USG Proceedings Journal

Meeting Abstracts | Open Access

Proceedings of the 6th International Conference on Carbon Chemistry and Materials (CCM-2026)

Keynote Presentations

Deciphering the Photophysical Properties of Covalent Organic Frameworks and Hydrogen-bonded Organic Frameworks Based Luminescent Materials

Mario de la Hoz Tomás[1], Taito Hashimoto[2], Boiko Cohen[1], Ryusei Oketani[2], Ichiro Hisaki[2] and Abderrazzak Douhal[1*]

[1]Department of Physical Chemistry, Faculty of Environmental Sciences and Biochemistry, and Institute of Nanoscience, Nanotechnology, and Molecular Materials, University of Castilla-La Mancha, Toledo, Spain

[2]Division of Chemistry, Graduate School of Engineering Science, The University of Osaka, Osaka, Japan

Abstract

Luminescent porous organic materials, including covalent organic frameworks and hydrogen-bonded organic frameworks, have emerged as an attractive class of carbon-based materials for optoelectronics, photonics, sensing, and light-harvesting technologies. Their highly tunable π-conjugated architectures, combined with permanent porosity and structural versatility, enable precise control over excited-state processes. However, the rational design of highly emissive materials remains challenging due to the aggregation effect which suppresses the emission properties of the materials. In this talk, I will present results on two representative luminescent porous organic materials. First, a hexadehydrotribenzo [12] annulene-based covalent organic polymer (T12-COP) which exhibits a remarkably large stokes-shifted emission band (~9000 cm^{-1}) arising from ultrafast intramolecular charge transfer and aggregate formation. Femtosecond (fs) time-resolved experiments reveal intramolecular charge transfer dynamics occurring within ~300 fs. Furthermore, T12-COP forms efficient donor–acceptor composites with Nile red, displaying ultrafast energy transfer processes on ~500 fs and ~6 fs governed by distinct electronic coupling degrees. Secondly, a perylene diimide-based hydrogen-bonded organic frameworks, whose layered crystal packing modulates the balance between monomer, H-type and J-type aggregates, and excimer formation. Fs-nanoseconds time-resolved spectroscopy experiments reveal that structural variations strongly influence the photophysical properties, with excimer formation occurring in less than 20 fs for the framework while steric hindrance significantly slows this process in related derivatives. These results provide fundamental insight into the excited-state dynamics governing luminescent porous organic materials and establish molecular design principles for next-generation carbon-based materials with enhanced optical performance for photonic and optoelectronic applications.

Mycelium-based Binders and Packaging Materials: High-performance, Circular Alternatives for Hygiene and Spill-control Applications

Sanjay Wahal*

Founder and President, Decarbonization, LLC, USA

Abstract

Mycelium-based binders and packaging materials emerge as scalable, biodegradable alternatives to fossil-derived foams and synthetic absorbent components, offering a rare combination of functional performance, circularity, and waste-to-value potential. This presentation examines recent advances in fungal biotechnology, substrate engineering, and modular manufacturing, with a specific focus on valorizing cellulose-rich residues from the pulp and paper industry as low-carbon feedstocks. Comparative performance and lifecycle data against expanded polystyrene, polyurethane, and bio-based foams demonstrate mycelium's advantages in key sustainability metrics—including substantially lower greenhouse gas emissions, reduced embodied energy, inherent microplastic-free end-of-life, and rapid compostability—while achieving application-relevant mechanical strength,

cushioning behavior, and absorbency. Use cases relevant to the hygiene and spill-control sectors—including absorbent cores, industrial spill management media, and protective packaging for sensitive products—are explored alongside commercial and pilot-scale case studies. These examples highlight both near-term opportunities and scale-up challenges, such as growth-cycle variability, material standardization, moisture sensitivity, and cold-chain requirements for spawn viability. The session further outlines priority research and development pathways in strain optimization, substrate formulation, hybrid mycelium-fiber composites, and industry-4.0-enabled process monitoring and control. Regulatory and market drivers, including plastic bags, green public procurement, and extended producer responsibility frameworks—are discussed as accelerating forces for adoption. By integrating material science, industrial ecology, and market insights, this presentation positions mycelium-based systems as a credible, high-impact pathway for delivering sustainable performance in hygiene, absorbent, and protective material applications—supporting Europe's circular-economy and decarbonization objectives.

Carbon Lattice Defects Single Atom Decoration Research of Meta-carbon Materials: Insights and Technology Opportunities

Mohini M. Sain[1*], Otavio Dias[1], Petr Shadrin[1], Jessica Ye[2], Athan Tountas[2], Shufang Ji[1] and Ritu Kumar[1]

[1]*Department of Mechanical and Industrial Engineering, University of Toronto, Canada*

[2]*Department of Chemistry, University of Toronto, Canada*

Abstract

Metal organic framework is a well establish support platform for heterogeneous catalysis. Metal organic framework facilitates surface to support enhanced electron sites promoting vacancy state influencing excitation energy, hence catalytic performance. The effect of such platforms is explored widely in new areas of catalysis such as photochemical and cold-hot plasma. In our presentation we documented facile transformation of gas phase hydrocarbon and other more polluting reactants including carbon dioxide to manufacturing nanostructured carbon as a co-product in a simultaneous activation of vacancy state of specific single atoms to produce hydrogen, methanol and dimethyl ethers. Density functional theory and molecular dynamics and machine learning study further elucidated the scope of expanding this single atom doping to create lower activation vacancy state and facilitated photochemical and photothermal processes in a wide range of wavelength. Our talk will focus on kinetics of several single atom doping state of metals and their selectivity on carbon nanomaterials production with carbon neutral hydrogen as a coproduct for modular deployment. We shall demonstrate our technology readiness level 4 technology scale up to produce nanotubes with unexpected functionalities and application of nanostructured carbon in target specific applications including hydrogen fuel cell, electrochemical cell ion transport, abnormal dielectric and paramagnetic applications such as conductors.

Oral Presentations

Designing Resilient Catalyst-sorbent Systems for Next Generation Flexible Sorption-enhanced Carbon Dioxide Hydrogenation Processes

Johannis A.Z. Pieterse[1*], Silvia Zanoni[2], Jonathan van den Ham[2], Pascal Buskens[2], Nicole Meulendijks[2], Alma Capa Tamargo[1] and Jurriaan Boon[1]

[1]*TNO STIP, Petten, Netherlands*

[2]*TNO MAS, Eindhoven, Netherlands*

Abstract

The transition to electrified, climate-neutral chemical manufacturing requires processes capable of operating dynamically, in response to fluctuating renewable energy supply. Sorption-enhanced carbon dioxide hydrogenation offers a promising route to achieve this flexibility, by shifting the reaction equilibrium through *in-situ* sorption of its (by-)products. Among the most mature implementations is sorption-enhanced dimethyl ether synthesis (SEDMES). Recent advances in SEDMES have substantially improved productivity by implementing pressure-swing regeneration, thereby eliminating the need for temperature-swing operation. However, the inherently cyclic operation of SEDMES imposes significant mechanical and chemical challenges on the functional materials. To address these challenges, a structured toolbox based on predefined stressors was developed using first-generation (commercial) SEDMES functional materials. These materials integrate a copper/zinc/aluminum-based methanol synthesis catalyst, a methanol dehydration catalyst, and a molecular sieve water adsorbent. Systematic performance and

degradation studies established a robust knowledge base to validate testing protocols and to define realistic stressor envelopes. Custom-built bench-scale reactors were employed to impose temperature and pressure swings, contaminant exposure, and extended time-on-stream operation, thereby replicating relevant degradation mechanisms, representative of the dynamic conditions anticipated in future energy-integrated and flexible chemical manufacturing environments. The validated insights guided the development of second-generation functional materials with engineered and experimentally verified tolerance to these stressors, while remaining compatible with established commercial catalyst manufacturing practices. The resulting toolbox enables material suppliers and end users to systematically map transient-operation stressors, benchmark durability and derive design rules for robust catalyst-sorbent systems, supporting adaptable carbon dioxide conversion processes capable of synchronizing production with renewable electricity availability.

Carbon Dioxide, Energy and Hydrogen Requirements for Carbon Capture and Utilization–A Simple Breakdown of the Energy Math

Georg Locher*

SCHWENK Building Materials Group, Germany

Abstract

The presentation analyzes the technical, energy-related, and infrastructural requirements for carbon capture and utilization as well as the role of carbon capture and storage in the context of German and European climate targets. While carbon dioxide from industrial processes would theoretically be sufficient to produce synthetic fuels and key chemical products, a comprehensive carbon capture and utilization strategy fails due to three major bottlenecks: limited biomass availability, insufficient expansion of renewable energy, and a severe shortage of green hydrogen. Carbon capture and storage, on the other hand, is considered indispensable by the intergovernmental panel on climate change for achieving climate goals. The presentation therefore calls for realistic prioritization: expanding renewable energy, building carbon dioxide and hydrogen infrastructure, prioritizing hydrogen use, and strengthening the role of carbon capture and storage to safeguard Europe's industrial base.

Amine-based Shaped Carbon Dioxide Solid Sorbents for Carbon Capture

Abdulkadir Bozarslan*, Michal Machovsky and Ivo Kuritka

Centre of Polymer Systems, Tomas Bata University, Zlin, Czech Republic

Abstract

The development of efficient and scalable solid sorbents remains a key challenge in carbon capture. Common shaping approaches such as granulation, palletization, and spheronization, are used to produce shaped forms. This work focuses on amine-based shaped sorbents, evaluating how shaping influences carbon dioxide adsorption performance. Amine-functionalized porous materials are structured into mechanically stable forms using suitable binders, improving handling and process integration. The relationship between shaping, material structure, and carbon dioxide adsorption behavior is evaluated, along with key performance parameters, including uptake, kinetics, and mass transfer limitations. While shaping can introduce diffusional resistance and partial pore collapse, it enhances structural stability and industrial applicability without significantly compromising equilibrium adsorption performance. Overall, this work provides insights into balancing amine accessibility and structural integrity of shaped sorbents for carbon capture and direct air capture applications.

Acknowledgments: This work was supported by the Ministry of Education, Youth, and Sports of the Czech Republic under the DKRVO program (RP/CPS/2024-28/007). Supports from the Internal Grant Agency of Tomas Bata University in Zlín under project No. IGA/CPS/2026/002 is also acknowledged.

Functional Carbon Modifications as Key Fusion Body Components within a Highly Flexible Material Programmed Inertial Confinement Fusion Power Plant

H.P. Berg[1*] and M. Maeder[2]

[1]*Brandenburg University of Technology, Cottbus, Germany*

[2]*Munich Garching Technical University, München, Germany*

Abstract

This work presents a comprehensive materials science concept for an advanced 50-megawatt electric material programmed inertial confinement fusion power plant, utilizing tailored carbon and nanographite structures within the key component of the main process. While the peripheral plant technology for internal closed-loop fluid processing relies on carbon-free, radiation-stable metallic and ceramic matrix components to prevent radiolytic methanation, the specific mechanical and anisotropic properties of carbon are systematically exploited within the injected fusion body itself. The primary materials science focus centers on establishing the cascade programming of the fusion target body within the extreme high-pressure regime. During the initial detonation and liner impulse onto the programmed core, transient shock pressures in the ultra-high gigapascal range are generated to drive a transformation into dense phases like lonsdaleite and diamond, thereby increasing the shock-wave velocity. A structurally textured, anisotropic nanographite matrix acts as a passive hydrodynamic waveguide. The pressure-dependent modification of sound velocities and the elastic anisotropy of the carbon layer lattice under these extreme conditions are utilized to mechanically absorb temporal and spatial ignition instabilities (jitter). This homogenizes the shock front for a highly symmetrical impact with high stagnation pressures onto the inner cryogenic capsule, ultimately achieving the required fusion hotspot conditions. This study outlines a transformative, material-based roadmap for laser-free fusion energy systems and identifies critical future research directions in the domain of programmable carbon and nanographite composite for extreme high-energy-density physics environments.

Evaluation of Mode II Fracture Energy in Adhesively Bonded Carbon Fiber-reinforced Polymer Laminates with Quad and Double-double Layups

Diego Schumacker dos Passos[1], Eduardo Martins Sampaio[1], Ranulfo Martins Carneiro Neto[2*] and Lucas Lisboa Vignoli[2]

[1]*University of State of Rio de Janeiro, Brazil*

[2]*Federal University of Rio de Janeiro, Brazil*

Abstract

In recent years, the demand for lightweight and high-performance structural materials has driven the widespread use of carbon fiber–reinforced polymer composites, particularly in the aerospace and offshore sectors, due to their high specific stiffness and strength. Nevertheless, a comprehensive understanding of the fracture behavior of adhesively bonded carbon fiber–reinforced polymer joints remain challenging, especially under different loading conditions. In this context, the assessment of mode II fractured toughness is of particular importance for predicting crack propagation and ensuring the structural integrity of bonded joints. Within this framework, the laminate stacking sequence plays a key role in governing the interlaminar properties of composite structures. Quad and double-double stacking configurations, although theoretically equivalent in terms of elastic modulus according to the Tsai criteria, may exhibit markedly different mechanical responses with respect to delamination resistance. Previous studies have shown that double-double layups tend to promote a more favorable stress distribution, leading to enhanced resistance to crack propagation. Accordingly, this work investigates three carbon fiber laminate configurations with distinct angular layups: (i) quad $[45/90/-45/0]_{2s}$, (ii) dd1 $[67.5/-22.5/22.5/-67.5]_4$, and (iii) dd2 $[67.5/22.5/-22.5/-67.5]_4$. The objective is to assess the practical equivalence of the elastic modulus among these configurations and to examine the influence of stacking sequence on the mode II critical fracture energy and the maximum load obtained from end-notched flexure tests. Mechanical testing is currently in progress.

Hydrogen Confinement in Ordered Porous Structures of Templated Carbon Materials

Rasmus Palm[1*], Iram Tufail[1], Miriam Koppel[1], Jaan Aruväli[1], Egert Möller[1], Nicholas P. Stadie[2], Emmanuel Osuagwu[2], Ove Korjus[3], Thomas C. Hansen[3], Jacques Ollivier[3], Ugne Miniotaite[4] and Martin Mansson[4]

[1]*University of Tartu, Taru, Estonia*

[2]*Montana State University, Bozeman, United States*

[3]*Institute of Laue-Langevin, Grenoble, France*

[4]*KTH Royal Institute of Technology, Stockholm, Sweden*

Abstract

Hydrogen adsorption in microporous systems is of interest for the fundamental understanding of interfacial phenomena and for energy storage, gas separation, and other applications. Templated carbon materials are excellent model materials with well-defined ordered porous and bulk structures. Zeolite-templated carbons (ZTCs) are of special interest for the possibility to control the presence of different heteroatom sites and, thus, investigate their influence on the structure and dynamics of the hydrogen adsorbed phase. To investigate the influence of different N-heteroatom sites on the formation of the hydrogen/deuterium adsorbed phase, *in situ* neutron powder diffraction and *in-situ* quasi-elastic neutron scattering were used with non-heteroatom-containing ZTCs containing dominantly graphitic and pyridinic N-heteroatom sites. The hydrogen confinement and self-diffusion inside the ZTCs porous structure are determined with *in-situ* quasi-elastic neutron scattering method. The temperature conditions at which an ordered adsorbed phase forms inside the porous structure are determined with deuterium as the adsorbate and with the *in-situ* neutron powder diffraction method. Thus, the influence of N-heteroatom sites on the formation of an ordered deuterium adsorbed phase and adsorbed hydrogen dynamics is presented and analyzed.

Engineered Biochar from Olive Mill Solid Waste as a Tunable Carbon Platform for Polyfluoroalkyl Substances Removal from Water

Sara P. Azerrad[1,2*], Shilat Parsha[1], Hassan Azaizeh[3] and Eyal Kurzbaum[1,3,4]

[1]*Shamir Research Institute, University of Haifa, Israel*

[2]*The Natural Resources and Environmental Research Center, University of Haifa, Israel*

[3]*Faculty of Sciences and Technology, Tel-Hai University of Kiryat Shmona, Galilee, Israel*

[4]*Department of Geography and Environmental Studies, University of Haifa, Israel*

Abstract

Olive mill solid waste, an abundant agro-industrial residue in Mediterranean regions, was converted into engineered biochar as a tunable carbon platform for the removal of persistent per- and polyfluoroalkyl substances (PFAS) from water. Biochar was prepared by pyrolysis followed by thermal or zinc/iron (Zn/Fe)-chemical activation to tailor surface area, pore structure, surface charge, and adsorption functionality. The materials were evaluated using two representative anionic PFAS with contrasting chain length and adsorption behavior: perfluorooctanoic acid (PFOA) and perfluorobutanoic acid (PFBA). Thermally activated biochar showed a clear preference for the longer-chain PFOA, achieving 69.4 ± 11.9% removal after 2 h, whereas PFBA removal was limited to 7.9 ± 3.4%. Zn/Fe modification substantially enhanced PFAS uptake. At pH 7, biochar-Zn/Fe achieved near-complete PFOA adsorption within 2 h (98.7 ± 0.1%), while PFBA removal increased from 32.7 ± 1.3% after 2 h to 51.3 ± 1.8% after 24 h. To elucidate the role of surface charge, biochar-Zn/Fe was further tested at pH 3, below its point of zero charge (pHzpc = 4.2), where the surface is positively charged. Under these conditions, PFOA was completely removed within 2 h, and PFBA removal increased markedly to 84.5 ± 1.2% after 2 h and 92.6 ± 0.3% after 24 h. The enhanced performance was attributed to the combined effects of developed porosity, hydrophobic interactions, and electrostatic attraction. Overall, olive mill solid waste-derived engineered biochar represents a sustainable, low-cost, circular-economy material for decentralized polishing of PFAS-impacted waters.

Graphene Oxide-enhanced Phase Change Composites for Thermal Management and Storage Applications

E.M. Anghe*, S. Petrescu, A. Neacsu, I. Atkinson, F. Papa and M. Tudose*

Institute of Physical Chemistry, Ilie Murgulescu of Romanian Academy, Bucharest, Romania

Abstract

The performance of miniaturized electronic devices is highly influenced by heat accumulation during operation and their service life. Using phase change materials represents one of the thermal management strategies. Since the most commonly used organic phase change materials are polymers with low thermal conductivity, the addition of thermally conductive fillers is required. Obtaining hybrid thermally conductive fillers with a dielectric shell covering the metallic core is a viable strategy for improving the thermal conductivity of polymer-based composites for thermal management applications and heat storage. Thus, graphene oxide (GO) facilitates heat transfer by forming continuous thermal networks while improving mechanical properties. Novel hybrid copper-GO fillers for thermal conductivity enhancement were obtained by a hydrothermal route. Filler dispersion and/or agglomeration, interfacial compatibility of fillers with the phase change materials (in this case polyethylene glycol (PEG6000) and matrices were a few parameters to adjust in order to improve the thermal conductivity of the resulting composites. Characterization of the hybrid GO-enhanced phase change composites was carried out by differential scanning calorimetry and thermal conductivity measurements, dynamic light scattering, Zeta potential, hydrogen temperature-programmed reduction, scanning electron microscopy, X-ray diffraction, and ultraviolet - and Vis-Raman spectroscopy. Thus, the obtained findings for copper@GO-PEG6000 are discussed in terms of GO interlayer spacing, "exfoliation", and restoring the graphene structure. Moreover, GO modifications of the degree of crystallinity and subcooling suppression of the phase change PEG6000 component ruled the thermal performance of the composites obtained.

Bio-based Pyrone–pyrrole Esters as Coupling Agents: A Novel Strategy for Grafting Reactive Moieties onto Carbon Black

D. Brighenti[1*], F. Magaletti[2], V. Barbera[1] and M. Galimberti[1]

[1]*Department of Chemistry, Materials and Chemical Engineering, Polytechnic University of Milan, Milan, Italy*

[2]*Pirelli SpA, Viale Piero e Alberto Pirelli, Milan, Italy*

Abstract

Sustainable mobility demands lower-emission tyre compounds and greener access to functional materials. This work addresses both via biobased chemistry. Carbon black (CB) nanofillers are essential for elastomer reinforcement, yet the filler-polymer interface creates a persistent trade-off between reinforcement and energy dissipation, the core of the tyre "magic triangle". 1) Reactive fillers forming covalent bonds with both the elastomer and the sulfur network can overcome this. 2) However, the traditional "pyrrole methodology" involves a Diels-Alder cycloaddition (air, 150 °C) that destroys the pyrrole ring, preventing its participation in vulcanization. 3) To resolve this, we designed "synergy molecules": bio-based esters, synthesized via Steglich esterification, combining a pyrrole subunit with a 2-pyrone moiety, derived from lignocellulosic biomass. Pyrroles are synthesized via solvent- and catalyst-free Paal-Knorr condensation of 2,5-hexanedione (from biobased 2,5-dimethylfuran) with primary amines. The 2-pyrone is obtained from mucic acid, retaining all six carbon atoms of its precursor (100% substrate carbon efficiency). 4) Both routes are scalable to kilogram quantities. With this strategy, the 2-pyrone anchors covalently to carbon black via mild Diels-Alder cycloaddition (Nitrogen gas, 130 °C), leaving the pyrrole ring intact. 5) Functionalization yields of 86.3% (Synergy A) and 92.0% (Synergy B) were achieved. During vulcanization, the tethered pyrrole integrates carbon black into the elastomer network. Carbon black/synergy B composites exhibit a reduced Payne effect and lower energy dissipation versus pristine carbon black, with lower rolling resistance and fuel consumption. This approach proves that green chemistry principles such as the use of biobased feedstocks, atom-efficient and solvent-free synthesis are fully compatible with high-performance elastomer composites.

Innovation in Topological Insulator based heterostructures for Room Temperature, Low Noise, Broad Band Infrared Photodetector Applications

Puja Dey[1,2*], Nitish Ghosh[1], Subhadip Paul[1], J.N. Roy[1,2] and Nibir K. Dhar[3]

[1]*Department of Physics, Kazi Nazrul University, Asansol, India*

[2]*Centre for Organic Spintronics and Optoelectronics Devices, Kazi Nazrul University, Asansol, India*

[3]*VCU College of Engineering, Virginia Commonwealth University, Richmond, USA*

Abstract

Innovation in topological insulators (TI), a new generation quantum materials exhibiting dissipation less charge transport, strong spin–orbit coupling, and spin–momentum–locked conductive surface states, has been aimed for the development of low noise, broadband infrared (IR) photodetector arrays at elevated temperatures. Investigation of direct current and alternating current transport properties on our fabricated indium tin oxide/TI (Bismuth selenide)/gold heterostructure revealed a bias voltage induced transition from a bulk insulating to a topological conducting surface state. This transition is probably because of fermi level shifting towards the Dirac point, with the conducting state retaining for at least 30 min. Positive photocurrent generation at near IR to mid-IR region, with photocurrent to dark current ratio of 56% and 1.6 × 106% for 5 nm and 58 nm TI thicknesses, respectively, was achieved using broadband IR light. Under 660 nm red laser light, a degradation of conducting topological state has been observed with the generation of negative photo response with an optimum photocurrent-to-dark current ratio of -70.48 % (5 nm TI) and -99.98 % (58 nm TI). Interfacial effects in our TI based heterostructures have been investigated through impedance spectroscopy, performed under dark, IR and red light amplification by stimulated emission of radiation illumination. High positive photosensitivity is further substantiated by an appreciable reduction in impedance magnitude nearly by 85% upon IR illumination. Likewise, negative photogeneration is confirmed with the high rise in impedance up to 6.6 x 104 % under red light amplification by stimulated emission of radiation illumination.

Acknowledgements: This material is based upon work supported by the Air Force Office of Scientific Research under award number FA2386-25-1 4052.

High Surface Area Catalysts for Enhanced Electrochemical Carbon Dioxide Reduction

Juqin Zeng[1,2*], Mitra Bagheri[1,2], Mario Gallone[1,2] and Candido Pirri[1,2]

[1]*Politecnico Polytechnic University of Turin, Turin, Italy*

[2]*Italian Institute of Technology – IIT, Genoa, Italy*

Abstract

To address the excessive carbon dioxide (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 mesoporous carbon supported nickel sulphide and ceria supported copper for selective production of carbon monoxide and methane, respectively. In addition, we also developed mesoporous organic metal frameworks for ethylene production. This work highlights the importance of high surface area of the catalysts to enhance the accessibility of the active sites.

Acknowledgements: This work is supported by the Clean Energy Transition Partnership Program (CET Partnership, 2024-2027, ELECTROMET, N. CETP23_00019).

An Experimental and Theoretical Study on Electronic Properties of Self-assembled 1,4-phenylenediacrylic Acid on Bilayer Graphite

Elaheh Mohebbi[1*], Eleonora Pavoni[1], Marina Petroselli[1], Cristina Minnelli[2], Luca Pierantoni[3], Davide Mencarelli[3], Martino Aldrigo[4], Masoud Seyyed Fakhrabadi[5], Emiliano Laudadio[1] and Pierluigi Stipa[1]

[1]*Department of Science and Engineering of Matter, Environment and Urban Planning, Marche Polytechnic University, Ancona, Italy*

[2]*Department of Life and Environmental Science, Polytechnic University of Marche, Ancona, Italy*

[3]*Department of Information Engineering, Marche Polytechnic University, Ancona, Italy*

[4]*National Institute for Research and Development in Microtechnologies, Ilfov, Romania*

[5]*School of Mechanical Engineering, College of Engineering, University of Tehran, Tehran, Iran*

Abstract

In this study, density functional theory calculations and ab initio molecular dynamics simulations were employed to expand the knowledge about the interaction of graphene and bilayer graphite surfaces with 1,4-phenylenediacrylic acid ($C_{12}H_{10}O_4$). We

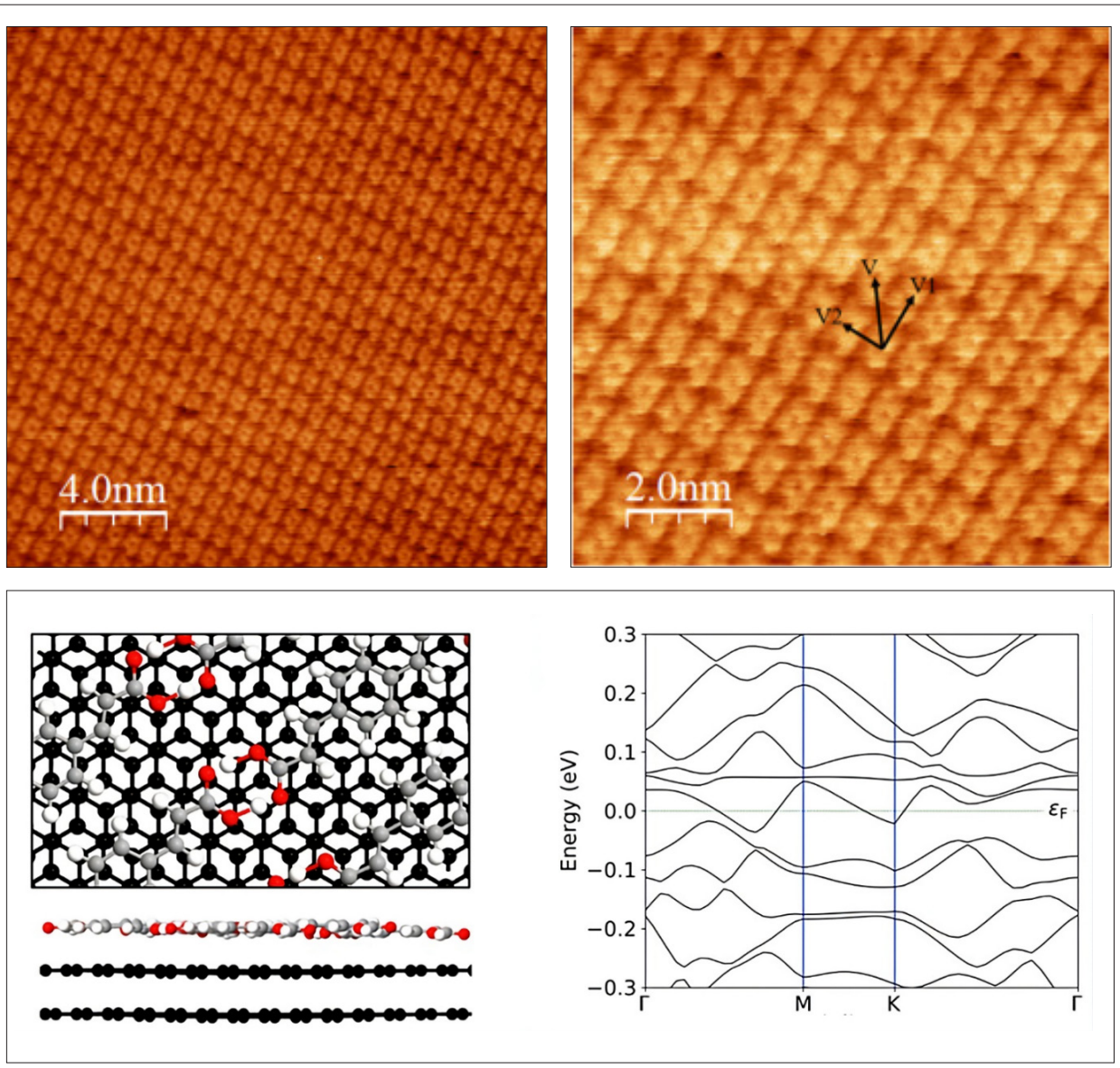


Figure 1: Scanning tunnelling microscopy images of the self-assembled 1,4-phenylenediacrylic acid ($C_{12}H_{10}O_4$) molecules on highly oriented pyrolytic graphite surface at two scales. The simulated top and side views of the $C_{12}H_{10}O_4$-layer, and its corresponding band structure on stacking structure of AB graphite.

proposed five modelled adsorbed structures from a single monomer to monolayer of $C_{12}H_{10}O_4$ organic molecules on graphene. Our density functional theory outcomes on assembled $C_{12}H_{10}O_4$ on graphene suggest that the magnitude of p-doping of graphene has increased by raising the lowest unoccupied molecular orbital energy level and the mixing of the molecular orbitals between the $C_{12}H_{10}O_4$ and graphene surface. The computations from the band structure calculations indicated a band gap of 0.0068 eV by the adsorption of 6 $C_{12}H_{10}O_4$ layer on the graphene, with valence energy of 0.0014 eV and conduction level of 0.0054 eV. The AB initio molecular dynamics calculations revealed that the modelled structures are reliable, since the molecules adopted the same displacements over time. The evaluation of the optical properties indicated the first peak intensity at 2.43 THz of $C_{12}H_{10}O_4$ on the graphene layer. Moreover, for all the adsorption structures, while a high dielectric constant has been observed for graphene, the real part of the dielectric constant and the dielectric losses values have been reduced from the monomer to layer $C^{12}H^{10}O^4$ on the graphene. Finally, the adsorption of $C_{12}H_{10}O_4$ layer on the AB stacking bilayer graphite has been considered to simulate the experimental scanning tunnelling microscopy image of self-assembled $C_{12}H_{10}O_4$ on highly oriented pyrolytic graphite surface. The zero-band gap has been predicted since the electronic structure of graphene near the K point varies by increasing its thickness (Figure 1).

Ecosystem Carbon and Nutrient Dynamics in *Pinus sylvestris* Forests after Clear-cutting in the Baltic Region

Iveta Varnagirytė-Kabašinskienė[1*], Dovilė Gustienė[2], Valentinas Černiauskas[1], Milda Muraškienė[1] and Aigars Indriksons[3]

[1]*Lithuanian Research Centre for Agriculture and Forestry, Lithuania*

[2]*Lietuvos Inzinerijos Kolegija Higher Education Institution, Lithuania*

[3]*Latvia University of Life Sciences and Technologies, Latvia*

Abstract

Scots pine (*Pinus sylvestris* L.) forests are key ecosystems of carbon and nutrient cycling in the Baltic region. Clear-cutting, a common forest management practice, substantially alters ecosystem structure and biogeochemical processes. This study examined changes in carbon and nutrient stocks in ground vegetation, forest floor, mineral soil, and deadwood across a Scots pine chronosequence in Lithuania. Study sites represented the *Vaccinium myrtillosum* forest type and included clear-cut and reforested stands aged 8 - 10, 15 - 20, 30 - 40, 70 - 80, and 101 - 130 years. Biomass of dominant mosses and vascular plants, forest floor and deadwood mass, and stocks of carbon, nitrogen, phosphorus, potassium, calcium, and magnesium were assessed in organic layers and mineral soil down to 40 cm depth. Clear-cutting led to substantial reductions in ground vegetation biomass and associated carbon and nutrient stocks. Forest floor carbon and nutrient stocks declined during early regeneration stages and recovered by 30 - 40 years, after which they remained relatively stable. In mineral soil, nutrient stocks increased shortly after harvesting and in young stands, then stabilized or decreased slightly in older stands. These results demonstrate that ground cover and soil layers respond differently to forest harvesting and recovery. Incorporating ground vegetation and forest floor parameters into forest inventories is essential for improving assessments of carbon ecosystem and nutrient dynamics.

Charge Transfer and Electron Injection Kinetics of Conjugated Versus Non-conjugated Porphyrin Sensitizers on Titanium Dioxide

Alvie Sin Voi Lo[*]

Faculty of Science and Technology, University of Malaysia Sabah, Kota Kinabalu, Malaysia

Abstract

Dye-sensitized solar cells are a promising low-cost, environmentally benign photovoltaic technology, in which porphyrins offer an attractive alternative to ruthenium-based sensitizers. The performance of a dye-sensitized solar cell is governed by the charge-transfer step: injection of the photoexcited electron from the dye into the conduction band (CB) of titanium dioxide (TiO_2). Here we examine how molecular structure governs this process for four porphyrin sensitizers — zinc-metalated, conjugated porphyrin, zinc-metalated, non-conjugated porphyrin, free-base, conjugated porphyrin and free-base, non-conjugated porphyrin — anchored on TiO_2. A uniform computational protocol was applied to all four systems, modelling the electronic structures with density functional theory/time-dependent density functional theory at the Becke, 3-parameter, Lee–Yang–Parr/6-31G(d) level (Gaussian09) and computing the injection rate constants (kinj) within Marcus-Hush theory, with the density of states of the TiO_2 CB treated as the accepting manifold. The calculated kinj are in close agreement with the experimental transient-absorption values in both magnitude and trend. The model shows that photoexcitation promotes an electron from the porphyrin

core into an acceptor orbital near the anchoring group; in the conjugated dyes, this orbital delocalizes along the linker toward the TiO_2 surface, whereas in the non-conjugated dyes, it remains localized on the macrocycle. In both cases, injections proceed into the manifold of TiO_2 CB states; no correlation was found between kinj and linker conjugation or metalation, indicating that the CB density of states, not any single molecular parameter, governs the injection rate. These results demonstrate that a unified density functional theory/time-dependent density functional theory-Marcus-Hush protocol, benchmarked against experiment, quantitatively captures charge transfer at the porphyrin/TiO_2 interface and offers a physically grounded basis for sensitizer design.

Poster Presentations

Controlled Functionalization of the 1,8-naphthalimide Core with Weak Nucleophiles: A Versatile Approach to Fluorescent π-conjugated Systems

Y. Zagranyarski[1*], M. Mutovska[1], K. Konstantinov[1,2], I. Zagranyarska[3], D. Sánchez[4], M. Allain[4], A. David[4], S. Angelova[5], S. Stoyanov[1] and C. Cabanetos[4]

[1]*Faculty of Chemistry and Pharmacy, Sofia University, Sofia, Bulgaria*

[2]*Faculty of Pharmacy, Medical University of Sofia, Sofia, Bulgaria*

[3]*Institute Organic Chemistry with Centre of Phytochemistry, Sofia, Bulgaria*

[4]*University of Angers, National Centre for Scientific Research, Angers, France*

[5]*Institute of Optical Materials and Technologies, Sofia, Bulgaria*

Abstract

Functionalized 1,8-naphthalimide derivatives represent an important class of π-conjugated compounds with widespread applications in fluorescence sensing, organic electronics, and bioactive systems. Despite significant advances in their synthesis, the selective modification of the naphthalimide core using weak nucleophiles remains challenging due to their low reactivity and competing side processes. Herein, we report a novel and efficient synthetic strategy for the controlled functionalization of the 1,8-naphthalimide core under mild, transition-metal-free conditions. The approach relies on the careful selection of the base and reaction temperature, enabling access to a diverse range of derivatives, including difluoro-, dialkoxy-, and mixed alkoxy–fluoro and alkoxy–hydroxy substituted products. Mechanistic investigations suggest a Halex-type process involving initial formation of peri-difluoro intermediates, followed by nucleophilic aromatic substitution with weak nucleophiles such as alcohols. The developed methodology demonstrates high efficiency, with short reaction times (up to 30 min), scalability to gram quantities, and excellent yields (80 - 97%). Importantly, fine-tuning of the reaction conditions allows precise control over the substitution pattern. The synthesized compounds were thoroughly characterized and exhibit typical photophysical properties of naphthalimide systems, including absorption in the near-ultraviolet region and strong blue–cyan emission. A pronounced dependence of the optical properties on the substitution pattern was observed, highlighting the potential of this approach for tailoring electronic and fluorescence behavior. Overall, this work provides a practical and versatile route to functional 1,8-naphthalimide derivatives from readily available starting materials, opening new opportunities for their application in sensing, photonic materials, and biomedical fields.

Acknowledgements: Authors are grateful to the Bulgarian National Science Fund project NSF KP 06-H79/8.

Design and Synthesis of π-conjugated Indolocarbazole Derivatives as Functional Organic Materials

Monika Mutovska[1*], Yulian Zagranyarski[1], Konstantin Konstantinov[1], Kalina Krastilova[1], Izabela Taneva[1] and Silvia Angelova[2]

[1]*Faculty of Chemistry and Pharmacy, Sofia University, Sofia, Bulgaria*

[2]*The Institute of Optical Materials and Technologies, "Academician Jordan Malinowski", Sofia, Bulgaria*

Abstract

Indolocarbazole-based π-conjugated systems have attracted increasing attention due to their unique electronic properties and potential applications in organic electronics and photonic materials. In this study, we report the design, synthesis, and characterization of novel indolocarbazole derivatives as functional organic materials with tunable photophysical properties. A series of indolocarbazole-based compounds were synthesized using efficient synthetic approaches, including transition metal-

catalyzed cross-coupling reactions. Structural modifications were introduced through the incorporation of electron-donating and electron-withdrawing substituents, enabling precise control over the electronic structure and extension of π-conjugation. The photophysical properties of the synthesized compounds were systematically investigated, revealing strong absorption in the ultraviolet–visible region and tunable emission behavior. Particular attention was given to the role of molecular design in promoting intersystem crossing and the formation of triplet excited states, which are crucial for applications involving phosphorescence and thermally activated delayed fluorescence. The results demonstrate that indolocarbazole-based systems represent a promising platform for the development of advanced metal-free organic materials. Their tunable electronic and photophysical properties make them attractive candidates for applications in organic light-emitting diodes, sensing, and optoelectronic devices.

Effect of Halloysite Nanotubes on the Mechanical and Thermal Performance of Epoxy and Bio-based Polyurethane Adhesives

Ranulfo Martins Carneiro Neto[1*], Matheus Viana Castilho Bichara[1], Ian Pellinca Braga Caetano[1], Jorge Amim Júnior[1], Eduardo Martins Sampaio[2] and Mariana Banea[3,4]

[1]*Federal University of Rio de Janeiro, Rio de Janeiro, Brazil*

[2]*University of State of Rio de Janeiro, Rio de Janeiro, Brazil*

[3]*Federal Center of Technological Education, Rio de Janeiro, Brazil*

[4]*Aveiro Institute of Materials, University of Aveiro, Portugal*

Abstract

Nanoreinforcement of structural adhesive materials has proven to be an effective strategy to enhance mechanical performance by improving stress transfer and interfacial interactions. This study investigates the effect of halloysite nanotubes (HNT) on two distinct adhesive formulations: a conventional epoxy resin and a bio-based polyurethane derived from castor oil. The main objective is to evaluate the reinforcing efficiency of HNT in a renewable adhesive and to compare its performance with that of a traditional epoxy system. Both materials were modified with different HNT contents and primarily characterized through tensile testing to assess changes in strength and stiffness. Complementary thermal analyses were performed to support the interpretation of the mechanical response and to identify modifications in thermal stability and transition behavior associated with nanotube incorporation. The bio-based polyurethane showed a strong response to nanofiller addition, reaching an increase in tensile strength of approximately 26% and nearly doubling its elastic modulus at an optimal loading of 1 wt% HNT. These improvements indicate efficient load transfer between the polymer matrix and the nanotubular reinforcement. The epoxy adhesive also exhibited mechanical enhancements, although to a lesser extent, accompanied by shifts in thermal transitions consistent with reduced molecular mobility. Overall, the results demonstrate that halloysite nanotubes effectively improve the mechanical performance of both adhesive systems, with more pronounced gains observed in the bio-based polyurethane. The findings reinforce the potential of nanoreinforced renewable adhesives as competitive alternatives for structural bonding applications.

Kraft Lignin Fractionation Enables Structure–property Control in Hard Carbon Anodes for Sodium-ion Batteries

Jonathan Berg[1*], Arpa Ghosh[1], Atte Mikkelson[1], Olli Sorsa[1], Kristoffer Meinander[2], Martin Kögler[1], Anna Kalliola[1] and Chamseddine Guizani[1]

[1]*VTT Technical Research Centre of Finland Ltd, Espoo, Finland*

[2]*Department of Bioproducts and Biosystems, School of Chemical Engineering, Aalto University, Aalto, Finland*

Abstract

Kraft lignin is an abundant yet underutilized bio-aromatic resource with strong potential as a precursor for hard carbon anodes in sodium-ion batteries. However, its complex structure often limits control over the properties of the resulting carbons. The inherent heterogeneity of lignin leads to inconsistent material properties, reducing process control and hindering efficient lignin valorization. Refining lignin into more homogeneous fractions therefore offers a viable strategy to reduce this heterogeneity and enable improved modification of lignin characteristics for downstream applications. In this work, Kraft lignin was fractionated using aqueous ethanol to produce precursors with distinct molecular differences, providing a controlled method for generating hard carbons with tailored physicochemical properties. These precursor-level modifications enable systematic investigation of how lignin structural features govern hard carbon structure and electrochemical performance. The results show that

precursor-level lignin modification enables direct control over hard carbon properties, allowing electrochemical performance to be linked to lignin structure and chemistry, rather than carbonization conditions alone. Specifically, variations in lignin molecular weight and compositional features were directly correlated with the structure and properties of the resulting hard carbons, with these parameters showing strong correlations with hard carbon microstructure. By linking these lignin features to subsequent electrochemical behavior, the results establish targeted modification of Kraft lignin as a rational pathway for controlling hard carbon properties and optimizing performance in sodium-ion batteries.

Received: October 30, 2026 **Accepted:** November 02, 2026 **Published:** November 06, 2026

Citation: Proceedings of the 6th International Conference on Carbon Chemistry and Materials (CCM-2026). *USG Proc J* 2(Suppl 18): S1-S12.

Copyright: © 2026. This is an Open Access article distributed under the terms of the Creative Commons Attribution 4.0 International License (CC-BY) (http://creativecommons.org/licenses/by/4.0/) which permits commercial use, including reproduction, adaptation, and distribution of the article provided the original author and source are credited.