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Keynote Session

Strategies for Regeneration of Hard Tissues

Jonathan Knowles

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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]

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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.

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

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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.

Reference: [1] N. Komatsu Acc. Chem. Res., 2023, 56, 106.
[2] Y. Wang, G. Reina, H. G. Kang, X. Chen, Y. Zou, Y. Ishikawa, M. Suzuki, N. Komatsu* Small, 2022, 18, 2204044.
[3] Y. Zhang, H. G. Kang, H. Xu, H. Luo, M. Suzuki, Q. Lan,* X. Chen,* N. Komatsu,* L. Zhao* Adv. Mater., 2023, 35, 2301479.

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]*

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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]*

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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]

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[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*

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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

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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

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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

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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 CaCO3 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 CaCO3. These advancements have enhanced our comprehension of CaCO3 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 Gd3+ 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

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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

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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.

Session 3: NanoSafety

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

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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

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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]

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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

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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.

Session 4: Innovations in Sensing and Recognition

Towards Discovering Aggregation Inhibitors Against Light Chain Amyloidosis

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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]

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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

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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

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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.

References: 1) P. Kishore Prasad, N. Eizenshtadt, I. Goliand, L. Fellus-Alyagor, R. Oren, L. Motiei*, D. Margulies* *Mater. Today Bio*. **2023**, 20 ,100669. 2) N. Lahav-Mankovski, P. Kishore Prasad, N. Oppenheimer-Low, G. Raviv, T. Dadosh, T. Unger, T. Meir Salame, L. Motiei*, D. Margulies* *Nat. Commun.* **2020**, 11, 1299. 3) J. Hatai, P. Kishore Prasad, N. Lahav-Mankovski, N. Oppenheimer-Low, T. Unger, Y. Fridmann Sirkis, T. Dadosh, L. Motiei*, D. Margulies* Chem. Commun. **2021**, 57, 1875.

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

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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

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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.

Young Researchers Presentations

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

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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

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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

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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

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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

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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

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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.

Symposium II: Materials for Electronics, Optics and Photonics

Session 1: Advances in Optoelectronics

Perovskite Photodetectors

Liang Li

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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

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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

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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 (≈ 2 and ≈ 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 responsivities 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

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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.

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Session 2: Detection Frontiers

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

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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

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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

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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

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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

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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.

Session 3: Heterostructures in Electronics

Switching of Perpendicular Magnetization by Magnon Torque in All Oxide Heterostructures

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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

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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.

Symposium III: Future Materials for Energy, Environment and Sustainability

Session 1: Materials for Environmental Sustainability

Nanoplastics Retention and Transport in Filtration Systems

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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

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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

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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

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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.

Session 2: Energy Production

Selective Absorber Coatings for Solar-thermal Energy Conversion

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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

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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 x 10-6 - 1x10-3 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

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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

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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

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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.

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

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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.

Session 3: Energy Harvesting

Advanced Materials for Near Ambient Temperature Energy Harvesting

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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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CO2 Capture for Energy Harvesting: Atomistic Modelling of the Working Mechanism

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Abstract:
It is well known that industrial process by-products pose a great threat for the environment. Among them, CO2 is considered one of the most harmful. CO2 release in the atmosphere can be avoided by exploiting carbon capture, the process of sequestration of CO2 thanks to a chemical reaction with a more stable compound. The technologies so far employed for capturing CO2 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 CO2, exploiting a supercapacitor setup in which an ionic liquid (IL) is both the electrolyte and the capturing agent. CO2 gas is fluxed through one of the two electrodes. The portion of the IL in proximity of the electrode captures the CO2 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 CO2 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 CO2 and to the difference in chemical potential between the two ends of the device.

Electrocatalytic Nitrate to Ammonia

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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.

Coarse-grained Ferritic Fe-10Al-4Cr-4Y2 O3 Nanocomposite as a Top Material for the Green Energetics

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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_2O_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_2O_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

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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 legislation3 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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(3) Regulation (EU) 2023/1542 of the European Parliament and of the Council of 12 July 2023 concerning batteries and waste batteries, amending Directive 2008/98/EC and Regulation (EU) 2019/1020 and repealing Directive 2006/66/EC

Composite Organic Ionic Plastic Crystal Membranes: The Effect of Etherfunctionalized Cations on Light-gas Separation Performance

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Abstract:
In light of increasing concerns about climate change, there is a growing need for innovative solutions to address CO2 emissions. Addressing this urgency, this work presents a unique approach to CO2 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 CO2 and an overall selectivity (CO2/N2) 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 CO2 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

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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.

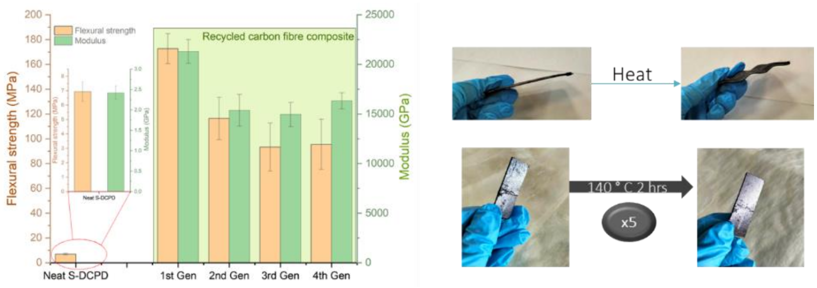

Figure 1. Flexural strength and modulus evolution of reclaimed carbon fiber composites that are tested to failure, repaired and retested over 5 cycles.