceramic materials based on partially stabilized zirconium dioxide (ZrO_2) are of great interest due to their high strength, hardness, corrosion resistance, and thermal stability. Recently, nanostructured ceramics have gained attention as ZrO_2 nanopowders offer superior mechanical and functional properties compared to coarse-grained

materials. A promising method for producing these nanopowders is electroconsolidation, involving hot pressing under high-amperage electric currents in a vacuum.

Our results were obtained using a patented hot-pressing installation in Ukraine and Poland, an advanced SPS technology variant. This installation's unique design and technological solutions enhance its industrial efficiency. Ensuring reproducibility of material properties is crucial for industrial application. The Weibull modulus evaluation is the optimal method for this, and our developed program enabled us to assess the reproducibility of composites based on ZrO_2 nanopowders.

Despite high Weibull modulus values, improving mechanical property stability requires better control of sintering parameters—temperature, pressure, and heating rate— which significantly affect sample quality and property reproducibility. Automating sintering parameter regulation, with diagnostic control, is planned. The heating rate, in particular, influences grain growth, microstructure, property uniformity, temperature fields in the graphite mold, and shrinkage rate during sintering. Optimal heating rate selection will enhance the reproducibility of mechanical properties in ceramic materials.

Generation of Paper Substrates Modified with Metallic Nanoparticles and Potential Applications in Remediation and Packaging

Nataly Silva[a]*, Paulina Contreras[a], Alejandra Amenábar[a], Sara Ramírez[a], Sebastián Salazar[a], Javiera Norambuena[a], and Jessica Martínez[b]

[a]Facultad de Diseño, Universidad del Desarrollo, Santiago, Chile
[b]Centro de Medicina Regenerativa, Facultad de Medicina, Clínica Alemana-Universidad del Desarrollo. Avenida Plaza 680, 7610658 Las Condes, Santiago, Chile

Abstract:
Paper is an exciting substrate composed of cellulose fibers. It is economical, versatile, globally accepted, and therefore possesses numerous applications [1]. Notably, it is used in remediation due to its high porosity and adsorption capacity, and in packaging due to its versatility in formats and types. To improve or incorporate new properties into the paper, nanotechnology has taken a leading role. Metallic nanoparticles (MNPs) possess attractive catalytic, optical, and antimicrobial properties, among others, mainly due to their size and high surface area-to-volume ratio. In this context, we have worked on various strategies to modify paper with MNPs, either through the chemical synthesis of MNPs and subsequent modification of the paper or by incorporating the MNPs during the *in-situ* paper formation process. Additionally, we have explored the *in-situ* generation of MNPs in cellulose paper[1], either through chemical methods, notably ultrasound-assisted[2], or through bio-fabrication using bacteria. We have characterized these composites using scanning electron microscopy, UV-Vis spectroscopy, Fourier-transform infrared spectroscopy, X-ray diffraction, and even their tensile mechanical properties.

Our research has practical implications. We have successfully used some of these materials as adsorbents for the remediation of organic pollutants, demonstrating a 47% increase in adsorption capacity compared to unmodified paper when gold nanoparticles modified with cyclodextrin were incorporated. Furthermore, we have shown the potential of paper packaging modified with silver and copper nanoparticles in reducing the growth of Botrytis cinerea on strawberry surfaces.

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Cobalt-Nitrogen Bonding for Triggering Low-power Dual Detection of NO_2 and NH_3 by Mixed Valence Co^{2+} and Co^{3+}

Mokhotjwa Simon Dhlamini[a]*, Bala Ismail Adamu[a,d], Lingxiang Jiang[b], and Weiguo Chu[c]

[a]Department of Physics, College of Science, Engineering and Technology, University of South Africa, Johannesburg 1710, South Africa

bSouth China Advanced Institute for Soft Matter Science and Technology, School of Emergent Soft Matter, South China University of Technology, Guangzhou 510640, China
cNanofabrication Laboratory, CAS Key Laboratory of Nanophotonic Materials and Devices, National Center for Nanoscience and Technology, Beijing 100190, China
dPhysics Department, Federal University Dutse, Jigawa 720101, Nigeria

Abstract:
Real-time detection of harmful gases like NO_2 and NH_3 is crucial for smart agriculture and the noninvasive diagnosis of kidney, liver, lung, and heart diseases. However, sensing these gases and understanding the primary sensing mechanisms can be challenging since the nitrogen site of NO_2 or NH_3 is the primary site that binds the sensing crystallite. Herein, we designed and fabricated low-cost sensors for dual NO_2 and NH_3 sensing using nanodevice-on-chips sensors (NDCS) with mixed valence Co_3O_4 (Co^{2+} and Co^{3+}). The Co_3O_4-NDCS detects NO_2 and NH_3 at low power, room temperature, and 70% relative humidity. It also exhibits stable, recoverable, reproducible sensing performance for NO_2 and NH_3, comparable to several high-performance sensors. The dual sensing performances are closely related to two distinct Co sites (Co^{2+} and Co^{3+}) in the Co_3O_4 crystal. Co^{2+} could host the nitrogen atom of either NO_2 or NH_3 to form Co-N bonding, preferable to NO_2 detection. Meanwhile, the N atom could replace one of the six oxygen atoms coordinating with Co^{3+} to form Co-N bonding, favourable to NH_3 detection. Looking forward, the strategy proposed here makes it possible to fabricate high-performance gas sensors with desired nanostructures and known sensing mechanisms.

Advanced Self-cleaning Paints: Sustainable Solutions with PNC-Doped TiO_2 Nanoparticles

Qaisar Maqbool[a,b]*, Francesca Tittarelli[b], and Günther Rupprechter[a]

aInstitute of Materials Chemistry, TU Wien, Getreidemarkt 9/BC, A-1060 Vienna, Austria
bDepartment of Materials, Environmental Sciences and Urban Planning (SIMAU), Università Politecnica delle Marche, INSTM Research Unit, via Brecce Bianche 12, 60131 Ancona, Italy

Abstract:
Self-cleaning photocatalytically active wall paints that operate in natural light are particularly promising. Given that a majority of both interior and exterior surfaces of buildings are coated with paint, there is substantial interest in improving paint properties by modifying polymeric paints with photocatalysts such as TiO_2 nanoparticles (NPs) [1–3] [4]. Adding photocatalytically active TiO_2 NPs to polymeric paints is a feasible route toward self-cleaning coatings. While paint modification by TiO_2 NPs can improve photoactivity, it may also cause paint-polymer photodegradation and release of toxic volatile organic compounds (VOCs), which can cause serious health issues [4,5]. This requires a targeted modification of TiO_2-NPs, which so far rarely resulted in stable TiO_2-NPs based paint formulations [4].

To counterbalance adverse effects, a green synthesis method for non-metal (P, N and C) doped-TiO_2-NPs is introduced, based purely on waste-valorization. PNC-doped-TiO_2-NPs characterization by vibrational and photoelectron spectroscopy, electron microscopy, diffraction and thermal analysis suggest that TiO_2-NPs were modified with phosphate (P=O), imine species (R=N-R) and carbon, which also hindered the anatase/rutile phase transformation, even after 700 °C calcination. When added to water-based paint, PNC-doped TiO_2-NPs achieved 96% removal of surface adsorbed pollutants under natural sunlight or UV, paralleled by stability of paint formulation, as confirmed by micro-FTIR surface analysis. The origin of the photoinduced self-cleaning properties was rationalized by 3D and synchronous photoluminescence spectroscopy, indicating that the dopants led to 7.3-times stronger inhibition of photoinduced e–/h+ recombination when compared to a benchmark P25 photocatalyst. The results are sumarized in figure 1.
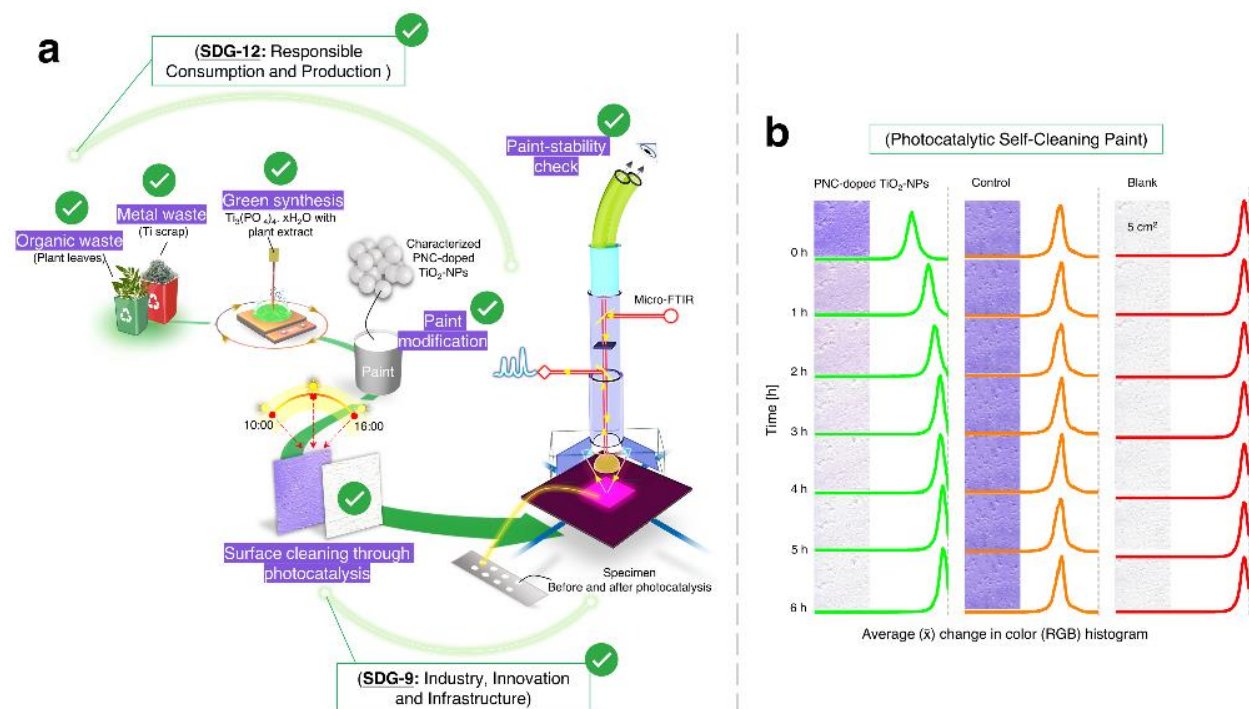
Figure 1. (a) End-to-end methodology, describing sustainable nanosynthesis (SNS), preparation/performance of photocatalytic paints and effect of NPs on paint stability. (b) Photocatalytic removal of surface adsorbed methyl violet by paint with 2.5% PNC-doped TiO_2-NPs, showing best performance.

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Morphological Effects in Metal Oxide Nanostructures: A Statistical Analysis of Ethanol Sensors Based on SnO₂

Andrea Ponzoni[a,b]

[a]National Institute of Optics, National Research Council (CNR-INO), Unit of Brescia, Brescia, Italy
[b]National Institute of Optics, National Research Council (CNR-INO), Unit of Lecco, Lecco, Italy

Abstract:
Metal oxide nanostructures are appealing materials for the development of solid-state gas sensors suitable for several applications, including environmental monitoring, food quality control and medical diagnosis. The capability to work in such different applications stems from the versatility of these nanostructures, whose sensing properties can be varied in a wide range by properly controlling the synthesis process. Crystallite size

and morphology are among the most investigated characteristics to optimize the sensor performance. However, differences in sensor configuration and measurement setups adopted by different authors often hinder the generalization of results and the comparison between different research groups. To overcome this limitation, we adopt statical methods to average over experimental differences and look for results having a general, statistical meaning. Specifically, we work on a dataset of more than 200 SnO_2 nanostructures reported in the literature for ethanol sensing. Ethanol is chosen as the target gas owing to its relevance in many applications, such as security and food fermentation. We discuss the impact of the morphological features of these nanostructures, such as the crystallite size, shape, the material porosity and specific surface area, on the main figures of merit of gas sensors, namely response intensity, response and recovery times.

Laser Patterned Polymer Graphene Composites for the Production of Sustainable Devices

Alessandra Scidà

National Research Council of Italy, CNR-ISOF, Bologna, Italy

Abstract:
In recent years, graphene and its related materials (GRM) have attracted a growing interest in both the scientific community and in industrial research, thanks to their remarkable structural and electronic properties[1][2][3]. Among the various GRM production technologies, laser scribed graphene looks promising for many applications such as sensors, energy storage, electrocatalysis and water treatment due to the fast, cost-effective, versatile and scalable process[4][5]. In this talk I will present the latest results we have obtained on laser patterning of polymers containing low percentages of different GRM. Appropriate laser parameters allow to ablate the polymer and connect graphene flakes dispersed in the matrix forming a porous conductive foam. With this method, conductive patterns with very low sheet resistance (<10 ohm/sq) can be produced by laser on insulating composites. Starting from conventional polymers, such as polypropylene or polyurethane, we have moved to biodegradable polymers, like Poly Lactic Acid, to produce more sustainable and disposable devices. Moreover, several devices like sensors and heaters were developed for automotive and healthcare applications. Potential benefits of this technology include metal replacement, easier recyclability and reduction of costs and production steps.

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Enhance the Thermal Conductivity of Phase Change Materials PCM Using Nanocomposites

Maha Alotaibi

The Center of Excellence for Advanced Materials and Manufacturing, King Abdulaziz City for Science and Technology, Riyadh 11442, Saudi Arabia

Abstract:
Research and improvement in phase change materials (PCMs) are very important due to their high-energy storage density, ability to store and release heat at nearly constant temperatures, and passive temperature control without the need for mechanical systems. Additionally, they are non-toxic and widely available, such as paraffin wax.

Paraffin wax has the properties of phase transition, meaning it absorbs heat when it melts and releases it when it solidifies, storing large amounts of thermal energy at nearly constant temperatures. PCMs are widely used in energy systems to store thermal energy, such as in solar energy storage, where they help store heat during the day and release it at night.

However, one of the limitations of phase change materials, especially organic ones like paraffin, is their low thermal conductivity. This means it takes a long time to either charge (store heat) or discharge (release heat).

In this work, we aim to improve its thermal conductivity so that heat can be transferred more quickly for thermal energy storage applications by using nanomaterials, which is multi-walled carbon nanotubes (MWCNT) and Titanium Dioxide (TiO_2). In this presentation, we will demonstrate the dispersion method for paraffin wax materials in PCM composites at various concentrations. Additionally, we will present the results of the thermal conductivity for PCM nanocomposites after modification.

Session 3: Nanomaterials for Bioapplications

Biosensing with Graphene Transistors: Advantages and Challenges

Pedro Alpuim[a,b]

[a]International Iberian Nanotechnology Laboratory (INL), Braga, Portugal
[b]Centro de Física das Universidades do Minho e Porto (CF-UM-UP), Braga, Portugal

Abstract:
Biosensing graphene transistors (GFETs), with their promising potential, are a significant area of research. Their inherent 2D nature, high carrier field-effect mobility and ambipolar transport, chemical inertness and robustness, and the possibility of surface functionalization make them a compelling choice.

The sensing principle, local gating by analyte molecules whenever they attach to the graphene channel, modulates graphene's Fermi energy (EF), causing a shift in the transistor transfer curve, typically detected by measuring the Dirac point voltage, the point of minimum conductance. Based on these principles, I will show the attomolar detection of single-stranded DNA containing a mutation occurring in brain tumor cells and results on neurotransmitter detection using a short-strand dopamine-specific DNA aptamer in different configurations for the graphene chip interrogation and signal acquisition. In particular, we use the DC and AC transistor modes and electrochemical impedance spectroscopy, and I will discuss their advantages and challenges.

Among the latter is the electrical instability that field-effect devices based on polycrystalline 2D materials often suffer due to the interaction of their charge carriers with the defects in the surrounding insulator layers [3]. Here, I present a complete model for the response of a GFET, showing that, at the transistor operating voltages, the graphene EF sits within the oxide bandgap between the two SiO2 defect bands. Our model shows that the electron capture and emission rates from and to the defect bands are responsible for the transistor drift. Once understood, this effect can be controlled, effectively removing the drift in most practical situations.

Essential Role of Chemistry in Shaping Graphene FETs for Biosensing

Alejandro Criado[a]* Adrián Martinez-Abelarias[a], Jesús Mosquera[a], Cecilia Wetzl[b], Alessandro Silvestri[c], and Maurizio Prato[b]

[a]Universidade da Coruña, Centro Interdisciplinar de Química e Bioloxía - CICA, A Coruña, Spain
[b]Center for Cooperative Research in Biomaterials (CIC BiomaGUNE), San Sebastián, Spain
[c]Department of molecular sciences and nanosystems, Ca' Foscari University of Venice, Italy

Abstract:
Graphene field-effect transistors (GFETs) have emerged as prominent diagnostic tools due to their remarkable sensitivity, selectivity, low detection limits, and suitability for *in vivo* applications. These attributes stem largely from graphene's high carrier mobility and additional properties such as biocompatibility, transparency, and flexibility. Consequently, GFETs can effectively detect various biomolecules, including proteins, DNA, and small molecules, with exceptional specificity and sensitivity across diverse media.

Achieving mandatory functionalization of graphene with various receptors or biorecognition elements has been accomplished through diverse chemical approaches, such as covalent binding, non-covalent binding, and electrostatic adsorption. However, the challenge remains in identifying the optimal immobilization strategy for receptors, as not all graphene chemistry strategies readily translate to transistor modification.

Through meticulous control of graphene functionalization and device design optimization, we have developed a range of GFET microarrays capable of detecting small molecules like neurotransmitters and air pollutants, as well as viruses, with remarkably low detection limits. These results could lay the basis for a new class of analytical platforms based on precisely engineered modifications of graphene. Such platforms hold significant potential for detecting a wide array of pathogens and biomarkers even before their isolation, thereby offering valuable contributions to health and environmental monitoring, as well as to the fight against future pandemics.

2D Carbon Nanomaterials as Photoactive Antiviral and Antibacterial Agent

Giacomo Reina[a]*, David Panacek[b,c], Krista Rathammer[a], Stefanie Altenried[a], Philipp Meier[a], Paula Navascués[a], Zdeněk Baďura[b,c], Paula Bürgisser[a], Vera Kissling[a], Qun Ren[a], Radek Zboril[b,c], and Peter Wick[a]

[a]Empa, Swiss Federal Laboratories for Materials Science and Technology, Lerchenfeldstrasse 5, 9014 St. Gallen, Switzerland
[b]Regional Centre of Advanced Technologies and Materials, Czech Advanced Technology and Research Institute (CATRIN), Šlechtitelů 241/27, 783 71, Olomouc – Holice, Palacký University Olomouc, Czech Republic
[c]Nanotechnology Centre, Centre of Energy and Environmental Technologies, VŠB–Technical University of Ostrava, 17. listopadu 2172/15, 708 00 Ostrava-Poruba, Czech Republic

Abstract:
The rising threat of antimicrobial resistance and the emergence of new infectious viral strains pose continuous challenges. Photoactive nanomaterials offer promising solutions in combating bacterial and viral infections by serving as catalysts that produce radicals and heat upon demand. In this presentation, we will propose nitrogen-doped graphene acid (NGA) as a photoactive agent with antibacterial and antiviral properties as a showcase. We will describe the preparation and characterization of metal-free biocompatible coatings suitable for various clinical settings. The catalytic heat and ROS generation of the coatings are maintained over a long shelf life, achieving a consistent performance using a clinically approved NIR light source. Finally, we will show that a few minutes of light irradiation is sufficient to hamper the spread of viruses and bacteria on the coating without producing skin irritation or sensitization. We believe that these coatings can find application in different clinical settings.

Describing the Mechanism of Interaction in the PAMAM Dendrimer and Doxorubicin Conjugated System by Ab Initio Calculations

Ernesto Osvaldo Wrasse*, Handriela de Oliveira Sobrinho, and Renato Eising

Technological Federal University of Paraná, Toledo, Paraná, Brazil

Abstract:
One of the biggest challenges in medicine is to provide efficient and selective treatment for cancer. A good alternative is drug delivery through a nanoparticle, in order to specifically target cancer cells, which would reduce adverse effects and increase the effectiveness of the treatment. Recently, it was experimentally demonstrated that a PAMAM dendrimer nanoparticle is capable of delivering the drug doxorubicin. Two targeting molecules were considered in the dendritic system: folic acid, linked to PAMAM; and cis-aconitic, bonded to doxorubicin. In this contribution, we employ ab initio simulations to describe the mechanism involved in this process. From our results we conclude that the doxorubicin/cis-aconite complex can indeed be conjugated to the PAMAM/folic acid nanoparticle by hydrogen bonds. The cis-aconitic anhydride molecule, which has the function of directing the complex through the recognition of the pH of the environment, showed performance in stabilizing this conjugated

system, as it promotes additional hydrogen bonds with the PAMAM/folic acid nanoparticle. We believe that our results will be useful for future theoretical and experimental studies in the area of drug delivery. Our contribution can be found in MSDE 8 (10), 1327, 2023 (https://doi.org/10.1039/d3me00060e).

New Tricks for Old Drugs: Utilisation of Novel Drug Delivery Systems to Overcome Cisplatinresistant Malignant Pleural Mesothelioma

Amalia Ruiz Estrada*, and Harriet Rose Walker

Institute of Cancer Therapeutics, University of Bradford, Bradford, United Kingdom

Abstract:
Mesothelioma is a rare, aggressive cancer with a prognosis of 9-12 months and most commonly develops in the pleural cavity of the lungs from exposure to asbestos. The most common approach to treatment is the combination of chemotherapy drugs, cisplatin and pemetrexed. However, it's highly resistant to chemotherapy agents, specifically cisplatin. In this work, we are discussing the repurposing of Auranofin and its loading in tumour-targeted nanoparticles to overcome MPM cisplatin resistance. Mechanism of action, therapeutic efficacy and the development of a targeted delivery system leveraging the pleural space have been developed to aid in better patient survival.

Innovative Pyroelectric Implantable Sensors for Cardiovascular Complications Real-time Monitorization

Mariana Rocha[a]*, Marta Nunes[a], Andreia T. Pereira[b,c], Inês C. Gonçalves[b,c], and André Pereira[a]

[a]*IFIMUP –Institute of Physics for Advanced Materials, Nanotechnology and Photonics, Department of Physics and Astronomy, Science Faculty, University of Porto, Porto, Portugal*
[b]*INEB – Instituto de Engenharia Biomédica, University of Porto, Porto, Portugal*
[c]*i3S - Instituto de Investigação e Inovação em Saúde, University of Porto, Porto, Portugal*

Abstract:
Cardiovascular diseases (CVD) are the primary cause of death globally, with an estimation of 17.9 million deaths/year. Stenting is the standard procedure used to widen narrowed or obstructed arteries (expected global market of ~19.8 billion € in 2030). Considerable post-implantation complications such as stent restenosis, thrombosis, and infection lead to their failure in up to 30% of the cases. This highlights the critical role of development of implantable sensors for diagnosis of stent-related complications. Smart stents with micro/nano-electromechanical sensing and communication systems have been developed for early failure diagnosis.[1] These sensors mainly measure pressure/blood flow and required external batteries for their operation, limiting their implantability.[2] This work proposes the development of self-powered sensors based on pyroelectric effect (conversion of thermal to electrical energy) implemented at the stent surface, and produced using low-cost, easy implementable and industrially scalable coating methods. For that, were produced PVDF-based devices and assessed their performance under temperature variations.

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Young Researchers Presentations

UV Sensors Based on Vertically Aligned Carbon Nanotubes (VA-CNTs)

Ravi Prakash Yadav[a,b]*, Ilaria Rago[a,b], Gianluca Cavoto[a,b], Francesco Pandolfi[b], Carlo Mariani[a,b], Sammar Tayyab[a,b], Alessandro Ruocco[c], and Alice Apponi[c]

[a]Department of Physics, Sapienza University of Rome, Rome, Lazio, Italy
[b]INFN Sezione di Roma, Rome, Lazio, Italy
[c]Dipartimento di Scienze, Universitá Degli Studi Roma Tre and INFN Sezione di Roma Tre, Rome, Lazio, Italy

Abstract:
We present an innovative UV light detector aimed at enhancing sensitivity. It comprises a photocathode to emit electrons through photoelectric effect upon UV light absorption, and an electron detector (MCP) to detect these emitted electrons. The revolutionary step lies in the use of vertically aligned Carbon Nanotubes (VA-CNTs) as a photocathode. Unlike conventional methods with a quantum efficiency of 20-25% our design minimizes the photoelectron reabsorption in the photocathode. The unique property of VA-CNTs, featuring negligible density along the tube axis, solves reabsorption issues. Carbon in its graphitic form possesses a 4.7 eV work function, rendering it insensitive to visible light and thermal noise, even when operating at room temperature.

To address challenges associated with thermal chemical vapor deposition (CVD) grown VA-CNTs, we adopt various strategies. The non-aligned top layer of dense, entangled CNTs is removed via plasma etching using Ar and O_2 as etching gas and are characterized via Atomic Force Microscope (AFM). We tackle the issue of waviness at nanoscale by transitioning to plasma enhanced chemical vapor deposition method (PECVD). A dedicated software is developed for defining and comparing VA-CNTs waviness from the Scanning Electron Microscope (SEM) images. Our approach ensures that the VA-CNTs, both as-grown and after modification through etching and improved waviness, are meticulously tested as a photocathode for the UV sensor prototype. The design represents a significant advancement in UV detection technology, poised to overcome reabsorption challenges and deliver improved sensitivity for a range of applications.

Iron Oxide Nanoparticles Modified with Cannabinoids and Anti-cancer Drugs

Jan Taudul*, and Dorota Nieciecka

Faculty of Chemistry, University of Warsaw, Warsaw, Poland

Abstract:
Superparamagnetic iron oxide nanoparticles are one of the most researched and used type of nanoparticles. Because of their magnetic properties, they have been used in targeted therapies, the anti-cancer drug attached to the carrier can be delivered to the tumor's environment. These kind of carriers are non-toxic and are easily removed from the organism. Lately, the growth in popularity showed compounds known as cannabinoids. The first identified cannabinoid was THC, which helped scientists to discover the cannabinoid receptors in the human organism. Because of THC's undesirable properties, in medicine we used different isomers like CBD and CBG. More and more scientific studies have demonstrated the anticancer properties of cannabinoids. They cause apoptosis of cancer cells, prevent their division, inhibits the development of new blood vessels within the tumor or they have antiproliferative effects. Cannabinoids can show synergistic effects combined with anthracyclines. In this project, a synthesis of iron oxide nanoparticles was developed modified with a cannabinoid and an anthracycline drug. Using the Dynamic Light Scattering method, the size of obtained nanostructures were examined and the value of the Zeta potential gave us information about the stability of conjugates. To confirm the modification with cannabinoids and anthracyclines, we used infrared spectroscopy, thermogravimetry, cyclic voltammetry and differential scanning calorimetry. The last three techniques were used to determine quantitative attachment of cannabinoids and anthracyclines. Additionally, using the magnetic hyperthermia, the ability to induce heat was tested. The finalizing point of the project was the determination of cytotoxicity of our conjugates.

Si Nanowire-based Schottky Sensors for Selective Sensing of NH3 and HCl via Impedance Spectroscopy

Valerii Kondratev[a]*, and Alexey Bolshakov[b]

[a]Alferov University, Saint Petersburg, Russia
[b]Yerevan State University, Yerevan, Armenia

Abstract:
This work is aimed at the development of a highly sensitive silicon (Si)-based sensor allowing for the selective detection and analysis of liquid solution compositions containing ammonia (NH3) and hydrochloric acid (HCl) in an indirect manner using electrochemical impedance spectroscopy (EIS). The best sensitivity results were obtained with Si nanowires based Schottky Sensors, which provided a detection limit of 4 µmol·L –1 and resistive sensitivities of 0.8% per µmol·L–1 for HCl and 4 µmol·L–1 , –0.2% per µmol·L–1 for NH3, respectively. Treatment with HF stimulated Si nanowires surface oxidation and increased the density of adsorption sites, making it promising for detecting analyte concentrations up to 1000 µmol·L–1 . The experimental data were confirmed via density functional theory (DFT) modeling of the processes of adsorption and redox interaction between ammonia and hydrochloric acid molecules and the surface of silicon nanowires. This study are particularly interesting from the perspective of developing sensors for biological markers of health based on silicon for personalized human medicine.

Deuterium Interaction with Carbon Nanotube Surfaces: Atomic-scale Insights and Hydrogen Storage Implications

Sammar Tayyab[a]*, Alice Apponi[d], Maria Grazia Betti [b], Gianluca Cavoto[a], Riccardo Frisenda[b], Francesco Pandolfi[c], Ilaria Rago[a], Alessandro Ruocco[d], Ravi Prakash Yadav [a], and Carlo Mariani [a]

[a]Physics Department and INFN, Sapienza University of Rome, Piazzale Aldo Moro 2, 00185 Rome, Italy
[b]Physics Department, Sapienza University of Rome, Piazzale Aldo Moro 2, 00185 Rome, Italy
[c]INFN Rome, Piazzale Aldo Moro 2, 00185 Rome, Italy
[d]Department of Science and INFN, University of Roma Tre, Via della Vasca Navale 84, 00146 Rome, Italy

Abstract:
Hydrogen can be an efficient energy carrier, a renewable, storable, abundant resource with reduced impact on the environment. Its efficient storage in solid-state materials will play a key role in many applications. Carbon Nano-Tubes (CNTs) are considered as one of the most effective potential candidates for hydrogen storage as they present high surface area, light weight, chemical and mechanical stability. CNTs are constituted by rolled graphene sheets made up of sp^2 bonding network of carbon atoms, and atomic hydrogen (H) chemisorption causes the C–C sp^2 bonds of pristine CNTs to be modified towards sp^3 H–C bonds. The chemical reactivity with H has been predicted to be enhanced by the local curvature of the C mesh, thus suggesting the use of CNTs as efficient storage systems. In this work, we present atomic deuterium (D) chemisorption on highly aligned multi-wall C nanotubes (MWCNTs), being D a H isotope with the same chemical reactivity and easily detectable in vacuum. High uptake of atomic D chemically bonded to the MWCNTs is observed, demonstrated by the C 1s core level line-shape, with the emerging of a neat sp^3 component, and by the opening of an energy gap in the valence band. Furthermore, the CNTs have been bombarded with rare gases, to increase the density of chemisorption sites. We analyze morphology, lattice deformation, and electronic state changes before and after ion irradiation. This research, beyond its importance for the storage, is also in line with new anisotropic detectors exploiting higher mass isotopes of hydrogen.

Poster Presentation

Ideal Metal Organic Frameworks' (MOFs)-platforms for the Development of Multifunctional MOF-Nanocarbon Hybrids

Giasemi K. Angeli*, Georgia Basina, Ioanna K. Sideri, and Nikos Tagmatarchis

aTheoretical and Physical Chemistry Institute, National Hellenic Research Foundation, 48 Vassileos Constantinou Avenue, Athens 11635, Greece

Abstract:

MOFs is a well-established class of periodic porous materials based on the meticulous combination of organic and inorganic building blocks[1]. The plethora of different building blocks that can be combined to build a MOF enables the formation of diverse possible porous networks with unique structural and physicochemical characteristics, that can be employed in applications regarding energy, environment, catalysis among others, bringing them at the forefront of materials' chemistry[2]. At the same time, this remarkable diversity that they present in terms of pore, shape, size and functionality, combined with their enhanced chemical stability, makes them excellent candidates for the preparation of hybrid materials. In detail, MOFs' networks can serve as highly promising platforms for the encapsulation and/or binding of guest materials or molecules (e.g., metal nanoparticles, dyes, nanocarbons, drugs, etc.), leading to the formation of smart functional hybrid materials with enhanced properties, expanding their field of application[3].

In this work, leveraging the merits of advanced functionalized 0D and 1D nanocarbons (fullerenes and carbon nanotubes (CNTs), respectively) in terms of light sensitization, redox activity and charge transport kinetics, we aim to the preparation of stable MOF-nanocarbon hybrids. These novel hybrids are anticipated to present enhanced photo and electrocatalytic behavior due to synergistic host-guest interactions overcoming existing limitations of pristine MOFs.[4,5] In this study, we will prioritize identifying the essential structural and physicochemical properties necessary for the formation of stable MOF-nanocarbon hybrid materials. Also, we will evaluate and discuss the experimental results by examining the hybrids' stability, along with their electrocatalytic and/or photocatalytic performance.

References: [1] *Chem. Rev.* 2012, 112, 673. [2] *ACS Omega* 2022, 7, 44507. [3]. *Chem. Sci.* 2018, 9, 4477. [4]. *Angew. Chem. Int. Ed.* 2023, 62, e202217897. [5]. *Chem. Sci.* 2018, 9, 4477.

A New Dual Emitting System Resulting from the Encapsulation of Rhodamine B Molecules within MOF-808 Cavities

G. Ficarra[a], A.Sciortino[a], L.G. Barbata[a], R. Ettilinger[b], V. De Michele[c], M. Cannas[a], R.E. Morris[b], and G. Buscarino[a*]

aDepartment of Physics and Chemistry "Emilio Segr`e", University of Palermo, Via Archirafi 36, 90123 Palermo, Italy
bEastChem School of Chemistry, University of St Andrews, North Haugh, St Andrews, UK
cUJM,CNRS,IOGS,LaboratoireH.Curien,UMRCNRS5516,UnivLyon,42000Saint-E´tienne, France

Abstract:

Metal Organic Frameworks (MOFs) are an emerging class of porous nanocrystals with promising application in sensing, catalysis, gas storage etc. They are hybrid ordered and porous structures where rigid rod-like ligand connect metal oxoclusters, showing outstanding values of internal surface area[1].

Along MOFs which display an optical activity, the ligands play the role of UV absorption centers, from which a charge or an excitation transfer can lead to the metal states. It's possible to exploit MOFs pores to introduce luminescent guest molecules[2].

We synthesized Zr-based MOF-808 ideal for molecules trapping due to its huge cages. We embedded Rhodamine B within the MOF cavities which results in a dual emitting system.

We found out that MOF-808 displays a broad emission band centered at 420 nm. We included nanosecond time-resolved measurements, estimating a 3 ns lifetime. By performing fs transient absorption measurements, we recorded an increase of the signal in 750 ns, suggesting the occurrence of an energy transfer from the electronic state of the ligand to the metal[3].

The host-guest system maintains the band associated to MOF-808 while displaying a second band related to the embedded Rhodamine. We observed a redshift of this second band and a lifetime change. The lifetime of the band attributed to the MOF resembles Rhodamine lifetime, suggesting the occurrence of an energy transfer.

References: [1] Vadia Foziya et al., ACS Omega 2022, 7, 44507–44531, [2] Mario Gutiérrez et al., Chem. Rev. 2022, 122, 10438-10483, [3] Jian-Xin Wang et al., ACS Appl. Mater. Interfaces 2022, 14, 9970-9986

Preparation of High-entropy Sulfides for Energy Conversion and Storage

E. Miliutina[a,b*], V. Buravets [a], V. Burtsev[a], V. Shilenko[a], V. Svorcik[a], and O. Lyutakov[a]

[a]Department of Solid State Engineering, University of Chemistry and Technology, 16628 Prague, Czech Republic
[b]Materials Centre, Faculty of Science, J. E. Purkyně University, 400 96 Ústí nad Labem, Czech Republic

Abstract:
2D high-entropy sulfides (HES) are a subclass of high-entropy materials characterized by multiple elements randomly dispersed at the atomic level, forming a homogeneous compound. Their composition and atomic arrangement include a huge variety of unique multielement redox active sites, which ensure superior surface properties and high surface activity in a wide range of processes. The synthesis of the sulfides itself is a complicated task, and the bottom-up approach requires sophisticated equipment and costly precursors (e.g., CVD or ALD methods) with very low yields of the obtained materials. On the other hand, the synthesis of high entropy materials (in particular, sulfides) is a challenge itself, as the induced strain is thermodynamically not favorable and thus clusterization of the elements in the materials can occur. In this work, we propose a novel, simple, and efficient approach for the synthesis and further functionalization of HES based on our experience with conventional sulfides. We proposed the utilization of salts of required metals as precursors and their mixing in an aqueous solution followed by instant freezing in liquid nitrogen to "capture" a high entropy metals arrangement. In the subsequent step, high entropy salts are freeze-dried and sulfurized using a home-made reactor. As a result, we have successfully obtained HES composed of different combinations of Co, Ni, Fe, Mn, Cr, Zn, and Ti. The obtained HESs were successfully tested for catalytic activity in the hydrogen evolution reaction and the oxygen evolution reaction.

Automated Characterization of Metal Organic Polyhedra

Andrea M. Oyarzún-Aravena[a,b*], Jethro Akroyd[b,c], Aleksandar Kondinski[b], and Markus Kraft[b,c,d,e]

[a]Universidad de Magallanes, Punta Arenas, Magallanes, Chile
[b]University of Cambridge, Cambridge, UK
[c]CARES, Singapore, Singapore
[d]Nanyang Technological University, Singapore, Singapore
[e]The Alan Turing Institute, London, UK

Abstract:
Advanced materials may be described by assemblies of smaller fragments, akin to the group contribution theory that was used to develop the UNIFAC model for fluids. One example is the family of metal-organic polyhedra (MOPs), which can be described by an assembly model and a set of building units. The building process requires several organized steps, the first of which is to discover and analyze patterns. This step was previously addressed using ontologies. Once the discovery is done, the molecular model can be built. In this work, we conceptualize the process of building new MOPs to obtain the final optimized structure and their properties.

On the Potential of Spatial Abstractions to Enhance Chemical Descriptions

Andrea M. Oyarzún-Aravena[a,b]

[a]Universidad de Magallanes, Punta Arenas, Magallanes, Chile
[b]University of Cambridge, Cambridge, UK

Abstract:
The representation of molecules could be improved by incorporating a description of their surroundings. Molecular file formats can describe atoms and their location. Some may incorporate a description of bonds and potentials associated with the species. However, understanding the reactivity of molecules requires to perform simulations such as *ab initio* or molecular dynamic ones. The simulations can shed light on the interaction between molecules. This is especially useful in the field of adsorption, as we try to understand the fundamental reasons for a specific experimental phenomenon. However, the advances in computing and the now extensive literature on molecular simulations, allow us to propose that the addition of additional features may improve the molecular descriptions. One example of the importance of spatial features is our previous work on gasification reactions, in which we used molecular orbitals to better understand the adsorption phenomena of water on graphene edges. We observed an out-of-plane reaction direction and a rotational phenomenon, associated to a comparatively low adsorption rate. Another example comes from the fact that some advanced materials may be described by assemblies of smaller fragments, akin to the group contribution theory that was used to develop the UNIFAC model for fluids. The building process requires to employ abstract connection points. In this work, we discuss the topic from different perspectives and suggest ideas for an enhanced molecular description.

In situ Electrosynthesis of MOF-type Nanomaterials of Zn-BTC, Cu-BTC and Zn/Cu-BTC on ITO Electrode for the Study of the Hydrogen Evolution Reaction

Carmen Castro-Castillo [a]*, Gonzalo García[b], Mónica Soler[a], Nataly Silva[a], and Rodrigo Espinoza-González[a]

[a]LabMAM, Department of Chemical Engineering, Biotechnology and Materials, FCFM, Universidad de Chile, Santiago, Chile
[b]Instituto Universitario de Materiales y Nanotecnología, Departamento de Química, Universidad de La Laguna, P.O. Box 456 Santa Cruz de Tenerife, Spain

Abstract:
The hydrogen (H_2) economy soon appears as the best and most appropriate way to produce a low-carbon energy source. The hydrogen evolution ratio (HER) has attracted even more attention during the last decades due to the growing energy demand and the great potential it presents in terms of energy storage and conversion in the future of renewable energies, such as the possibility of use fuel cells as ecological devices for energy consumption[1]-[2].

 In this work, the use of BTC ligand MOFs of Zn-BTC, Cu-BTC and Zn/Cu-BTC as electrocatalysts is proposed, which were synthesized by *in situ* electrosynthesis on an ITO (indium tin oxide) surface without no binder or functional group to evaluate its efficiency in HER electrocatalysis. The novelty of this study is the synthesis of MOF derived on the surface of an electrode without any binder at the nanometer scale. This method proposes a new route to manufacture high-performance electrocatalysts on different substrates with high production speed and excellent response in the hydrogen evolution reaction.

References: [1] Electrochem 2020, 1, 75–86; doi:10.3390/electrochem1020008
[2] Chem Rev 2020 Jan 22;120(2):851-918; doi: 10.1021/acs.chemrev.9b00248.

Synthesis and Characterization of Cobalt Nanoparticles for Enhanced Oxygen Evolution Reaction in Alkaline Environments

Borislava Mladenova*, Galin Borisov, Mariela Dimitrova, and Evelina Slavcheva

Institute of electrochemistry and energy systems Acad. Evgeni Budevski – Bulgarian Academy of Science, Sofia, Bulgaria

Abstract:

In recent years, there has been increased academic and global political interest in green hydrogen production due to its potential as a clean energy source capable of replacing internal combustion engines. Consequently, research into new materials for hydrogen energy applications is ongoing. This study presents the synthesis of Co nanoparticles using Cobalt (II) 2,4-pentanedionate ($C_{10}H_{14}CoO_4$) via a high-temperature method. The electrochemical activity of the Co particles towards the oxygen evolution reaction (OER) was investigated. Electrodes with varying catalytic loadings (0.5 mg cm^{-2}, 1 mg cm^{-2}, 1.5 mg cm^{-2}, and 2 mg cm^{-2}) were prepared for this purpose. Electrochemical tests were conducted in a three-electrode cell in an alkaline environment (25% KOH). The synthesized materials underwent structural and morphological characterization using X-ray diffraction (XRD), transmission electron microscopy (TEM), X-Ray Fluorescence (XRF), and scanning electron microscopy-energy dispersive X-ray analysis (SEM-EDX). The results revealed predominant particle sizes around 100 nm and crystallite sizes ranging from 8 nm to 16 nm. Furthermore, the Cobalt nanoparticles demonstrated promising catalytic activity for the oxygen evolution reaction with the highest performance observed at a catalytic loading of 2 mgcm^{-2}.

Investigating the Effect of pH on the Growth of Coprecipitated Ni(OH)$_2$ Agglomerates as Precursors of Cathode Materials for Li-ion Batteries

Son, Jong-Tae*, Hong, Tae-Whan, Kim, Il-Song, and Kang, Jeong-Won

Nano Polymer Science and Engineering Department, Korea National University of Transportation, Chungju-si, Chungcheongbuk-do, Republic of Korea

Abstract:

Understanding how the morphology and microstructure of secondary particles are affected by pH is essential to design spherical and dense hydroxide aggregates as precursors of high-performance cathode materials for lithium-ion batteries. the decrease in pH causes a significant increase in the complex ion concentration, thereby facilitating the growth of crystals along the [104] direction. We will explain the effect of battery property of high Ni cathode material as a function of pH.

Inner/Outer Side Chain Engineering of Non-fullerene Acceptors for Efficient Large-area Organic Solar Modules Based on Non-halogenated Solution Processing in Air

Sabeen Zahra[a,b]*, Seungjin Lee[a], Muhammad Jahankhan[a,b], Muhammad Haris[a,b], Du Hyeon Ryu[a], Bumjoon J. Kim, Chang Eun Song[a,b]**, Hang Ken Lee[a,b], Sang Kyu Lee[a,b], and Won Suk Shin[a,b]**

[a]*Energy Materials Research Center, Korea Research Institute of Chemical Technology (KRICT), Daejeon, Korea*
[b]*Advanced Materials and Chemical Engineering, University of Science and Technology (UST), Daejeon, Korea*

Abstract:

Achieving efficient and large-area organic solar modules via non-halogenated solution processing is vital for the commercialization, yet challenging. The primary hurdle is the conservation of the ideal film-formation kinetics and bulk-heterojunction (BHJ) morphology of small-area organic solar cells (OSCs) even in large-area modules. A cutting-edge non-fullerene acceptor (NFA), Y6, shows efficient power conversion efficiencies (PCEs) when processed with toxic halogenated solvents, but exhibits poor solubility in non-halogenated solvents, resulting in

suboptimal morphology and PCEs. Therefore, in this study, we investigated the impact of modifying the inner and outer side-chains of Y6 on OSC performance. Our study reveals that blending a PM6 polymer donor with one of the modified NFAs, namely N-HD, achieved an impressive PCE of 18.3% on a small-area OSC. Due to the longer alkyl-chains, this modified NFA displayed improved solubility in a non-halogenated solvent (*i.e.*, *o*-xylene) at room temperature, which facilitated the formation of a favorable BHJ morphology. A large-area (55 cm^2) sub-module delivered an impressive PCE of 12.2% based on N-HD using *o*-xylene under ambient conditions. These findings underscore the significant impact of the modified Y6 derivatives on structural arrangements and film processing over a large-area module at room temperature. Consequently, these results are poised to deepen our comprehension of the scaling challenges encountered in OSCs and may contribute to their commercialization.

ZnS-Ag in Form of Janus Nanoparticles and Multi-headed Structures for Hydrogen Evolution in Visible Light

H. Głowienke[a]*, W. Lisowski[b], T. Klimczuk[c], A. Mikolajczyk[d,e], D. Falkowski[d,e], M. Pawlyta[f], A. Zaleska-Medynska[a], and A. Gołąbiewska[a]

[a]*Department of Environmental Technology, Faculty of Chemistry, University of Gdansk, Gdansk, Poland*
[b]*Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland*
[c]*Department of Solid State Physics, Faculty of Applied Physic and Mathematics, Gdansk University of Technology, Gdansk, Poland*
[d]*Laboratory of Environmental Chemoinformatics, Faculty of Chemistry, University of Gdansk, 308 Gdansk, Poland*
[e]*QSAR LAB, Gdansk, Poland*
[f]*Institute of Engineering Materials and Biomaterials, Silesian University of Technology, Gliwice, Poland*

Abstract:
Photocatalysts comprising zinc sulfide (ZnS) and silver compounds with diverse configurations (Janus, Janus-like, and multi-headed) were synthesized via a two-phase method involving hydrothermal synthesis and the deposition of silver compounds onto the ZnS surface. These nanoparticles (NPs) were then assessed for their ability to photocatalytic generation of hydrogen under visible light (wavelengths greater than 420 nm). The highest efficiency in this photocatalytic process was demonstrated by material exhibiting Janus morphology. Various analytical techniques (including TEM, SEM, UV-Vis spectroscopy, XPS, XRD and PCA analysis) were employed to elucidate the role of surface chemistry in the photocatalytic performance of these structures. Two potential mechanisms for the photocatalytic reaction were postulated, one involving the excitation of silver particles and the other implicating the Ag_2S semiconductor.

Edge-sharing Octahedrally Coordinated Ni–Fe Dual Active Sites on ZnFe$_2$O$_4$ for Photoelectrochemical Water Oxidation

Zhiyong Jiang[a]*, Xiaodi Zhu[a]*, Zhiyu Wang[a], Wei Liu[b], Wensheng Yan[a], Kevin Sivula[c], and Jun Bao[a]

[a]*National Synchrotron Radiation Laboratory University of Science and Technology of China, Hefei, Anhui, China*
[b]*State Key Laboratory of Fine Chemicals School of Chemical Engineering Dalian University of Technology, Dalian, Liaoning, China*
[c]*Laboratory for Molecular Engineering of Optoelectronic Nanomaterials, École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland*

Abstract:
The structural properties of octahedral sites (B_{Oh}) in spinel oxides (AB_2O_4) play vital roles in the electrochemical performance of oxygen-related reactions. However, the precise manipulation of AB_2O_4 remains challenging due to the complexity of their crystal structure. Here, a simple and versatile molten-salt-mediated strategy is reported to introduce Ni2+ in B_{oh} sites intentionally on the surface of zinc ferrite ($ZnFe_2O_4$, ZFO) to promote the active sites for photoelectrochemical (PEC) water splitting. The as-created photoanode (ZFO-MSNi) shows a remarkable cathodic shift of ≈540 mV (turn-on voltage of ≈ 0.6 VRHE) as well as three times the 1-sun photocurrent density at 1.23 VRHE for PEC water oxidation in comparison with bare ZFO. A comprehensive structural characterization

clearly reveals the local structure of the introduced Ni^{2+} in ZFO-MSNi. Fewer surface trapping states are observed while the precisely introduced Ni^{2+} and associated neighboring $Fe^{(3-\sigma)+}$ ($0<\sigma<1$) sites unite in an edge-sharing octahedral configuration to function as Ni–Fe dual active sites for PEC water oxidation. Moreover, open circuit potential measurements and rapid-scan voltammetry investigation give further insight into the enhanced PEC performance. Overall, this work displays a versatile strategy to regulate the surface active sites of photoelectrodes for increasing performance in PEC solar energy conversion systems.

New Organic Cathodes based on Polyperylenediimides and Graphene-type Structures for Ca-multivalent Secondary Batteries

Belén Martínez-Moral*, Antonio Peñas-Sanjuán, Celeste García, M. Dolores López, M. Luz Godino, and Manuel Melguizo

University of Jaén, Jaén, Spain

Abstract:
Lithium-ion batteries have dominated the energy storage sector since the 1990s, but a recent global trend has brought about the need to develop transition-metal-free energy storage systems. Calcium metal based rechargeable batteries have recently gained a great deal of attention, however, although Ca batteries are expected to provide efficient, safe and cost-effective battery solutions, a key challenge in their practical implementation is the lack of suitable and efficient cathode materials.

Several studies have assessed the electrochemical properties of Organic Electrode Materials (OEMs) such as conductive polymers, organosulfur compounds, carbonyl compounds, etc. However, despite the fact that some strategies based on structure engineering, polymerization, hybridization, and amorphization of OEMs have been performed to reach high cathode performances, the application of OEMs for multivalent batteries has been hindered by their low cell voltage, low specific power/energy, poor electric conductivity and dissolution in electrolyte. Herein, we present our latest investigation focused on the development of organic cathodes based on polyperylenediimide redox-active materials integrated with graphene-type structures, through efficiently directed methodologies, which provided high conductive hybrid cathodes, with a redox-active molecule content up to 90%-95% and 2-3 mAh/cm^2. These new cathode materials were obtained through an unprecedented synthetic procedure based on feasible, reproducible, cost-effective and sustainable methodologies, avoiding costly and polluting solvents (DMF, DMSO, etc.).

A Study on the Processing and Microstructure of High Strength Ti Alloy with Solute Element by Metal 3D Printing

Choon-Man Lee[a]*, Tae-Wook Kim[b], Jae-Hyun Kim[a], and Young-Tae Cho[b]

[a]Mechatronics Research Center, Changwon National University, Changwon-si, Republic of Korea
[b]Dept. of Smart Manufacturing Engineering, Changwon National University, Changwon-si, Republic of Korea

Abstract:
Ti6Al4V stands out as one of the most widely utilized titanium alloys, boasting exceptional biocompatibility and impressive mechanical attributes, including a favorable strength-to-weight ratio, heat resistance, and corrosion resistance. This makes it a preferred choice for crafting crucial components in aerospace, marine, and biomedical applications. However, a significant challenge in the metal 3D printing of titanium alloys lies in the production of coarse columnar grains due to a high thermal gradient. The presence of columnar grains in titanium, manufactured through metal 3D printing, is undesirable as it can lead to anisotropic mechanical properties. Consequently, addressing this issue of easily generated columnar grains in titanium alloys via metal 3D printing becomes imperative.

Primary method is addition of solute elements. Unlike more common alloys like aluminum, there is a scarcity of commercially available grain refiners for titanium alloys that effectively refine the alloy's grains, so that researchers have increasingly focused on the addition of solute elements as an alternative method.

This study specifically explores the deposition of Ti6Al4V with solute elements using directed energy deposition, aiming to assess both the microstructure and mechanical properties of the resulting material. Consequently, the Ti6Al4V with solute element exhibited a finer grain size than the Ti6Al4V alloy, and the workpiece demonstrated a higher hardness than the Ti6Al4V workpiece. The excellent mechanical properties observed can be attributed to the fine grain size achieved through rapid cooling, the solid solution strengthening, and precipitation strengthening because of Cu addition.

On the High Photodarkening Values of Some Amorphous Thin Films of the Ge-As-S System

P. Kutálek[a]*, P. Knotek[b], E. Černošková[b], Z. Černošek[b], E. Samsonova[b], and L. Tichý[b]

[a]Center of Materials and Nanotechnologies, Faculty of Chemical Technology, University of Pardubice, Cs. Legii 565, 530 02 Pardubice, Czech Republic
[b]Department of General and Inorganic Chemistry, Faculty of Chemical Technology, University of Pardubice, Studentská 573, 532 10 Pardubice, Czech Republic

Abstract:
Amorphous chalcogenide glasses exhibit interesting properties such as a wide range of infrared transparency, high linear and nonlinear refractive index, low phonon energies and tunable properties by compositional tailoring. These unique properties make chalcogenide glasses and thin films good candidates for many applications such as sensors and detectors, lasers, optical fibers or waveguides. They also exhibit several photo-induced phenomena, such as photo-induced expansion or photodarkening. In bulk glasses of the Ge As-S chalcogenide system, the magnitude of photodarkening reached as much as 5% of the band gap value for the specific chemical compositions. The reason for this maximal photodarkening remains unanswered.

Amorphous thin films were prepared by the vacuum-thermal evaporation from the previously synthesized bulk glasses ($Ge_{16}As_{26}S_{58}$, $Ge_{20}As_{25}S_{55}$ and $Ge_{30}As_{30}S_{40}$). Annealed thin films were illuminated with different light sources (band gap, over-band gap and sub-band gap photons) to induce the photodarkening. The nanophase separation of the thin films after the annealing and illumination was studied using the Raman microscopy and PeakForce Quantitative Nanoscale Mechanical mode of atomic force microscopy.

Our main aim is to present some literature findings and our experimental results which suggest that the nanophase separation is likely to contribute significantly to the observed pronounced photodarkening within a limited region of a Ge-As-S chalcogenide system. It is characterized by a sulfur-poor chemical composition, with an arsenic content ranging approximately from 15 to 50 at%.

Effect of Incorporation of Nickel/Cobalt Ions on the Structure and Physical Properties of ZincPhosphate Glasses

Jana Holubová*, and Zdeněk Černošek

Department of General and Inorganic Chemistry, Faculty of Chemical Technology, University of Pardubice, Studentská 573, 532 10 Pardubice, Czech Republic

Abstract:
Phosphate glasses have been intensively studied in recent years because they provide some unique physical properties compared to classic silicate glasses, including the ability to hold large amounts of transition metal ions without crystallization. Transition metals, embedded in a phosphate glass network, improve the various important glass properties, such as their mechanical strength, chemical durability and what is important – also optical and magnetic properties, which implies their potential use in optical communication, photonic devices

and laser materials. The invention of new glass materials with the exact composition corresponding to the desired properties is closely related to the knowledge of the structure, which is far from being understood.

Glasses containing 3d transition metal ions were found to exhibit interesting magneto-optical properties due to the distinct orbital configuration, various valences and coordination states. The aim of our work was to study the influence of nickel and cobalt, i.e. a typical transition metals, on the structure and some physico-chemical properties of zinc-phosphate glasses. The glasses of the system $NiO-ZnO-P_2O_5$ were prepared by the conventional melt–quenching technique in two compositional series formally expressed (in oxides): the first series (A) $xNiO/CoO-(50-x)ZnO-50P_2O_5$ and the second one (B) $xNiO/CoO-(50-0.75x)ZnO-(50-0.25)P_2O_5$. The Raman spectroscopy, ^{31}P MAS NMR spectroscopy, magnetic susceptibility, UV-VIS-NIR spectroscopy and electron paramagnetic resonance were used to obtain information on their short as well as intermediate-range structure. Thermal properties of glasses were studied by thermomechanical analysis.

Advanced SiOC 3D Microstructures: Fabrication via Laser Lithography and Pyrolysis

Greta Merkininkaitė[a,b*], Darius Gailevičius[c], Mangirdas Malinauskas[c], and Simas Šakirzanovas[a,b]

[a]Center for Physical Sciences and Technology, Vilnius, Lithuania
[b]Institute of Chemistry, Faculty of Chemistry and Geosciences, Vilnius University, Vilnius, Lithuania
[c]Laser Research Center, Faculty of Physics, Vilnius University, Vilnius, Lithuania

Abstract:
In recent years, there has been a growing interest in ceramic materials and their derived 3D structures, owing to their outstanding mechanical, chemical, and thermal properties. We present a novel approach for fabricating robust ceramic SiOC 3D microstructures by combining precursor synthesis, laser lithography, and pyrolysis. Hybrid organosilicon precursors, prepared using trimethoxymethylsilane and 3-(trimethoxysilyl)propyl methacrylate through a sol-gel method, enable laser photopolymerization due to the acrylate functional group. After high-temperature pyrolysis under a nitrogen atmosphere, hard ceramic objects with exceptional mechanical properties are achieved, surpassing those of soft organometallic derivatives. The attained mechanical properties and tunability of materials, including amorphous SiOC and crystalline SiC, α,β-Si3N4, represent a significant advancement in manufacturing mechanically robust devices. Notably, the our prepared MTMS:MAPTMS 8:2 material annealed at 1200 °C exhibits a hardness of 14.33 ± 1.17 GPa, a reduced elastic modulus of 104.99 ± 1.81 GPa, low density of 2.21 ± 0.09 g/cm3, and an amorphous SiOC state. This material is ideal for pressing molds in micro-optic fabrication using fused quartz and for producing microscopic apertures due to its opacity. In summary, the results highlight multi-photon lithography and thermal post-processing as a powerful tandem for creating ultra-resilient multifunctional 3D microscale ceramic structures. These achievements effectively tackle the challenges associated with producing solid and precise 3D structures, expanding the potential applications of this technology in the industry.

Detecting Drugs on the Air an SERS and Artificial Neural Network

V. Burtsev[a*], A. Trelin[a], E. Miliutina[a,b], V. Svorcik[a], and O. Lyutakov[a]

[a]Department of Solid State Engineering, University of Chemistry and Technology, 16628 Prague, Czech Republic
[b]Materials Centre, Faculty of Science, J. E. Purkyně University, 400 96 Ústí nad Labem, Czech Republic

Abstract:
The most commonly used methods for determining the presence of narcotic substances in the air are specially trained dogs or ion mobility spectrometry (IMS) and gas chromatography-mass spectrometry (GC-MS). These methods offer high sensitivity and accuracy but have a number of limitations. Dogs can only work efficiently for

a limited time and training them is time-consuming and expensive. IMS and GC-MS also have high costs for the equipment as well as sample preparation. In addition, both of these methods may be less sensitive to some new or rarely occurring substances. In this work, we propose a new alternative procedure for air composition determination with the main focus on the detection of illicit psychoactive and stimulant substances using SERS analysis. For this purpose, we prepared plasmon active surfaces based on commercially available filters made of polypropylene membranes covered by a thin silver film. The air is drawn through the obtained filter from a climatic chamber simulating different conditions (temperature and humidity changes) and with different analyte concentrations. We chose phenylethylamine as a commercially available model analyte. Subsequent training/validation of the neural network was performed on the spectra obtained. The use of a neural network improves the accuracy and reliability of detection of target molecules, including detection against spectrally complex backgrounds without the need for manual interpretation. The detection limit of phenylethylamine content was 150 μg/m^3.

Detection of Microplastics in Water Using SERS and Machine Learning

Karolina Kukralova[a*], Andrii Trelin[a], Elena Miliutina[a,b], Vaclav Svorcik[a], and Oleksiy Lyutakov[a]

[a]Department of Solid State Engineering, University of Chemistry and Technology, 16628 Prague, Czech Republic
[b]Centre for Nanomaterials and Biotechnology, Faculty of Science, J. E. Purkyne University, 40096 Ústí nad Labem, Czech Republic

Abstract:
In this work, we used nanostructured plasmon-active substrates for microplastics (MP) detection in water using the combination of surface Enhanced Raman Spectroscopy (SERS) and machine learning. Microplastics of different forms are commonly found in water around the world. Their concentrations can range up to several grams per liter and their effects on the human body are not clearly determined. At the same time, there are no standardized methods for MPs detection. One of the more efficient analytical approaches, SERS, has not been widely used for MPs detection, because the analytes must reach a plasmon-active spot (with nanometer size) on the nanostructured plasmon-active surface, while MPs are well beyond these hot spots in size. Therefore, in our work, the deposition of MPs on the nanoporous plasmon-active substrate was followed by annealing, with the aim of melting the plastic(s) and tuning the material(s) inside the plasmon-active hot spot. Due to the high sensitivity of SERS, MPs were detected using the proposed approach even at very low concentrations against a sophisticated sample background (that is, the presence of various organic molecules, which are commonly present in 'natural' water). In turn, machine learning was used to evaluate the SERS spectra, making it possible to find MP particles that are indistinguishable in the complex spectra and thus determine the corresponding MPs in the 'real' water samples. We anticipate that such an approach will provide a universal method that will allow any user/operator to quickly and without additional knowledge determine the type and concentration of MPs.

Low-temperature Reactions and Interface Formation Between Ga and Electrode Materials Used in Microelectronic System

Yoonchul Sohn

Dept. of Welding & Joining Science Engineering/Chosun university, 309 Pilmoon-daero, Dong-gu, Gwangju 61452, Korea

Abstract:

Alloys based on gallium, such as eutectic Ga-In and Galinstan, have garnered significant attention due to their potential for deformability, miniaturization, low eutectic temperatures during manufacturing, and low toxicity. Leveraging their low melting point and capacity to form intermetallic compounds (IMCs) with diverse metals, gallium and gallium-based alloys have recently been explored as promising soldering materials in the realm of microelectronics. Despite their fundamental significance, in-depth investigations into the interactions between gallium (and its alloys) and foundational electrode metals have been notably scarce. This study delves into the detailed examination of interfacial reactions between gallium and base metals such as copper, nickel, palladium, gold, and copper/nickel/gold(palladium) multilayers.

Regarding reactions involving copper/nickel/gold(palladium) multilayers, it's observed that at lower reaction temperatures, the presence of gallium-rich IMCs, particularly Ga_xNi (x = 89 to 95 at%), on the Ga_7Ni_3 layer is distinctly confirmed. With increasing reaction temperature and duration, there is a gradual consumption of the nickel layer, leading to the formation of gallium-copper IMCs, specifically $CuGa_2$ and $\gamma3\text{-}Cu_9Ga_4$, beneath the Ga-Ni IMC layer. Concurrently, the gap between the Ga-Ni and Ga-Cu IMC layers widens, facilitating the infiltration of molten gallium. The rate of Ga_7Ni_3 growth exhibits a time exponent ranging approximately from 1.1 to 1.7. The activation energy for Ga_7Ni_3 growth is determined to be 61.5 kJ/mol. It is hypothesized that the growth of Ga_7Ni_3 is primarily steered by the diffusion of gallium atoms along grain boundaries, with the porous microstructure inherent in the Ga_7Ni_3 layer offering additional diffusion pathways.

Integrating Flexible Optical Waveguides into Soft Robotics: Advancing Multimodal Sensing for Enhanced Control and Operational Precision

Xiang Zhang*, Sunquan Yu, Wen Yao, Teng Yi, Yibing Liu, and Xiaoqian Chen

Defense Innovation Institute, Beijing, 100071, China

Abstract:
This research delves into innovating soft robotics by integrating flexible discrete optical waveguides with soft materials, aiming to transcend current limitations in sensor integration and real-time feedback. The focus is on enhancing the multimodal sensing capabilities—encompassing stretching, compression, and bending—of soft robotic arms through the novel application of soft materials coupled with discrete optical waveguide structures. This fusion is pivotal for advancing the precision control and robustness of soft robots in complex operations. Central to our investigation is the exploration of the mechanics-optics coupling mechanism inherent to these waveguide structures, alongside optimizing their design for superior sensory devices. We are pioneering algorithms for the succinct decoupling of color space from multimodal deformations, which is crucial for precise signal processing. Additionally, our work includes the advancement of manufacturing techniques and rigorous testing protocols for these optical devices. The potential applications of this research are vast, ranging from healthcare to rescue operations, where the enhanced operational performance and reliability of soft robotic systems could have transformative impacts. By melding materials science with robotics, this work not only pushes the boundaries of what's possible in soft robotics but also sets the stage for future innovations in intelligent systems designed for complex environmental interactions.

Characterizing Scaled Integrated Quantum Photonic Devices Based on Machine Learning Approaches

Teng Yi[a], Xiang Zhang[a], Wen Yao[a], Yibing Liu[a], and Xiaoqian Chen[b*]

[a]Defense Innovation Institute, Academy of Military Science, Beijing, 100071, China
[b]Academy of Military Science, Beijing, 100091, China

Abstract:
Programmable on-chip optical network plays a key role in the application of optical quantum information processing and optical neural network. It is the core device. With the increase of the scale of the optical network

on chip, it is difficult to calibrate the configurable elements on the network. On the one hand, there is a contradiction between a large number of configurable elements and a limited input-output interface; on the other hand, it leads to cross-talk among configurable elements, including the cross-talk of heat, light and other factors, which makes the behavior of the whole optical network difficult to model and test, and involves a large number of data fitting. Machine learning has unique advantages in dealing with complex models, especially with the increase of the number of components in the network. Many methods and tools of machine learning can play an important role in the calibration of this large-scale optical network. This work is mainly based on machine learning to provide accurate calibration of large-scale programmable photonic quantum chips, and even to build models to provide technical support for the development of integrated optical quantum chip technology.

Plasmonic Anisotropy of Ordered Subwavelength Metal Nanostructures Deposited on Corrugated Sapphire Templates

Ephraim Mathew[a*], Jacek Jenczyk[a], Szymon Murawka[a], Andriy Serebryannikov[a], Igor Iatsunskyi[a], Tomas Tamulevičius[c], Sigitas Tamulevičius[c], Patryk Florczak[a], Mikołaj Lewandowski[a], and Maciej Wiesner[b]

[a]*NanoBioMedicalCentre, Adam Mickiewicz University, Wszechnicy Piastowskiej 3, 61-614 Poznań, Poland*
[b]*Faculty of Physics, Adam Mickiewicz University, Uniwersytetu Poznańskiego 2, 61-614 Poznań, Poland*
[c]*Institute of Materials Science of Kaunas University of Technology, K. Baršausko St. 59, LT-51423, Kaunas, Lithuania*

Abstract:
Structural modulations in metal surface reorders the collective oscillation of surface charges, resulting in the excitation of different types of plasmon resonance modes, as in a roughened metal surface the EM near field is focused on its rough tips due to the localization of surface plasmon resonance in its sharp lateral cross-sections. Substrates decorated with metal nanoparticles of different size, shape and arrangements exhibit tuneable (LSPR)localized surface plasmon resonance modes[1] and are most commonly used in surface enhanced spectroscopies. Non-percolated metal films with semi-continuous networks exhibit unique plasmonic properties with enhanced scattering cross-section. Percolation theory and its recent experimental studies of optical, electrical and morphological properties provided evidence of both localized and de-localized plasmon modes coexisting in near-percolated metal films[2]. In this poster we discuss the plasmonic properties of non-percolated Au films deposited by electron beam evaporation in ultrahigh vacuum conditions onto corrugated transparent sapphire dielectric[3]. This causes the nucleation of Au clusters to self-assemble based on the template topography as ordered, anisotropic subwavelength metal arrays. Analysis revealed an unique property of the sample which transmits or scatters light based on the excitation polarization. The LSPR scattering further exhibited a dichroic property dependent on the excitation polarization. We studied the topographical and optical properties of these samples and specifically analyse its dependence on light attributes such as polarization and wavelength. These substrates with tuneable (LSPR) throughout the visible –NIR region are highly beneficial in various applications such as meta-surfaces, optical filters, SERS sensing and on-chip communications.

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Novel Synthetic Bio-architectures Configured with S-layer Technology

Breitwieser, A.*, Reuning, U., Darren, T.C., Zayni, S., Sleytr, U.B., and Ehmoser, E.

Institute of Synthetic Bioarchitectures, Department of BioNanoSciences, University of Natural Resources and Life Sciences, Vienna, Austria

Abstract:

Nanotechnology has revolutionized the field of biology, enabling advancements beyond traditional biological applications. In this study, we generated synthetic bio-architectures functionalized with S-layer protein coatings. S-layer proteins have the intrinsic property to recrystallize by self-assembly into a monomolecular network, allowing to coat almost all surfaces in a highly ordered and oriented manner. These assemblies provide a robust framework and could have a therapeutic function by combining S-layer assemblies with biomaterials like liposomes or emulsomes. Thus, we create a synergistic effect that further improves the stability and delivery of therapeutic agents as we can introduce specific binding epitopes to cellular receptors by genetic engineering. The so functionalized pathogen-like particles will compete with native pathogen binding to their specific receptors, preventing or lowering their cellular uptake or induce immune responses. As proof of principle, we constructed a fusion protein with the S-layer responsible for coating polystyrene particles and the RBM or RBD region of the SARSCoV-2 spike protein for specific receptor binding. The applicaKon potenKal of recrystallized S-layer fusion proteins on nanoparKcles mimicking the surface architecture of the virus was investigated by cell uptake studies. In such mimicking synthetic bio-architectures counteracting pathogen intrusion, such as viral entities, the S-layer technology offers an ideal molecular toolkit leading to applicaKons in materials science and nanomedicine.

Summarizing, this study demonstrates the potential of nanotechnology in advancing therapeutic applications beyond traditional biology. The stabilization of natural compounds using S-layer protein assemblies enabling the targeted delivery represents a significant step forward in the field of nanotechnology-based therapeutical approaches.

Boosting the Acetone Gas Sensing of WS$_2$–ZnO Nanosheets by Codecoration of Pt/Pd Nanoparticles

Jae-Hun Kim

Materials Science and Engineering, Inha University, Incheon 22212, Republic of Korea

Abstract:

WS$_2$-based gas sensors are used for detection of toxic gases at low temperatures due to their high surface area, weak interlayer van der Waals force, and high electrical conductivity. However, in their pristine form, they exhibit poor selectivity. Herein, to increase the selectivity of WS$_2$ sensors, ZnO shells (10-50) nm were fabricated on WS$_2$ nanosheets (NSs) using atomic layer deposition. The sensor with a ZnO shell thickness of 10 nm displayed an improved gas response under 4.2 V applied voltage in the self-heating condition. Next, Au, Pt, Pd, and Pt/Pd nanoparticles (NPs) were decorated on WS$_2$–ZnO (10 nm) NSs, and the Pt/Pd decorated WS$_2$–ZnO (10 nm) NSs exhibited the highest response of 13.77 to 10 ppm acetone under the fixed applied voltage of 4.2 V. The enhanced output was related to the catalytic nature of the Pt and Pd noble metals, formation of WS$_2$–ZnO heterojunctions, and Pt/ZnO and Pd–ZnO Schottky barriers. This study illustrates the promising role of bimetallic Pt/Pd decorations in enhancing the performance of resistive gas sensor.

Adaptation of the Electronic Properties of Bi$_2$O$_2$Se Through Surface Modification and Magnetic Doping

José Mejía-López[a]*, I. M. Arias-Camacho[b], and A. M. León[c]

[a]Pontificia Universidad Católica de Chile, Santiago, Chile

bFaculty of Physics, University of Warsaw, PL-02093 Warsaw, Poland
cFaculty of Physics, University of Warsaw, PL-02093 Warsaw, Poland

Abstract:

Current research is primarily focused on finding a two-dimensional material with properties suitable for usage in spintronics and optoelectronics, such as a tolerable bandgap, robust in plane carrier mobility, and good environmental stability. If magnetism is also present, its utility is greatly extended. Bi2O2Se, a non-van der Waals system with a recently discovered monolayer, is one of the intriguing materials that possess these properties. This study investigates the structure and electrical properties of several monolayers that can be generated experimentally using a theoretical framework. It has been discovered that these monolayers are extremely sensitive to the introduction of "extra" electrons, changing their electrical properties from semiconductor to conductor Furthermore, we look into how the characteristics of each analyzed monolayer alter when the system is doped with magnetic atoms. As a result, doping introduces low-dispersion bands created by d orbitals of impurities, which can hybridize with the oxygen and bismuth atoms in the monolayer. This significantly alters the material's electronic characteristics, resulting in variations in the valence of specific Bi atoms, which can cause symmetry breaking in the perpendicular plane. Depending on the metal doping, such processes provide either metallic or semiconducting properties.

Superheating Nature of REBCO Nanofilms and their Applications in the Growth of REBCO Superconductors

Xin Yao

School of Physics and Astronomy, Shanghai Jiao Tong University, Shanghai, 200240, China

Abstract:

Recently, we reported a superheating phenomenon of REBCO (RE= Y, Sm, Nd) nanofilms, e.g. the complete decomposition of a c-oriented YBCO film occurs at a temperature of 50 K higher than its peritectic temperature (T_p). The origins and influential factors of superheating property were investigated, involving film orientation, substrate material, buffered structure, chemical processing condition and phase diagram nature. On the other hand, making full use of their highly thermal-stable properties, we employed REBCO nanofilms as superior seed materials to induce the growth of high-performance REBCO crystals in a variety of aspects, which are unsuccessful by the prior art seeding techniques.

Plasmon-produced Solvated Electrons: A New Approach with Utilization of Hybrid Structures

V. Shilenko[a]*, E. Miliutina[a,b], A. Zabelina[a], V. Burtsev[a], V. Svorcik[a], and O. Lyutakov[a]

aDepartment of Solid State Engineering, University of Chemistry and Technology, 16628 Prague, Czech Republic
bMaterials Centre, Faculty of Science, J. E. Purkyně University, 400 96 Ústí nad Labem, Czech Republic

Abstract:

Solvated electrons are free electrons that are in solution and stabilized by interaction with solvent molecules. One of their interesting properties is the ability to chemically activate molecules that are difficult to activate by alternative chemical approaches, which is useful in organic chemistry, photochemistry, and electrochemistry. The goal of this work is to produce and use hydrated electrons in an efficient way with the utilization of middle-energy photon illumination and plasmon-active nanostructures coated with low-yield work materials. The photon energy can be efficiently converted into hot electrons excited by the plasmons. These electrons are then injected into the low work function material (scandium oxide). Depending on the residual energy, the electrons can either "wait" for the second photon and be injected into surrounding electrolyte through a two-photon process, or they can be injected directly into the electrolyte under a single photon process. Several methods, including Kelvin probe, electronic paramagnetic spectroscopy, and fiber-based optical spectroscopy, were used to establish the

generation of solvated electrons. Then, the obtained materials were subsequently used for the nitrogen reduction reaction in photoelectrochemical and photoelectrochemical modes. As a result, the excellent efficiency of the nitrogen-to-ammonia conversion was demonstrated.

High-fluence Nitrogen Ion Implantation into Titanium and its Effects on Surface Saturation

Vojtěch Smola[a]*, Petr Vlčák[a], Josef Šepitka[b], and Zdeněk Weiss[c]

[a]Department of Physics, Faculty of Mechanical Engineering, CTU, Prague, Czech Republic
[b]Department of Mechanics, Biomechanics and Mechatronics, Faculty of Mechanical Engineering, CTU, Prague, Czech Republic
[c]Institute of Physics, Czech Academy of Sciences, Prague, Czech Republic

Abstract:
High fluence nitrogen ion implantation into commercially pure titanium grade 2 was investigated. Nitrogen ions were implanted with fluences ranging from $1 \cdot 10^{17}$ to $27 \cdot 10^{17}$ cm^{-2} using an accelerating voltage of 90 kV. Here we present the influence of high nitrogen fluence on the structural changes of the nitride surface layer and the impact of nitrogen saturation on the surface properties. Several analytical techniques were used to assess the implanted surfaces, including atomic force microscopy for characterizing the surface morphology and roughness, glow discharge optical emission spectroscopy for analyzing nitrogen depth distribution, and nanoindentation for measuring nanomechanical properties. Our findings demonstrate that surface saturation with nitrogen was achieved in the examined interval of applied fluences. Blisters, craters, and cracks, typical signs of oversaturation, were observed. Oversaturation resulted in a reduction in surface hardness compared to titanium implanted with lower fluences.

A Novel N-doped Porous Carbon/g-C$_3$N$_4$ Composite for Enhanced Photocatalytic Reduction of CO$_2$

Roopesh Mekkat*, Edith Mawunya Kutorglo, Milena Setka, and Miroslav Šoóš

University of Chemistry and Technology, Department of Chemical Engineering, Technická 3, Prague 160 00, Czech Republic

Abstract:
Solar light-driven CO$_2$ conversion into hydrocarbon fuels is regarded as one of the most crucial inventions for reducing CO$_2$ abundance in the atmosphere and fulfilling energy needs. Graphitic carbon nitride (g-C$_3$N$_4$) has garnered considerable attention and emerges as a promising candidate for photocatalytic CO$_2$ reduction, owing to its visible light absorption, metal-free and environmentally benign nature. However, its ability to effectively achieve this is currently hindered by several factors such as relatively low surface area, fast electron hole recombination rate and poor CO$_2$ adsorption capacity, which constrain its practical applicability.

In this work, a novel photocatalyst was synthesized by incorporating a suitable amount of Zeolitic Imidazolate Framework (ZIF-8) derived N-doped porous carbon into g-C$_3$N$_4$ without affecting its light absorption capacity. The as-prepared samples were characterized by X-ray diffraction (XRD), transmission electron microscopy (TEM), Fourier transform infrared spectroscopy (FT-IR), X-ray photoelectron spectroscopy (XPS), UV–Vis diffuse reflectance absorption spectra (UV-DRS) and photoluminescence spectroscopy (PL).

Compared to g-C$_3$N$_4$, the optimized photocatalyst showed improved surface area, 3.5 times enhancement in CO$_2$ adsorption, reduced optical bandgap and a superior activity on photocatalytic reduction of CO$_2$ with CH$_4$-production rate of 70.87 µmol h^{-1} g^{-1} and C$_2$H$_6$-production rate of 35.31 µmol h^{-1} g^{-1}. The enhanced activity of the composites is attributed to the synergistic effect of the N-doped carbon and g-C$_3$N$_4$. This approach offers a promising strategy for future development of C$_3$N$_4$-based catalysts for efficient solar to fuel conversion.

Regrowth-free InGaN/GaN Super Lattice Capped GaN CMOS and Ring Oscillator with InGaN Back Barrier

Mahalaxmi*, and D. Saha

Indian Institute of Technology Bombay, Department of Electrical Engineering, Mumbai, Maharashtra, 400076, India

Abstract:

The exceptional properties of Gallium nitride (GaN) and its alloys (AlxGa1−xN), showcase their considerable potential as semiconductor materials for advanced high-power and high-frequency device applications. The presence of a two-dimensional electron gas (2DEG) at the heterointerface of AlGaN/GaN devices commonly manifests an "ON" state behavior. But, in power electronics, it is essential to employ devices that are normally in an "OFF" state, which guarantees safety and simplifies the design of the gate driver circuitry. To reduce the circuit complexity, monolithic integration of gate driver circuitry and power transistor on the same chip is essential. A CMOS-like technology is significant in improving the efficiency of GaN-based Integrated Circuits. Difficulties in achieving monolithic integration of high-performance enhancement mode GaN n-channel transistor and early developmental stage of enhancement mode GaN p-channel transistor are the roadblocks for achieving GaN CMOS technology. In this work, we present a regrowth-free GaN-based CMOS and Ring Oscillator with p-doped InGaN/GaN superlattice (SL) pairs as capping layers on AlGaN barrier layer, and an InGaN as back barrier layer. The frequency of operation of the inverter can be improved by reducing the gate length of the transistor which leads to short channel effects (SCEs). The purpose of InGaN back barrier is to reduce the short channel effects and reduces the leakage current. The frequency of oscillation increased from 0.44 GHz, 1.1 GHz, and 18 GHz to 1.35 GHz, 3.31 GHz, and 26 GHz respectively for 1 μm, 500 nm, and 200 nm gate lengths of transistors with InGaN back barrier.

Efficient Microfluidic-based Synthesis of Polymer Brushes

Markéta Vrabcová[a,b*], Monika Spasovová[a,b], Volkan Cirik[a,b], Judita Anthi[a], Alina Pilipenco[a,b], Milan Houska[a], Hana Vaisocherová-Lísalová[a], and N. Scott Lynn Jr.[a]

[a]FZU – Institute of Physics of the Czech Academy of Sciences, Na Slovance 2, Prague, 182 00, Czechia
[b]Institute of Physics, Faculty of Mathematics and Physics, Charles University, Ke Karlovu 5, Prague, 121 16, Czechia

Abstract:

Polymer brushes (PBs), ultrathin coatings formed by polymer chains tethered to a surface, offer tunable chemical and physical properties tailored through the selection of appropriate monomers. Zwitterionic PBs have shown great potential in biosensing applications, especially when used as antifouling surfaces that resist non-specific biomolecule adsorption. However, traditional methods of PB synthesis like surface-initiated atom transfer radical polymerization (SI-ATRP) are consuming large volumes of polymerization solution relative to the surface area treated. Recent advancements have focused on optimizing these methods, including the use of microfluidics, which allows for efficient PB synthesis and precise spatial and temporal control of low volumes per sample.

In this study, we present a novel microfluidic-based approach to SI-ATRP that significantly reduces the required volume of polymerization solution while maintaining the high quality of the PB coatings. This method also facilitates the synthesis of more complex PB architectures, such as block copolymers, with controlled surface properties. We synthesized various PBs – poly(carboxybetaine methacrylamide) (pCBMAA) and poly(hydroxypropyl methacrylamide) (pHPMAA), a random copolymer p(CBMAA 20%-HPMAA 80%), and linear di-block copolymers p(CBMAA-HPMAA) and p(HPMAA-CBMAA) – using both standard Schlenk line reactors and innovative microfluidic stack reactors. The properties and bioanalytical performance of these PBs were evaluated using advanced surface-sensitive techniques such as spectroscopic ellipsometry, infrared reflection-absorption spectroscopy, surface plasmon resonance, and contact angle measurements. Our results demonstrate that the microfluidic approach not only reduces the consumption of chemicals but also enhances the versatility and

scalability of PB-coated surfaces, making it a promising tool for the large-scale production of high-performance biosensing platforms.

Peptide/Graphene Nanocomposites: An *in Silico* Investigation

Elena Markopoulou[a]*, Gregory Savvakis[b], and Anastassia N. Rissanou[c]

[a]*Department of Materials Science and Engineering, University of Crete, GR-71409, Heraklion, Crete, Greece*
[b]*Physics Department, University of Ioannina, GR-45110 Ioannina Greece*
[c]*Theoretical & Physical Chemistry Institute, National Hellenic Research Foundation, 48 Vassileos Constantinou Avenue, 11635 Athens, Greece*

Abstract:
In the current work, the self-assembly of dipeptides on a graphene layer, in aqueous solution, is investigated, through all-atom Molecular Dynamics simulations [1]. The effect of graphene surface on the self-assembly propensity of dipeptides, as well as on the formed structures, as they have been observed in the corresponding bulk systems (i.e., dipeptides solutions in water) [2], is examined. Two graphene materials have been used, pristine graphene and graphene oxide (GO) with two different dipeptides, diphenylalanine (FF) and Cyclo-diphenylalanine (Cyclo-FF) at room temperature. Atomistic details about the conformational preferences, the orientation of dipeptides with respect to the surface and the hydrogen bond network are investigated. Length and time scales of the formed structures are quantified providing important insight into the adsorption mechanism of dipeptides onto the graphene surface. A hierarchical formation of dipeptide structures is observed involving two sequential processes: a stabilized interfacial layer of dipeptides onto the graphene surface, followed by the development of a structure of self-aggregated dipeptides on top of this layer. Strong $\pi - \pi^*$ interactions between the dipeptides and the graphene lead to a parallel to the graphene layer orientation of the phenyl rings, especially in the case of pristine graphene. Reduction in the number of hydrogen bonds between dipeptides is observed because of the graphene layer, since it disturbs their self-assembly propensity. The differences between pristine graphene and GO nanostructures with both FF and Cyclo-FF are highlighted.

Factor Analysis of ssNMR Spectroscopy Data of Alginate-pectin Based Systems Crosslinked by Ca^{2+} vs. Zn^{2+} vs. Cu^{2+}

Martina Urbanova[a]*, Miroslava Pavelkova[b], Katerina Kubova[b], and Jiri Brus[a]

[a]*Department of Structure analysis, Institute of Macromolecular Chemistry, Czech Academy of Sciences, Czech Republic*
[b]*Department of Pharmaceutical Technology, Faculty of Pharmacy, Masaryk University Brno, Czech Republic*

Abstract:
The most commonly used polyuronates are alginate and pectin. Their flexibility, biodegradability, biocompatibility and non-toxic nature make cross-linked alginates or pectin invaluable in creating innovative solutions for diverse industrial challenges. The gelation mechanisms of alginate and pectin, known as egg-box model, were believed to be basically the same. However, studies have found that the formation and the structure of egg-box dimmers between alginate and pectin were different. Therefore, this study was proposed to summarize the structural factors that can influence the gelation of alginate and pectin. As an experimental tool to provide a detailed insight into the molecular structure, distribution of cross-linking ions and interactions of individual components, we used a Solid-State nuclear magnetic resonance (ss-NMR) spectroscopy techniques. Factor analysis (FA) was then applied to enhance the information content of the spectroscopic data obtained. Specifically, we focused on finding the key structural motifs that preferentially occur in the cross-linked polysaccharide matrix.

Architecture of Multicomponent Polycrystalline Materials at Atomic Resolution

Jiri Brus[a*], Martina Urbanova[a], and Jiri Czernek[a]

[a]Department of Structure Analysis, Institute of Macromolecular Chemistry, Czech Academy of Sciences, Czech Republic

Abstract:
A growing number of currently discovered drugs may never reach their true potential. This is due to unfavorable physicochemical properties. Recent efforts to optimize their therapeutic efficacy have led to the development of multi-component drug delivery solids that perform multiple functions. However, the development of these materials is dependent on precise structural analysis at the level of atomic resolution. This contribution addresses our attempt to formulate an efficient strategy for obtaining deep insight into the structure of polycrystalline pharmaceutically active materials with micro- and nanodomain architecture. This strategy is demonstrated on representative systems including injectable polyanhydride microbead formulations of decitabine, *liquisolid* mesoporous-silica-based drug-delivery systems loaded by tapentadol and double-crosslinked hybrid alginate/pectin microparticles encapsulating self-emulsifying systems (SES) for the delivery of lipophilic phytotherapeutics.

Self-assembled Capsid: Synthesis and Characterization

Anca Aldea[a,b*], Ana-Maria Ignat[c], Monica Enculescu[a,b], and Victor Diculescu[a,b]

[a]CIFRA- Centre International de Formation et de Recherche Avancées en Physique, Măgurele, Romania
[b]National Institute of Materials Physics, Măgurele, Romania
[c]Department of Electricity, Solid Physics and Biophysics, Faculty of Physics, University of Bucharest, Măgurele, Romania

Abstract:
The aim of this study is to investigate the synthesis conditions on the size distribution of gold nanoparticles and to correlate their size with their functionalization with different ligands, playing an essential role for the development of virus-like particles. Gold nanoparticles were synthesized using gold chloride trihydrate (which, upon reduction of gold ions forms the core of the nanoparticle) and trisodium citrate dihydrate (which provides the citrate groups that form stabilizing coat for the individual nanoparticles). Addition of tannic acid, which serves as a reductant for gold ions, was shown to play an important role in determining the size of gold nanoparticles. In order to obtain different sizes of synthesized gold nanoparticles three different volumes of tannic acid were added: 47, 50 and 52 μL. It is important to study whether nanoparticle size can be influenced by other parameters such as concentration and number of washes. Thus, the obtained gold nanoparticle solutions were diluted 4 and 8 times and washed 3 times before characterization.
UV-Vis absorption spectra of gold nanoparticle solutions (concentrated, diluted and washed) were analyzed. Scanning electron microscopy (SEM) technique was used to characterize the morphology of gold nanoparticles. The size of the gold nanoparticles was obtained analyzing the images with the ImageJ software. Nanoparticles with sizes between to 11-13 nm were selected for functionalization with PEG as a ligand. The nanoparticles-ligand assemblies were characterized by UV-Vis spectrophotometry, scanning and transmission electron microscopy and used in assemblies with capsid proteins to mimic the virus shell.

Optical and Morphological Characterization of Gold Nanoparticles Synthesized Using Tannic Acid

Maria-Lorena Jinga[a,b,c]*, Anca Aldea[b] Monica Enculescu[b], and Victor Diculescu[b]

[a]International Center for Advanced Training and Research in Physics (CIFRA), Magurele, Romania
[b]National Institute of Materials Physics (NIMP), Magurele, 077125, Romania
[c]University of Bucharest, Doctoral School of Physics, Magurele, Romania

Abstract:
Nanoparticles have opened new frontiers in various scientific fields due to their extremely small size and unique physicochemical properties. These particles exhibit different characteristics compared to bulk materials, such as quantum effects, large specific surface area and enhanced optical, magnetic and mechanical behavior. In this paper, we will analyse the latest advancements in the synthesis, characterization and application of nanoparticles in obtaining viromimetic particles. These biomimetic particles are engineered to mimic the structural and functional properties of viruses but are they are used in therapeutic applications like gene therapy or targeted drug delivery. We also explore the design and synthesis of these particles, highlighting their potential to enhance the precision and efficiency of treatments.

We report results of the studies regarding the influence of fabrication parameters on the optical and morphological properties of the size and shape of the gold nanoparticles. The particles were synthesized using different concentrations of tannic acid leading to a shift in the nanoparticles' sizes. Thus, stable gold nanoparticles (Au NPs) obtained by this method are found to have average sizes between 8 and 20 nm, depending on the reducing agent's concentration. The optical properties were evaluated using UV-Vis absorption spectra of gold nanoparticle solutions and the morphological evaluation was made by using scanning electron microscopy (SEM) technique. The Au NP were functionalized in order to be further used for proteins' assembling.

A Small-diameter Vascular Graft Promotes Rapid and Benign Remodeling of the Neointima Through Dual Release of Nitric Oxide and Hydrogen Sulfide

Fubang Liang[a]*, Dawei Jin[b], Lijuan Wang[c], Jingyi Zhang[a], Pengfei Li[c], Jiang Yuan[c], Yanjun Pan[a], and Meng Yin[a]

[a]Department of Cardiothoracic Surgery, Shanghai Children's Medical Center, School of Medicine, Shanghai Jiao Tong University, 1678 Dong Fang Road, Shanghai, 200127, PR China
[b]Department of Cardiac Surgery, Zhongshan Hospital, Fudan University, Shanghai, 200032, PR China
[c]Jiangsu Collaborative Innovation Center of Biomedical Functional Materials, Jiangsu Key Laboratory of Bio-functional Materials, Department of Materials Science and Engineering, School of Chemistry and Materials Science, Nanjing Normal University, Nanjing, 210023, PR China

Abstract:
Coronary artery bypass grafting often requires autologous veins as alternatives. The limited source and problem of over-expansion are major obstacles for vein grafts, which could be solved by small-diameter artificial vascular graft. However, their clinical application is limited by thrombosis and restenosis caused by incomplete endothelialization and abnormal smooth muscle cells (SMCs) proliferation. Nitric oxide (NO) and hydrogen sulfide (H_2S) are crucial signaling molecules in the cardiovascular system, known to regulate endothelial cells (ECs) and SMCs proliferation, migration, reduce oxidative stress, and inhibit inflammation to prevent intimal hyperplasia. In this study, we developed a new method to prepare a keratin based H_2S donor (KAT) complexed with copper ions and electrospun it with PCL to prepare PCL/KAT-Cu small-diameter tissue-engineered vascular graft, which is capable of dual release of NO and H_2S. We investigated the effects of NO and H_2S release on human umbilical vein endothelial cells (HUVECs) and human umbilical arterial smooth muscle cells (HUASMCs) proliferation and migration, evaluated the graft's selectivity for HUVECs, and assessed its effects on macrophage phenotypic transitions and its protective effect on HUVECs under reactive oxygen species (ROS) conditions. Additionally, we tested the graft's ability to rapidly endothelialize under shear force using an *in vitro* 3D-perfusion

system. After one month of *in situ* transplantation in rat abdominal aorta, the PCL/KAT-Cu small-diameter tissue-engineered vascular grafts demonstrated satisfactory intimal remodeling, comparable to natural blood vessels. In conclusion, our study presents a promising new strategy for remodeling small-diameter vascular grafts.

High Temperature Superconductivity - Exciton Mechanism

Junhui Cao*, and Alexey Kavokin

Westlake University, Hangzhou, Zhejiang Province, China

Abstract:
Starting from the exciton-induced superconductivity, here we showed theoretically that the interplay between exciton- and phonon-induced superconductivity may lead to a higher critical temperature Tc for the superconducting state, while the conventional BCS or Brinkman-Rice-Bardeen-Cooper-Schriefer (BR-BCS) mechanisms would result in a much higher critical magnetic field for the same Tc. Such phenomenon might be experimentally observed in the superconducting quantum well, where the stable electronic Cooper pairs can be created by the scattering between free electrons and excitons.

Enhancing Emission of Perovskite Films Using Soft Lithography

Mathias Bizimana[a]*, Arynn O.Gallegos[b], Qi Zhou[b], and Daniel N. Congreve[b]

[a]*African Leadership College, Pamplemousses, Mauritius*
[b]*Stanford University, Stanford, CA, USA*

Abstract:
This research investigates the enhancement of optoelectronic properties in metal-halide perovskite thin films via nanopatterning with soft lithography. The study focuses on the impact of nanopatterning on emission wavelength and photoluminescence quantum yield (PLQY). The experimental procedures included the preparation of polydimethylsiloxane (PDMS) stamps and perovskite precursor solutions, followed by the patterned film-making process. Results reveal that stamping with weights of 500 g and 1000 g significantly improves the uniformity and emission efficiency of perovskite films compared to unstamped control films. Stamping with 500 g achieves high pattern transfer efficiency, while a 1000 g stamping weight yields the highest PLQY and sharpest emission peaks. These findings highlight the critical role of precise patterning in optimizing perovskite-based optoelectronic devices. However, the study notes a tradeoff between pattern transfer efficiency and PLQY between films stamped with 500 g and 1000 g. Given this tradeoff and the limited number of experiments conducted, further research is recommended to identify the optimal stamping weight. Future studies should also focus on the scalability, stability, and integration of nanopatterned films in practical applications, such as perovskite LEDs and lasers. By addressing these aspects, the development of high-efficiency, stable optoelectronic devices using nanopatterned perovskite films can be realized, advancing the field of optoelectronics and broadening the scope of their application.

High-order Harmonic Generation in the Giant Fullerene Molecules

A. G. Ghazaryan*, Kh. A. Manukian, H. H. Mikayelyan, and Kh. V. Sedrakian

Centre of Strong Fields Physics at Research Institute of Physics at Yerevan State University, Yerevan, Armenia

Abstract:
Among nanostructured materials with potential for nonlinear extreme optical applications, carbon allotropes, such as fullerenes, are of particular interest for the investigation of the one of the basic processes in intense laser-matter interaction such as high-order harmonic generation (HHG). HHG phenomenon involves highly

multiphoton processes[1], offering access to extreme time resolution and enabling attosecond physics. Fullerenes being large molecules formed by closing a graphite sheet, and their stable closed topological structure makes them intriguing objects for matter-light coherent interaction with large groups of symmetry. Large fullerenes have since been the subject of active investigation. In the present work the investigation of HHG in the large fullerene molecules under intense laser field has been presented. To model of the large fullerene molecule and its interaction with the laser field, we employ the tight-binding mean-field approach. Our detailed analysis of the HHG power spectrum reveals the multiphoton resonant nature of harmonic generation, shedding light on the underlying quantum processes involved. We demonstrate that the large fullerenes exhibit a significantly stronger high harmonic intensity compared to the more widely studied C_{60}.

References: [1] H. K. Avetissian, Relativistic Nonlinear Electrodynamics: The QED Vacuum and Matter in Super-Strong Radiation Fields (Springer, New York, 2015).

Rheological Behavior of Polymer Materials Filled by Microwave-modified Bentonite

Zuzana Mičicová*, Slavomíra Božeková, Petra Skalková, Ivan Labaj, and Mariana Pajtášová

TnUAD of Trenčín, Faculty of Industrial Technologies, I. Krasku 491/30, 020 01 Púchov, Slovakia

Abstract:
Bentonite finds widespread application across various industrial sectors due to its physicochemical properties, including a specific surface area, high chemical and mechanical stability, as well as a variety of surface and structural properties. However, to further enhance its properties, natural bentonite requires pre-treatment. The microwave method has recently been employed for clay activation and the synthesis of nanomaterials. Microwave heating ensures uniform and thorough moisture removal from clay materials even at lower temperatures, thereby minimizing both time and energy required for the process. The paper was focused on the investigation of microwave-modified bentonite effect on rheological behavior of polymer materials. Bentonite was subjected to microwave processing at different time intervals to achieve optimum processing. Subsequently, the modified bentonite samples were characterized by FTIR and thermal analysis to assess the changes in structure and thermal properties. After incorporating our prepared microwave-modified bentonites into polymer blends, which partially replaced the commonly used filler, carbon black. The rheological behavior of the resulting polymer materials was evaluated using a rubber process analyzer.

Modified Wood Flour and its Effect in Polymer Matrix

Slavomíra Božeková*, Zuzana Mičicová, Ivan Labaj, Petra Skalková, and Darina Ondrušová[a]

TnUAD of Trenčín, Faculty of Industrial Technologies, I. Krasku 491/30, 020 01 Púchov, Slovakia

Abstract:
Preliminary experiments have shown the excellent mixing ability of wood flour with all widely used rubbers: natural rubber, isoprene rubber, styrene rubber, butadiene rubber, acrylonitrile-butadiene rubber, etc. For the reinforcement of rubber, a high degree of filler dispersion is crucial. In this paper, wood flour derived from the production of wood pellets was used as filler. In addition, the interaction between the filler and the rubber contributes significantly to the desired reinforcement induced by chemical or physical mechanisms. Therefore, modification of the wood flour is necessary. This paper deals with the incorporation of modified wood flour with

different fractions into a polymer matrix and then it's the effect on selected rheological behavior and mechanical parameters of polymer blends and vulcanizates compared to polymer blends filled with unmodified wood flour was studied. The measured results suggest that proper selection of the fraction of modified wood flour can lead to an improvement in the resulting properties of polymer blends.

The Effect of Temperature on the Parameters of the Mixing Process in the Preparation of Elastomeric Composites

Ivan Labaj*, Petra Skalková, Zuzana Mičicová, Slavomíra Božeková

Alexander Dubček University of Trenčín, Faculty of Industrial Technologies, I. Krasku 491/30, 020 01 Púchov, Slovakia

Abstract:
Elastomeric composites are among the key engineering materials that find wide application in industrial and domestic applications. The work deals with the preparation of elastomeric composites based on natural rubber (NR) filled with 20 phr cellulose (CEL). The reason for preparing a composite filled with biopolymer is the environmental point of view, to replace synthetic polymers at least partially with natural materials. When using cellulose in an elastomeric matrix, high processing temperature can cause problems, leading to degradation of the cellulose. The solution could be the preparation of polymer composites at lower temperatures. The influence of processing temperature (50-90 °C), torque during the preparation of elastomeric composites filled with cellulose was investigated. Rheological tests made it possible to determine the optimal processing parameters and properties of elastomeric composites filled with cellulose. Hardness, mechanical properties, particle size of cellulose fibres and phase morphology were also studied on the prepared NR/CEL composites.

Design of a Sustainable System Based on Paper-Cyclodextrin Nanosponges-Copper Nanoparticles for the Remediation and Detection of Organic Pollutants

Sebastián Salazar Sandoval*, and Nataly Silva

Facultad de Diseño, Universidad del Desarrollo. Av. Plaza 680, Las Condes, Santiago, Chile

Abstract:
Pesticides, while effective in controlling pests, pose significant environmental and health risks through water contamination, leading to acute and chronic poisoning, and carcinogenic effects. Consequently, there is an urgent need for innovative approaches to mitigate these risks. This study proposes a ternary system comprising paper, cyclodextrin nanosponges (NSs), and copper nanoparticles (CuNPs) for efficient pesticide removal from water sources. Paper was chosen as a substrate for its high porosity and surface area. NSs offered multiple interstitial sites for enhanced pollutant adsorption via molecular recognition, while CuNPs contributed to increased remediation capacity due to their larger surface area. The synthesis of the ternary system adopted a green and sustainable approach, employing mechanical milling for the fabrication of both NSs and CuNPs. Two synthetic routes were explored: simultaneous synthesis of a NSs-CuNPs binary system and subsequent immobilization on the paper substrate, or separate fabrication of each component followed by their deposition on the paper.

Characterization techniques including field emission scanning electron microscopy (FE-SEM), energy dispersive spectroscopy (EDS), X-ray powder diffraction (XRD), ultra-violet visible spectroscopy, X-ray fluorescence (XRF), Brunauer-Emmer-Teller (BET) surface area, Raman, and Fourier-transform infrared spectroscopy (FT-IR) were performed to analyze and confirm the formation of a paper-NSs-CuNPs system. Results indicate that the ternary system exhibits superior adsorption capacity towards the pesticide thiram (THR) compared to the individual components. These findings underscore the efficiency and viability of the fabricated ternary system for pesticide removal from aqueous matrices.

Potential Occupational Exposures to Nanoparticles by Aircraft Mechanics at A Flight Training Facility

Cynthia T. Pugh

Embry-Riddle Aeronautical University: School of Graduate Studies, Daytona Beach, FL, USA

Abstract:
Occupational exposures by aircraft mechanics and ground personnel primarily focus on heat, ergonomics, or noise since most of these workers are exposed to the outdoor environment as a function of their occupation. Nevertheless, the potential for occupational exposures to particulate air emissions and metals exists given the associated job tasks mechanics are required to perform on engine repair and the proximity to aircraft emissions mechanics and ground personnel. Piston-engine airplanes primarily use aviation gas (avgas) with a designated rating of 100 octane AVGAS 100, or low lead (AVGAS100LL) or, in some cases, 100 octane very low lead (AVGAS100VLL). To decrease lead air pollution and minimize lead poisoning, tetraethyl lead was eliminated from all types of gasoline except avgas. Avgas contains tetraethyl lead, and additional chemical components include benzene, toluene, ethylbenzene, and xylenes (BTEX), known and probable carcinogens. Common routes of occupational exposure to particulate air emissions and metals include the skin, eyes, nose, and lungs. Bulk wipe samples are used to identify potential cross and take-home contamination of metals. Particulate analyses are conducted using area air monitoring equipment to determine a difference in the background concentration of particulates from air monitoring equipment and the concentration post a specific task. Analytical results from the area air sampling and bulk wipe data provide baseline data of potential occupational exposures, which may be measured against known exposure limit standards. Similarly, particulate air emissions are measured at the size range and concentration to develop a baseline exposure assessment.