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Meeting Abstracts

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Keynote Presentations

Indium Tin Oxide Thin Films as Protective Coatings for Space Applications

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Abstract

Thin conducting films (TCFs) are of considerable interest for commercial and space applications, particularly in solar cells, flat panel displays, and electrochromic windows. Recently, NASA space travel applications have established requirements for environmentally robust anti-reflection (AR) TCFs that require <0.5% total losses (e.g., reflection, absorption, and scattering). The guidance, navigation, and control (GNC) light detection and ranging (LIDAR) systems utilized in NASA's volatiles investigating polar exploration rover (Space qualified rover lidar), Dragonfly (Ocellus), and on-orbit servicing, assembly, and manufacturing-1 (Kodiak) missions require pulsed transmit beams with exceptionally high-power densities. In this talk, I will discuss the development and manufacturing of an environmentally friendly, transparent, conductive, and AR coating suitable for use in GNC LIDAR and other space-flight applications using indium tin oxide (ITO) thin films. We have deposited and optimized ITO thin films utilizing a radio frequency (RF) sputtering process with varying gas flow, substrate temperature, and pressure, employing AR as the working medium. Various properties of ITO thin films such as surface morphology, optical and electrical properties will be presented. We found that the transmittance of ITO thin film at 1064 nm wavelength was 100%. Additionally, the sheet resistance measured was 362.1 Ohms per square, which closely aligns with conditions found in outer space, thereby ensuring the mitigation of static dust particle accumulation. We also built a six-layer thin film-designed device optimized for spectral characteristics at the targeted wavelength of 1064 nm using sputter deposition and conventional photolithography. This design incorporates a thin layer of ITO positioned between the outermost TiO_2 and SiO_2 layers. The performance of this structure will be presented as well.

Laser Engineering Nanocarbon Phases within Diamond for Science, Sensors and Electronics

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Abstract

Diamond, as the densest allotrope of carbon, displays a range of exemplary material properties that are attractive from a device perspective. Despite diamond displaying high carbon-carbon bond strength, ultrashort (fs) pulse laser radiation can provide sufficient energy for highly localized internal breakdown of the diamond lattice. The less-dense carbon structures generated on lattice breakdown are subject to significant pressure from the surrounding diamond matrix, leading to highly unusual formation conditions. By tailoring the laser dose delivered to the diamond, it is shown that it is possible to create continuously modified internal tracks, with varying electrical conduction properties. In addition to the widely reported conducting tracks, here conditions leading to semiconducting and insulating written tracks have been identified. This holds great promise for future devices, where nitrogen-carbon nanostructures can be controllably manufactured within a diamond wafer, providing not only buried conductive wires, but 3D structures with active device junctions (depletion or tunnelling). High resolution transmission electron microscopy (HRTEM) is used to visualize the structural transformations taking place and provide insight into the different conduction regimes. The HRTEM reveals a highly diverse range of nanocarbon structures are generated by the laser irradiation, including many signatures for different so-called diaphite complexes which have been seen in meteorite samples, and seem to mediate the laser-induced breakdown of the diamond. The work offers insight into possible formation methods for the diamond

and related nanocarbon phases found in meteorites. In addition to discussing the fascinating nanoscience occurring in this work, practical technology examples, currently undergoing commercial development, of radiation detectors, chemical sensors and even 3D transistors for power electronics fully embedded in single crystal diamond wafers (20 x 20 mm) using this methodology will be described. 'Show and tell' samples will be available.

Drug-loaded Emissive and Photothermal-cyclodextrin Carbon Nanodots: Antimicrobial, Antioxidant, and Anti-Inflammatory Properties

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Abstract

Carbon nanodots (Cdots) have gained great interest due to their optical properties and low cytotoxicity. In the present study, we report the synthesis of biocompatible Cdots derived from β-cyclodextrin (β-CD) via a novel one-pot mild-thermal method. The resulting Cdots-βCD are composed of an emissive C-sp2 core covered by an outer shell of β-CD. Thanks to the known capacity of the β-CD cavity to form inclusion complexes, the synthesized Cdots-βCD were used to produce supramolecular systems with various molecules, including iodine, ciprofloxacin (CPX), curcumin (CUR), and carvacrol. The supramolecular systems were characterized by optical absorption, emission, nuclear magnetic resonance, and fourier-transform infrared spectroscopy techniques. The nanoscale dimensions of the synthesized structures were confirmed through dynamic light scattering measurements and atomic force microscopy. Antimicrobial, antioxidant and anti-inflammatory activities of the inclusion complex have been widely investigated. The structure of the Cdots-β-CD/drug inclusion complexes was explored by molecular modelling simulations. Furthermore, polyvinyl alcohol blend films loaded with Cdots-β-CD containing CPX or CUR were fabricated and their antimicrobial, antioxidant, and anti-inflammatory activities as well as thermal stability were studied. This work has been funded by the European Union (Next Generation EU), project PRIN PNRR "Novel biomedical devices combining antimicrobial and anti-inflammatory activity by embedding bioactive loaded nanoconstructs in polymer films for more effectiveness in infectious disease treatment (BIONANOF)" (grant number P20229ZLSA).

Carbon Materials for Gas Sensors

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Abstract

This lecture will review the recent advances in carbon gas sensors for practical applications including environmental sensing, greenhouse gas monitoring, volatile organic compounds detection. The research achievements at the state-of-the art will be presented and discussed from carbon-based materials to devices, systems and related technologies.

Oral Presentations

Metal-terminated Diamond Negative Electron Affinity Surfaces for Thermionic Emission Applications: A Competitor for Photovoltaic Solar Cells?

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Abstract

Over the past few years, significant work has been done studying electron emission from diamond surfaces terminated with metals such as lithium (Li), magnesium (Mg), etc., to afford a negative electron affinity (NEA) surface stable at high temperatures. NEA enables electrons in the conduction band to escape to the vacuum without overcoming a potential barrier. Thermionic emission is therefore possible with NEA diamond at around 600 °C, rather than the 1500 - 2000 °C typically required for metals. Results from many groups worldwide suggest that NEA is maximized when the adsorbate is small, highly electropositive, and readily forms stable bonds with C and O. Various metal terminations, such as Li, Mg, aluminum, titanium, vanadium, nickel, and zinc have been studied both theoretically and experimentally, affording varying degrees of thermal stability and emission efficiency. A metal that meets the criteria mentioned above, but has only recently been studied, is scandium. A series of recent papers suggests that 0.25 monolayer Sc-terminated bare and oxidized diamond (100) surfaces may be among the most promising reported for diamond electron emission. These surfaces produce low work function, highly NEA characteristics, are stable to ~800 °C, permit high emission yield at low temperatures (~500 °C), resist degradation, are unaffected by air exposure, and are compatible with thermionic solar converters. In this talk, we briefly reviewed metal and metal-oxide terminations for NEA diamond surfaces as candidates for thermionic devices. We then discuss new results with scandium and scandium oxide terminations and speculate on whether this technology could become a viable competitor to photovoltaic solar cells.

Assessment of the Feasibility of Fractionation of Natural Biomass as a Circular Source for Biocarbon and Minerals

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Abstract

Diverse biomass residues were utilized in biorefining processes, providing new insights into the value-added applications of biomass resources. Raw materials such as pine bark, corncob, coconut fiber, grape pomace, vine pruning, fruit post-harvest loss, and marine macroalgae were fractionated by using deferent physical and chemical techniques to obtain high-value molecules, giving new conceptions into the value-added application of biomass resources. Appropriate pretreatment strategies were used to overcome the recalcitrance of lignocellulosic materials and facilitate their disintegration. Methods such as enzymatic and autohydrolysis, saccharification, fermentation, osmosis, microwave-assisted extraction, and ohmic heating were used for the biomass fractionation. Additionally, various analytical techniques such as fourier transform infrared spectroscopy, scanning electron microscopy, differential scanning calorimetry, derivative thermogravimetry, X-ray diffraction, and proton nuclear magnetic resonance were used to observe chemical structure differences. Molecules such as alginate, xanthan gum, bioethanol, cellulose, α-cellulose, holocellulose, and lignin were obtained in high yield and purity. Mixtures of extractives with antioxidant and antimicrobial activity were also obtained. These approaches also result in the obtention of mineral mixtures that may qualify these residues for various types of uses. These residues and byproducts derived are a significant reservoir of valuable bio compounds that hold substantial industrial value. Their fractionation through the application of the biorefinery approach not only aids in their recuperation but also plays a pivotal role in advancing the principles of the circular economy.

Integrated Pyrolysis of Vineyard Residues for Dual Production of Bio-pesticides and Functionalized Biochar Fertilizers

Gregor Tond*, Anna Willfarth, Dibin Davis, Christoph Kroiss, Wolfgang Gabauer, Christoph Pfeifer and Gerhard Soja

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Abstract

Conventional pyrolysis research tends to pursue either high-yield bio-oil production for energy purposes or biochar generation for agricultural use. This study introduces an integrated thermochemical valorization pathway for vineyard residues that targets both goals simultaneously: the production of a bio-based pesticide and a nutrient-enhanced fertilizer. The core process is a tailored pyrolysis system optimized to yield two functional product streams. The first is a bio-oil fraction, which is processed via nano-encapsulation for application as a biological pesticide. The second is a biochar fraction that undergoes functionalization with nitrogen-rich compounds and subsequent nanoencapsulation, enhancing nutrient retention and enabling controlled release when applied to soil. To address the complexity of this dual-output system, a validated thermochemical process model has been developed using IPSEpro. This model simulates key mass and energy flows and allows for the calculation of unmeasured variables based on experimental inputs. The modeling framework supports the interpretation of lab-scale results and offers a basis for industrial process design. By linking experimental findings with process engineering, this approach demonstrates a scalable route for circular resource use in viticulture, aligning with sustainability goals and carbon reduction strategies in agriculture.

Activated Porous Carbon Fiber: New Adsorbent for Sampling and Analysis of Siloxanes

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Abstract

The increasing global demand for energy necessitates the continuous development and optimization of sustainable and renewable energy sources. Within the framework of the circular economy, the conversion of waste into biogas and biomethane represents a promising strategy to enhance energy recovery and reduce environmental impact. However, the injection of biomethane into distribution networks and its utilization in energy conversion systems require rigorous quality control and efficient purification processes. Consequently, the development of innovative, cost-effective, and time-efficient sampling and analytical techniques is essential. This study evaluates the potential of activated porous carbon fiber (APCF), a highly versatile adsorbent suitable for thermal desorption analysis, as an alternative to conventional materials traditionally employed for siloxane monitoring. Siloxanes are among the primary contaminants in biogas and biomethane; if not adequately removed, they compromise fuel quality and damage equipment surfaces. During combustion, these compounds generate abrasive quartz particles and exhibit radical-scavenging properties that diminish the energy efficiency of biomethane. The adsorption performance of APCF tubes was assessed in comparison with standard multilayer tubes through both laboratory-scale and real-scale sampling at a biogas production facility. Thermal desorption coupled with gas chromatography-mass spectrometry analysis demonstrated that APCF offers superior siloxane capture and recovery efficiency. Overall, the findings indicate that APCF constitutes an innovative and effective material for improving sampling and analytical procedures in siloxane determination, thereby enhancing the monitoring of biomethane quality and contributing to more reliable and sustainable bioenergy production.

Catalytic Processing of Bio-based Materials for Graphitizing Functional Carbon

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Abstract

In the pursuit of sustainable replacements for synthetic graphitic materials, this research investigates the catalytic graphitization of biomass residues utilizing iron-based systems under moderate thermal conditions ranging from 800 to 1000 °C. Olive pomace, a readily accessible agricultural by-product, served as the model precursor and was functionalized with iron chloride, subsequently undergoing thermal processing and purification. The optimized procedure attained a graphitization degree of 0.81, a d-spacing of 0.338 nm, and a crystalline exceeding 60%, with yields reaching 30%, thereby presenting substantial advancements over uncatalyzed methods. Comprehensive characterization techniques (Raman spectroscopy, X-ray diffraction, transmission electron microscopy, and X-ray photoelectron spectroscopy) validated the formation of well-aligned graphitic structures with minimal defects. A techno-economic evaluation indicated that catalytic processing diminished operational expenditures and energy consumption by as much as 40% in comparison to traditional graphitization, with production costs projected at approximately $1670 per ton. Furthermore, life cycle analysis indicated reduced environmental impacts relative to the Acheson or electrochemical approaches, particularly in relation to ozone depletion and acidification metrics. These results establish catalytic

biomass graphitization as a scalable, low-carbon approach for the advancement of high-performance graphitic materials suitable for applications in supercapacitors, battery electrodes, and environmental remediation.

Theory of Friction for Periodic Water Structures and for Ions Moving Through a Sub-nanometer Carbon Nanotube

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Abstract

In this talk, we present a unifying theoretical framework that underpins the flow of water and ions in carbon nanotubes (CNTs) with diameters of the order of a nanometer. Previous molecular dynamics simulations show that under such circumstances, water forms one-dimensional water wires or hollowed cylindrical periodic structures. Since these structures are likely incommensurate with the nanotube, they exhibit very low friction, analogous to "superlubricity" in solids. This fact provides a qualitative explanation for the high flow velocity of water observed in sub-nanometer CNTs. Since the one-dimensional nature of these structures dictates that they do not exhibit long range order, they are not pinned by defects. We calculate the sliding friction arising from phonon excitation in nanotubes and in water structures and show that it scales linearly with the sliding velocity, and the interfacial friction coefficient is consistent with the results of the molecular simulations. Next, we consider the effects of random defects in the water structures and show that they give rise to a friction that is largely independent of the sliding velocity, i.e., dry friction, and demonstrate, based on the Langevin equation for a particle subject to both dry and viscous friction, that our model can account for the water flow measured in experiments. Lastly, we argue that there is also dry friction for ions moving in CNT's and demonstrate that this provides a natural explanation for the breakdown of the Nernst-Einstein relation for an ion moving in a sub nanometer CNT, as observed in recent experiments.

Scalable Continuous-flow Synthesis of PtNiRu@Graphene Nanoalloys for Enhanced Hydrogen Evolution Reaction Performance in Acidic Media

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Abstract

The growing demand for sustainable energy solutions highlights the urgent need for efficient and durable electrocatalysts for hydrogen production. Platinum-group metal-based catalysts exhibit excellent hydrogen evolution reaction (HER) activity; however, their widespread adoption is limited by high cost, scarcity, and performance degradation in acidic environments. To address these limitations, we developed a trimetallic PtNiRu nanostructured catalyst supported on graphene nanosheets, synthesized via a scalable continuous-flow method. This strategy enables precise control over metal composition and promotes uniform alloy formation. An optimized thermal sintering step enhances crystalline and structural stability. The resulting PtNiRu@graphene catalyst demonstrates significantly enhanced HER activity and long-term durability in acidic media, outperforming commercial Pt/C (40 wt.%). The improved electrocatalytic performance stems from a synergistic interplay among the constituent metals: Ruthenium enhances interfacial proton transfer and hydrogen recombination kinetics, while Nickel optimizes hydrogen adsorption by tuning the electronic and geometric structure of Platinum active sites. Thermal sintering promotes atomic diffusion and alloy homogeneity, mitigating the leaching of less noble metals and enhancing corrosion resistance. These results highlight the potential of continuous-flow nanoengineering as a scalable, reproducible, and cost-effective route for manufacturing next-generation HER electrocatalysts. Detailed insights into the synthesis, structural evolution, and electrochemical performance will be presented at the conference.

Microwave-assisted Pyrolysis of Waste for Xylene Adsorbent Preparation

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Abstract

Disposing of waste materials, particularly polymers (e.g., scrap tires), biomass (e.g., corn cob, waste from tomato production) and animal by-products (e.g., waste animal bones from slaughterhouse), has become an urgent environmental issue. Microwave pyrolysis and/or co-pyrolysis is a promising way to convert these waste materials or mixture of this waste into valuable carbon-based adsorbents. Compared to conventional pyrolysis, microwave-assisted processes offer greater controllability and efficiency (e.g., lower retention time), as well as being more cost-effective. Carbons produced by microwave pyrolysis, such as pyrolytic carbon black and chemically activated pyrolytic carbon black, exhibit excellent adsorption properties for polar and non-polar volatile organic compounds (VOCs) in gaseous streams. The adsorption performance of these materials is strongly influenced by the type of feedstock and the preparation parameters (e.g., microwave power, residence time, and the presence of chemical activators). This study investigates the adsorption behaviors of carbons derived from various waste sources, both with/without chemical activation. A comprehensive characterization of the textural, chemical and surface properties of the adsorbents is conducted. Furthermore, adsorption experiments are performed using xylene as a model VOC in the gas phase. The results provide insights into the key factors that govern adsorption capacity and highlight the potential of carbons derived from microwave pyrolysis as cost-efficient adsorbents for environmental remediation applications.

Engineering Carbons Prepared from Corn Cobs and Red Mombin Seeds by Using Microwave Pyrolysis for Xylene Adsorption

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Abstract

Biochars and activated carbon are widely used carbon materials for wasting air and water purification and soil remediation. They are also used for functionalization by photo/catalytic nanoparticles to have hybrid photo/catalytic-sorption function. This contribution presents the results of optimization of microwave pyrolysis of agricultural wastes, corn cobs and red mombin seeds, to yield high-quality biochars and activated carbons suitable for volatile organic compounds (VOCs) (xylene) adsorption from waste air. The effect of raw material loading (20 g vs 60 g), nitrogen atmosphere (batch vs flow) and $ZnCl_2$ activation on the carbon textural properties and micro/structure was studied. The mass balance of microwave pyrolysis process was done, and the quality of pyrolytic gas was also determined with respect to valuable compounds such as H_2, CO_2 and CH_4. Produced activated carbons were investigated for xylene adsorption in laboratory scale, using the adsorption column with 1.5 - 2.5 mm carbon particle-size fraction, 1000 ppm of xylene in an air flow, connected to online fourier transform infrared. The research value of this work consists in the fundamental understanding of microwave pyrolysis process of two different types of agricultural waste and identification of carbon material properties leading to their highest xylene adsorption capacity.

Porous Carbon Materials Derived from Renewable Biomass and Waste Feedstocks

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Abstract

Porous carbon materials derived from renewable biomass and waste feedstocks have been developed via controlled pyrolysis and chemical activation at LLC Perechin Timber and Chemical Plant. These materials exhibit very high specific surface areas (Brunauer–Emmett–Teller method up to 1833 m^2/g) and large pore volumes (~1.2 cm^3/g), with tunable porosity depending on activation conditions. For example, increasing the activating reagent concentration from 0% to 45% raised the BET surface area from ~55 m^2/g to ~1830 m^2/g, while the BJH pore volume increased from 0.07 to 1.23 cm^3/g. The resulting mesoporous structure (average pore diameter ~7 nm) enables outstanding performance across diverse applications. In energy storage, the biomass-derived carbon serves as an anode material for lithium-ion and sodium-ion batteries, accommodating lithium ion/sodium ion insertion with improved capacity retention and cycling stability. It also functions as a high-surface-area electrode in supercapacitors. Carbon further acts as a versatile catalyst support or solid acid catalyst in chemical reactions, and as an effective stationary phase for chromatographic separation of sugars and polyphenols. In environmental applications, it demonstrates

strong CO_2 adsorption capacity and selective uptake of metal ions, enabling efficient CO_2 capture and the separation of precious metals (Gold, platinum, and palladium) from base metals.

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

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Abstract

Water dissolves various substances, and many essential chemical reactions occur in aqueous solutions. The behavior of protons (H+) in an aqueous solution is also crucial in biochemical reactions and proton transfer in living organisms. On the other hand, the behavior of deuteron (D+) in heavy water (D_2O), an isotope of water, is still unclear. In this study, thus, we have applied the on-the-fly path integral molecular dynamics simulation, which can incorporate both the nuclear quantum effect and thermal effect. To elucidate the isotope effects of H^+/D^+ behavior in an aqueous solution, we calculated the systems of H^+ in light water solvent and D^+ in heavy water. We found a significant isotope effect around the Eigen H_3O^+/D_3O^+ region. First, the structures with Zundel H_5O^{2+}, H_7O^{3+}, and H_9O^{4+} were confirmed at the system of H+ in a light water solvent, while such structures are less at that of D^+ in heavy water. We also found the H/D isotope effect at the radial distribution function of O-O distances.

Photochemical Synthesis of Hybrid Carbon-Gold Nanostructures: Optical and Photothermal Properties

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Abstract

Metal-carbon based nanohybrid systems have attracted considerable interest due to their distinctive optical, electronic, and chemical properties, which are typical of both metal- and carbon-based low-dimensional materials. C-nanodots are low-dimensional materials produced through a novel, gentle thermal treatment of organic precursors such as glucose, fructose, agarose, polymers, amino acids, and others, developed in our laboratory. The resulting C-nanodots consist of an emissive and photothermal carbon sp^2 core encased by a carbon sp^3 shell derived from precursor molecules. These C-nanodots demonstrate very low cytotoxicity, along with luminescence, photothermal activity, and excellent photocatalytic capabilities. Building upon the photophysical characteristics of these C-nanodots, we have recently devised a new photochemical approach to synthesize hybrid gold-Cdots nanostructures via a photo-assisted mechanism. In this method, the C-nanodots act as photo-reducing and stabilizing agents for the formation of metal plasmonic nanostructures. When irradiated with UV light (around 300 nm), the sp^2 core of the C-nanodots produces free electrons (e^-) and holes (h^+). The photogenerated electrons promote the reduction of gold ions (Au^{3+}) to metallic gold (Au^0), while the carbon shell stabilizes the newly formed hybrid gold nanostructures. The resulting hybrid gold-Cdots nanostructures exhibit excellent optical and photothermal properties, which are highly dependent on the type of precursor used to create the carbon shell. We have shown that both the localized surface plasmon resonance band and the photothermal efficiency of these hybrid structures are influenced by the specific C-shell precursor. Finally, these nanostructures have been characterized in terms of molecular composition, morphology, size, and optical features.

Nanostructured Hybrid Materials for Sensing of Cardiac Disease Biomarkers

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Abstract

Label free biosensors for nucleic acid quantification are pivotal for the development of point-of-care diagnostic platforms. The approach offers significant advantages such as cost-efficiency and real-time analysis without the need for complex labelling procedures. Our study explores the use of 0-dimensional gold nanocluster (AuNCs) and 2-dimensional nanostructures for the de-

velopment of a label free platform for biosensing. A photochemical approach was developed to prepare emissive GSH-capped AuNCs and further ligand exchange process was performed for anchoring of specific biomolecules as ssDNA and protein. The self-assembly monolayer of (3-Glycidyloxypropyl) trimethoxy epoxy silane was prepared and properly modified for specific and specific recognition of DNA targets. The engineering of the surface with hybrid nanocoating allows the control over the biocompatibility, surface robustness and fine tuning of binding affinities. Both nanostructure materials were characterized in terms of optical and surface properties. Controlling the sensor surface properties is essential for the development of sensitive and reproducible biomolecular sensors. The sensing of DNA and protein was investigated and the results reported. Both platforms exhibit good potential for the development of label free, precise, sensitive and specific biosensors for nucleic acids and protein biomarkers. These can in turn be developed in low-cost point-of-care platforms for nucleic acid and protein-based biomarker diagnostics such as miRNAs and IL-6. This work has been funded by Linea di Intervento 1- Progetti di Ricerca Collaborativa del "PIAno di in CEntivi per la RIcerca di Ateneo 2024/2026" (University of Catania). Title Project: MhyNano: Multifunctional hybrid nanomaterials for cancer diagnosis and personalized targeted therapy.

Influencing Chloride Oxidation by a Novel Boron-doped Diamond Electrode Design

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Abstract

The extensive formation of perchlorate is one of the major drawbacks of Boron-doped diamond (BDD) technology in the field of electrochemical oxidation for water treatment. Without understanding why potentially toxic by-products are generated and consequently knowing how to prevent formation, a widespread deployment of the technology for water purification is not possible. A novel generation of BDD electrodes is discussed to address this issue, which brings new opportunities as well as challenges through its design: the integrated double diamond electrode (iDDE). The iDDE is based on the idea of an electrically insulating substrate for BDD in combination with a subsequent laser structuring of the BDD layer to electrically separate it into two or more regions. Depending on the electrical contact, those regions will function as anode or cathode with an interelectrode spacing distance below 50 µm. The primarily electrochemically active surface area is thus determined by the laser structure and less by the global dimensions of the electrode. Due to an increase in current density in this region, the oxidation behavior of the electrode system changes significantly depending on the chosen structure. This makes it possible to create multiple electrode systems without changing the BDD layer quality or global parameters (e.g., interelectrode spacing, electric current, flow conditions). Initially, the increased current density in the laser-structured gap promotes the formation of perchlorate; however, the iDDE concept simultaneously offers new opportunities to mitigate the generation of undesirable by-products.

Theoretical Study of Electron Transport in the Interface of Manganese dioxide/Carbon with Potential Applications for Energy Storage Devices

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Abstract

Manganese dioxide (MnO_2) is well-regarded for its potential in supercapacitor applications, offering both high energy and power densities. These characteristics can be further improved by integrating MnO_2 with carbon nanostructures. The electronic double layer effect at the interface of these composite materials plays a vital role in charge storage capability. To explore this interaction, the relationship between alpha-MnO_2 and nanostructured carbon was examined. A theoretical analysis using density functional theory and the non-equilibrium green function method was conducted to study electron transport within the alpha-MnO_2/carbon composite. Electron transmission simulations provided current–voltage (I – V) data over a voltage range of -3.0 to 3.0 V, with the maximum current reaching 90.0 µA at 3.0 V, indicating a significant improvement in electronic conductivity due to the carbon support. Additionally, quantum capacitance (QC) analysis offered insights into the system's energy storage capability, showing values between -0.5 and 0.5 V and peaking at 767.52 µF/cm^2. Both the QC and electron transport characteristics at the alpha-MnO_2/carbon interface were identified as key elements for guiding the design and optimization of advanced electrode materials for future energy storage technologies.

Optics with a Twist: Switching with Dirac Fermions in Graphene

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Abstract

The dynamics of 2-dimension Dirac fermions in graphene, driven by the symmetries of their underlying pseudospins, can manifest in wavefunctions and current transmissions in ways that are fundamentally different from conventional optical interfaces. I will present numerical simulations and experimental demonstrations of several textbook optical effects mirror in graphene, albeit with a twist-specifically (i) trajectories set by Snell's Law but with negative index of refraction, (ii) angular transmission set by Fresnel's equation but with universal transmission at normal incidence, (iii) Brewster angles set by electron pseudospin rather than photon polarization, and (iv) polarizer-analyzers following Malus' law but with half angles. These subtleties all arise because the photon like band structure comes with particle-antiparticle pairs, so that the corresponding band effective mass flips signs at a split-gated PN junction, even while electrons across differently gated graphene segments are unable to alter their group velocity. Symmetry dictates that the pseudospins (mixing coefficients of its frontier dimer pz orbitals) for an N-layer Bernally stacked graphene execute N rotations around the Fermi surface, with a fixed Berry phase Nπ and Chern number of N/2. This implies that the reflectivity at small incident angle θ across the PN junction resembles sinNθ for odd N and cos Nθ for even N, giving alternately perfect headon transmission (Klein tunneling) or head-on reflection (anti-Klein tunneling), with an angular sweet spot (Brewster angle). At the same time the higher angle electrons collimate with increasing voltage barrier (refractive index mismatch), so that by placing multiple junctions at an angle, the overall transmission can be quenched much like Malus' law in a polarizer-analyzer pair. The result is a gate tunable transmission gap that can be used to turn graphitic electrons off for bulk samples, both for digital and analog electronic applications.

Novel Thermally Reduce Graphene Oxide Microsupercapacitor Fabricated via Mask–free Axidraw Direct Writing

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Abstract

We report a simple and scalable method for fabricating all-solid-state thermally reduced graphene oxide (TRGO) micro supercapacitors (μ-SCs) using atmospheric pressure horizontal tube furnace, spray coating, and a mask-free AxiDraw sketching apparatus. TRGO thin films were deposited on microscopic glass substrates and characterized using X-ray diffraction, scanning electron microscopy, energy-dispersive X-ray spectroscopy, ultraviolet–visible spectroscopy, and Fourier transform infrared spectroscopy. These analyses revealed a significant reduction in oxygen functional groups with increasing reduction in temperature (RT), accompanied by changes in film transparency, color, and stacking behavior. Raman spectroscopy provided insights into crystallite size, defect density, and amorphous content. Electrochemical performance of the μ-SCs was evaluated using cyclic voltammetry (CV), electrochemical impedance spectroscopy (EIS), and Bode plot analysis. The μ-SCs exhibited rectangular CV curves across a 0 - 0.8 V window at scan rates ranging from 5 - 1000 mV s^{-1}, confirming electric double-layer capacitor behavior. Devices with 14 digits per cm^2 demonstrated a 46% increase in capacitance over those with 6 digits per cm^2, outperforming configurations with 22 and 26 digits per cm^2. TRGO reduced at 500 °C (TRGO-500) achieved volumetric energy and power densities of 14.61 mWh cm^{-3} and 142.67 mWh cm^{-3}, respectively. EIS showed a decrease in equivalent series resistance with increasing RT, while Bode plots showed a phase angle of -85° for TRGO-500. Power law and Trasatti analyses revealed that low-temperature μ-SCs are diffusion-controlled, whereas higher-temperature devices exhibit surface-controlled behavior. These results demonstrate tunable electrochemical performance through temperature, electrode density, and configuration adjustments.

Advanced Carbon Nanocapsules for Neutron Cancer Therapy

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Abstract

Cancer remains one of the leading causes of mortality worldwide, and conventional therapies often show limited effectiveness. Neutron capture therapy (NCT) offers a targeted alternative in which stable isotopes are delivered to tumor cells and activated by neutron irradiation, producing localized nuclear reactions that can destroy malignant tissue. Although boron-10 has been the focus of most NCT research and clinical applications, current boron-based agents suffer from limited tumor selectivity and the need for high intracellular concentrations, restricting their clinical efficacy. Lithium-6 has recently emerged as a promising isotope for NCT due to the higher energy released by its nuclear reaction products. Our group pioneered the use of lithium as a neutron-active element by developing carbon nanocapsules (CNCs) filled with lithium (Li) iodide. These 6Li@CNCs demonstrated excellent cellular biocompatibility (>90%), and after neutron irradiation, cancer cell survival decreased dramatically to 1.8%. Expanding on this approach, we engineered carbon dots doped with lithium-6 (6Li@CDs) using optimized microwave-assisted and hydrothermal syntheses. Comprehensive characterization (Transmission electron microscopy, atomic force microscopy, high-resolution transmission electron microscopy, fourier transform infrared spectroscopy, X-ray photoelectron spectroscopy) confirmed their structural and chemical composition. The 6Li@CDs also exhibited green photoluminescence, supporting their potential as theragnostic platforms. Cytotoxicity assays in MRC-5 fibroblast cells confirmed high biocompatibility. These findings position 6Li@CDs as a promising nanoplatform for Li-based neutron capture therapy. By integrating therapeutic and diagnostic functionalities, this approach could overcome critical limitations of current boron agents and accelerate the translation of NCT nanodrugs into preclinical trials.

Chiral Nematic Mesoporous Organosilica Films: Preparation, Modification and Applications

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Abstract

In the Nature, unique materials can be found whose building blocks are arranged in chiral (helical) structures that affect their optical and mechanical properties, e.g., the wings of *Morphous* butterflies. In the laboratory, chiral, iridescent materials are obtained from cellulose nanocrystals (CNCs), whose structure results from the formation of a left-handed helix by the building blocks. CNCs are also used in the preparation of bio composites and in the template synthesis of chiral and organic silica. Chiral, nematic, mesoporous organic silica (CNMO) has unique sorptive, iridescent and optical properties that make it used as a decorative and sorptive material. CNMO is prepared using bridged alkoxysilanes and a suspension of CNCs. However, the limited number of commercially available organosilicon precursors for the formation of these materials means that they have a limited range of chemical and mechanical properties. This presentation will describe the development of an efficient method to functionalize CNMO films that does not destructively affect the chiral, nematic structure of the material. The modified materials exhibit additional hydrophobic and/or complexing properties that can be used as moisture indicators or membranes for ion sequestration.

Unveiling The Origin of Ph-dependent Catalytic Performance of Bi_2O_3 Nanostructure for Electrochemical Co_2 Reduction

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Abstract

To address the excessive CO_2 emissions from burning fossil fuels, various strategies, including CO_2 capture and storage technologies, have been implemented. A promising next step is converting captured CO_2 into value-added chemicals and renewable fuels, which would reduce dependency on fossil fuels and support the advancement of the Circular Economy. Among the potential conversion methods, electrochemical CO_2 reduction powered by renewable electricity is particularly promising, as it also enhances the integration of electricity into the energy mix. However, despite its potential, electrochemical CO_2 conversion faces several challenges, such as the low energy content of CO_2, high reaction energy barriers, slow electroreduction kinetics, and low product selectivity. To overcome these obstacles, the development of highly active, selective, and stable catalysts, as well as the optimization of the electrolysis process, is crucial. Our research focuses on advancing catalyst development to enable effective CO_2 reduction and contribute to a more sustainable energy future. We have recently developed Cu-based, Ag-based and Bi-based materials for selective production of C_2 products, carbon monoxide (CO) and formic acid (HCOOH), respectively. Additionally, by advancing the electrolysis process, we have increased the current density from tens of milliamps to hundreds of milliamps, bridging the gap between laboratory results and industrial requirements.

Scalable Microwave-assisted Continuous Flow Synthesis of Silver Nanowires

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Abstract

In this investigation, we introduce a pioneering methodology integrating microwave irradiation with continuous flow techniques for the efficient, eco-friendly, and scalable synthesis of silver nanowires. Utilizing a growth kinetics model tailored for microwave-assisted synthesis, we optimized conditions to achieve higher yields and complete conversion of the metal precursor. The integration of conventional and microwave growth kinetics contributes to achieving 100% selectivity in nanowire production. Our study underscores a notable reduction in reaction time with increased nanowire yields. Precise modulation of the growth rate across three distinct stages governing nucleation and growth processes enable enhanced selectivity in nanowire production. The capability to adjust reactor temperature and microwave power at different stages of the reaction process empowers the fabrication of silver nanowires with customizable dimensions, achieving a production rate of 4 grams per hour. We systematically examined key reaction parameters, including the concentration of metal ions, residence time, and different reactor configurations. Our approach successfully yielded AgNWs with 40 - 60 nm diameter and 15 µm length. The cost associated with this process for synthesizing AgNWs was USD 9 per gram. This study highlights the potential of continuous, high-throughput processes for controlling particle size through reactor engineering.

Performance Investigation of Micro Tools Coated with Carbon Nanotubes and Graphene in Micro-electro Discharge Machining Process

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Abstract

In micro electro discharge machines, a high tool wear rate affects the geometric accuracy of machined features. The purpose of this research was to develop a methodology for reducing tool wear rate of micro tool electrodes. In this work, the effect of thin film coating of graphene and carbon nanotube (CNT) on tungsten carbide micro-electrode on tool wear rate (TWR), over the cut and depth of machining (Z coordinator) during micro-drilling of Ti-6Al-4 V were studied. Experimental work is examined in a comparative study of graphene-coated, CNT-coated, and non-coated tools. The experimental work includes development of thin film coatings of graphene and CNT. The design of experiments was performed using the Taguchi method with an L9 orthogonal array and the results are discussed using ANOVA of each response variable. The machine results showed that TWR decreases, and the material removal rate increases with coated tools. In comparison, CNT-coated graphene-coated tools provide the best outcomes, and both coated tools outperform uncoated tools.

Carbon-doped Chitosan Hydrogels-synthesis and Characterization

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Abstract

Chitin and chitosan are biopolymers obtained mainly from crustacean shells and characterized by a structure similar to cellulose. Chitosan does not exhibit toxic reactions in the environment, which allows for its safe use in medicine, pharmacies or environmental applications such as purification of water reservoirs e.g. from heavy metals. Chitosan can be crosslinked with the use of different chemicals leading to hydrogels. The methodology of hydrogels' synthesis, as well as the reaction conditions influence the final structure of the resulting material. Moreover, numerous substances can be incorporated into polymer matrix, among others carbon microparticles obtained from waste biomass. In this study chitosan was crosslinked with different organic acids under microwave radiation leading to hydrogels additionally doping with biochar. The synthesis parameters, as well as preparation procedure affected the structure and sorption properties of resulting materials.

Electric Vehicles and CO_2 Emissions: The Case of Turkey

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Abstract

Reducing carbon emissions is one of the top priorities on countries' agendas. In recent years, electric vehicles have begun to play a role in reducing CO_2 emissions. The use of hydrocarbon-based fuels in electricity generation has a significant impact on CO_2 production. To this end, the effects of two best-selling electric cars in Turkey and a diesel car with similar characteristics on CO_2 production were compared in three different scenarios. In the first scenario, the sources used for electricity generation in Turkey in 2024 were employed. In the second scenario, the contribution of coal power plants to electricity generation was increased by 50%, while the contribution of natural gas power plants was reduced by 50%. In the third scenario, renewable energy sources were excluded, and electricity generation was provided solely by coal and natural gas power plants. In the first scenario, CO_2 production decreased by 40.1% and 47.6% compared to diesel vehicles, while in the second scenario, it decreased by 21.2% and 31.1%. In the third scenario, a 2.3% decrease and an 11.8% increase were observed. For electric vehicles to reduce CO_2 emissions, electricity production must focus on solar, wind and hydroelectric energy instead of hydrocarbon-based fuels.

Highly Flexible, Low-cost Carbon Fabric-rubber Composite Sheets from Discarded Jute Bags and Natural Rubber Latex for Efficient Electromagnetic Interference Shielding

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Abstract

The waste-to-wealth concept is proven in this work by using cast-off jute bags for the preparation of flexible electromagnetic interference (EMI) shielding materials of high shielding effectiveness. Carbonization of jute fabrics in a rolled condition enables large-scale production of carbon textiles in a conventional inert atmosphere box furnace. The thin (0.47 mm), turbostratic carbon textile produced is robust with a tensile strength, Young's modulus, and strain-to-failure of 0.44 MPa, 43.76 MPa, and 2.7%, respectively. The flexible carbon textile is amenable to bending, twisting, and cutting using scissors. The high EMI shielding effectiveness (38 dB) of the carbon textile is due to its adequate electrical conductivity, dielectric constant, and the presence of a large area of interfaces. The multiple internal reflections due to hierarchical porosity, consisting of grid-like pores between yarns, inter-fiber pores within the yarn, macropore channels in the fiber cross-section, and micro-mesopores present in the fiber, contribute to enhanced EM wave absorption. The durability for prolonged use is ensured by embedding the carbon textile in the natural rubber matrix by *in situ* coagulation of rubber latex within the pores using acetic acid as a coagulating agent. Multilayered carbon-textile rubber composites fabricated by a simple hand layup achieve a high EMI shielding effectiveness of 77.8 dB at a thickness of 2.38 mm. The absolute EMI shielding effectiveness of 3185 and 419-888.4 dB cm^2 g^{-1} obtained for the carbon textile and the carbon textile-natural rubber composite, respectively, are among the highest reported in the category of biomass-derived carbon and polymer matrix composites.

Sequential Novel Use of *Moringa Oleifera* Lam, Biochar, and Sand to Remove Turbidity, *Escherichia Coli*, and Heavy Metals from Drinking Water

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Abstract

This research investigates the individual and combined use of *Moringa oleifera* Lam., biochar, and sand to remove turbidity, pathogens, and heavy metals from drinking water. Contaminated water was synthetically prepared using kaolin, standard nickel/lead solutions, and *Escherichia coli.* The optimal dose of *M. oleifera* seed protein, extracted in 1 M NaCl solution, was determined using a jar test flocculator. *M. oleifera* treatment reduced water turbidity from 200 to 4 nephelometric turbidity unit (NTU) and achieved a 1 - 2 log reduction in *E. coli*. Subsequently, the *M. oleifera* -treated water was passed through a biochar column

supported on a sand bed, revealing clear water with 1 NTU turbidity. The sequential process of using biochar and sand reduced nickel and lead by 97.5% and 99.3%, respectively.

Poster Presentations

Microwave-assisted Reduction of Graphene Oxide to Reduced Graphene Oxide

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Abstract

In this communication, a microwave-assisted hydrothermal technique and a thermal annealing method were used in the reduction of graphene oxide (GO) to make reduced GO (rGO). Graphite powder was oxidized using the improved Hummers' method, exfoliated, and freeze-dried. Thereafter, an aqueous suspension of GO was reduced under microwave (MW) irradiation for 10 min at 600 W with and without the help of a reducing agent (hydrazine hydrate). Thermal annealing reduction was also conducted under a nitrogen atmosphere at 300 °C for 1 h. Prepared samples were analyzed using Raman laser spectroscopy, X-ray diffraction (XRD), transmission electron microscopy, the Brunauer–Emmett–Teller method, and X-ray photoelectron spectroscopy. A successful reduction in the GO functional groups between the sheets was established using XRD. From the Raman analysis, the ratio of the intensity of the D and G band (ID/IG) in graphene sheets assisted in assessing the quality of the graphene films. An increase in the ID/IG ratio after both oxidation and reduction processes was observed. The defect densities of both MW-treated samples were comparable while an increased defect density was evident in the thermally annealed sample. Transmission electron microscopy micrographs confirmed the sheetlike morphology of the samples. It was also evident from XRD analysis that thermal treatment promoted the coalition of graphitic layers, such that the estimated number of layers was larger than that of GO. The elemental analysis showed that the C/O ratio of GO increased from 2 to 7.8 after MW hydrazine reduction.

Versatility of Diamond Electrodes-opportunities by Electrode and Cell Design

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Abstract

The use of Boron-doped diamond (BDD) electrodes in water treatment is limited due to the formation of potentially harmful by-products. Therefore, effective water treatment technologies that utilize BDD require a reliable strategy to control the formation of these byproducts. Part of this strategy is not only to modify the diamond itself but to tailor the electrode design and the associated flow dynamics. This is done in flow-through mode by changing the geometry and porosity of the electrodes to generate channels in different configurations and sizes. In this way, it is possible to influence the various reactions that occur during the water treatment process. A particular focus of this research is on chlorinated byproducts to prevent serious health issues caused by chlorate and perchlorate, as chloride is commonly found in almost any water matrix. In addition, BDD not only enables the anodic oxidation of pollutants, but also potentially the direct reduction of the by-products produced during these reactions. By adjusting the cathode material and design, the aim is to achieve simultaneous electrochemical reduction of the byproducts produced in an undivided cell.

DFT Insights into CO_2 Adsorption Mechanisms on Doped Graphene Oxide Nanoribbons

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Abstract

Graphene oxide nanoribbons (GONRs) doped with heteroatoms have attracted growing interest for their potential in CO_2 capture applications. In this preliminary study, we explore how single (Boron (B), Nitrogen (N), Phosphorus, Boron–Nitrogen

(BN)) and binary (BN) doping a Gect the interaction of CO_2 with edge-functionalized ketidic GONRs using density functional theory. Early results suggest that nitrogen and phosphorus dopants promote weak, reversible adsorption via physisorption, whereas boron and BN cooping enable stronger interactions consistent with chemisorption. The most notable adsorption energy so far is observed for B-doped systems (ca. -3.33 eV), where the CO_2 molecule binds to both a boron atom and a carbonyl oxygen, stabilizing a closed-edge configuration. BN co-doping also leads to strong adsorption (ca. -3.24 eV), though through a distinct interaction pattern involving both dopants. Electronic structure analyses (Density and partial density of states) indicate dopant-induced modifications in orbital hybridization and bandgap, particularly in the BN system. Charge density studies reveal localized and delocalized charge rearrangements depending on the dopant type. These preliminary findings underscore the importance of dopant selection in tuning the reactivity and sensing potential of GONRs. Ongoing work includes systematic evaluation of adsorption reversibility, thermal eGects, and dopant configuration optimization.

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