2D Materials
Room 122 - Session 2D+EM+QS-ThA
2D Materials: Applications

Moderators: Matthias Batzill, University of South Florida, **Fei Yao**, University at Buffalo

2:15pm **2D+EM+QS-ThA-1 Tuning Functionality: Graphene Oxide (GO)/Few Layers Graphene (FLG) Membranes for Water Treatments**, *J. Flores-Arciniega, S. Acosta, H. Ojeda-Galván,* CICSaB, Universidad Autónoma de San Luis Potosí, Mexico*; B. Yáñez-Soto,* Instituto de Física, Universidad Autónoma de San Luis Potosí, Mexico*; **Mildred Quintana**,* Facultad de Ciencias, CICSaB, Universidad Autónoma de San Luis Potosí, Mexico

Graphehe oxide (GO) and few layer graphene (FLG) are exciting platforms with a huge potential for developing new advanced technologies. The unique combination of properties, such as high specific surface area, charge transport, chemical stability, mechanical strength, flexibility, high electrical and thermal conductivity, make them the ideal substrates for several applications in water remediation. Here, I will describe the synthesis and processing of GO and FLG, their characterization, handling, and performance towards advanced membranes for water treatments. In particular, we aim to address the production of van der Waals heterostructures for the development of micro and nanofiltration membranes for bacteria removal, organic molecule adsorbents, and desalination. The properties of 2D materials modulate mechanical and chemical stabilities, while active sites are created by the effective construction of van der Waals heterostructures allowing charge and mass transfer producing cost-effective and highly efficient membranes for water purification.

Acknowledgments

CONAHCYT basic science project CB-A1S-8817 and Sinergía-UNAM 1564464, JF thanks to CONAHCYT for Ph.D. scholarship No. 744836. The authors want to thank Laboratorio Nacional de Ingeniería de la Materia Fuera de Equilibrio (LANIMFE), for the use of equipment and technical support.

2:30pm **2D+EM+QS-ThA-2 New Graphene Oxide-based Nanozymes for Cancer Theranostics**, *A. Foti, S. Sciacca, G. Tranchida, S. Petralia, R. Fiorenza, S. Scirè, L. D'Urso, C. Bonaccorso, A. Fraix,* University of Catania, Catania, Italy*; A. De Bonis,* University of Basilicata, Italy*; **Cristina Satriano**,* University of Catania, Catania, Italy

Graphene oxide (GO) and plasmonic nanoparticles (Pd, Au, Ag NP) nanocomposites were scrutinized in this study as combinative multimodal platform with enzyme-like, photocatalytic and photothermal properties. A green one-pot chemical reduction method by using D-glucose as reducing agent and polyvinylpyrrolidone (PVP) as capping agent, was used to fabricate the hybrid 2D platforms (NP@G) and the reference plasmonic nanoparticles alone. Different molar ratios of the metal precursor/reducing agent were tested to get the best results in terms of stability, reproducibility and reaction yield, as monitored by the plasmonic band of the NPs. The physicochemical characterization of the morphological, compositional, structural, and functional properties of NP@G nanozymes was carried out in terms of X-ray photoelectron spectroscopy (XPS), X-ray diffraction (XRD), transmission electron microscopy (TEM), UV-visible, Raman spectroscopy, Fourier Transformed Infrared Spectrocopy (FTIR), thermocamera, atomic force microscopy (AFM), dynamic light scattering (DLS) and zeta potential (ZP). The enzyme-like activity was tested by colorimetric assays in a cell-free environment to confirm the maintenance of the nanozymes capability in the NP@G samples.The photocatalytic properties were tested in the H_2 evolution by water splitting reaction under simulated solar light. Further, the nanoplatforms were tested in prostate cancer cells (PC-3 line) in terms of cytotoxicity, cell migration and reactive oxygen species (ROS) production, to prove the antitumoral action of the developed nanomedicine. Cell imaging by laser scanning confocal microscopy (LSM) demonstrated the theranostic capability of the developed platforms, including dynamic processes at the level of sub-cellular compartments.

Acknowledgements: ADB and CS acknowledge the financial supported by MUR in the framework of PRIN2022-PNRR call under project CoMu4CaT.

2:45pm **2D+EM+QS-ThA-3 Graphene and Copper Nanoparticles Based Electrochemical Sensors for the Detection of Glyphosate in Water**, ***Uswah Yasin**, F. Torrisi,* University of Catania, Italy

Glyphosate is commonly used as a herbicide to control weeds in agricultural and non-agricultural applications (Carretta, et al. J. Chromatography. A 1600, 2019), resulting in significant adverse impacts on the environment, especially contaminated soil and water, with potential effects on human health (Richmond, AESS 8, 2018). Such environmental threat recently triggered the development of enhanced and scalable glyphosate sensing technologies.

Commercial sensors for glyphosate based on gold nanoparticles (AuNPs), silver nanoparticles (AgNPs), quantum dots, show a sensitivity ranging from 0.88 μM to few pM (Zúñiga, et al. Water 14, 15, 2022). Graphene is an excellent material for sensing applications (Fenech-Salerno, et al. Nanoscale 15, 7, 2023) (Schedin, et al. Nat. Mater 6, 9, 2007). Due to the high mobility, large surface area, high mechanical strength, and chemical stability, graphene provides a versatile platform for the detection of a wide range of analytes, including glyphosate. For the detection of glyphosate, graphene-based sensors can achieve a high sensitivity of the order of 0.30×10^{-12} M (Gonçalves, et al. Mater. Today Commun. 36, 2023). In addition, graphene inks enable a large range of printed, sustainable and flexible devices (Carey, et al. Nat. Commun. 8,1, 2017).

Here, we present the preparation of a glyphosate sensor based on graphene and Cu nanoparticles, deposited by a scalable spray-coating process on flexible substrate, such as polyimide (PI) and polyethylene terephthalate (PET). The graphene ink is prepared by liquid phase exfoliation, reaching a graphene concentration of ~ 0.7 mg/ml. The spray-coated graphene ink resulted in electrodes with a sheet resistance of ~ 240 Ω/☐, subsequently spray coated with Cu nanoparticles synthesized using Pulsed Laser Ablation in Liquid (PLAL), with the concentration of 12.5 μg/ml, to form the Graphene/Cu nanoparticle (G:Cu) electrode.

The concentration of glyphosate was determined by Multiple Cyclic Voltammetry (CV) using the G:Cu electrode as the working electrode in a glass electrochemical cell loaded with a solution of glyphosate was prepared in Milli-Q water. The CV curve of G:Cu showed the presence of a redox reaction related to the oxidation states of copper ($Cu \rightarrow Cu^{2+}$), compared to a plain graphene electrode, thereby affirming the sensing efficacy of the glyphosate sensor.

Our G:Cu sprayed sensor offers a flexible, sustainable, and scalable solution to detect glyphosate with excellent selectivity and sensitivity making it the perfect approach to address the need for accurate and efficient monitoring of glyphosate contamination in environmental and agricultural settings.

3:00pm **2D+EM+QS-ThA-4 Engineering Novel Hybrid Membranes for Battery Separators from Sustainable Sources**, ***Suvash Ghimire**, P. Makkar, M. Islam, K. Mukhopadhyay,* University of Central Florida

The surge in device use in transportation, biomedical sectors, and other industries is escalating at an alarming rate, coupled with grave concerns about pollution and global warming that underscores the urgency for developing efficient, safe, and environmentally friendly energy storage devices. There is a growing urgency to reduce planet-warming pollution through mining and other activities at the federal level to drop carbon emissions by half this decade and reach close to zero by the middle of the century to prevent some of the most devastating effects of climate change. Research groups worldwide are developing metal-based substitutes that address sustainability by eliminating the use and generation of hazardous substances during the synthesis and developing cheap, recyclable substitutes for electrode materials, electrolytes, membranes, and separators that are the pivotal components of energy storage devices.

Materials and their interfaces play an essential role in energy storage devices by facilitating ion transports and impeding short circuits by separating anode and cathode. Ion exchange membranes have broad applications in water electrolysis, fuel cells, and flow batteries. To date, Nafion® membranes and polyolefin-based separators are considered the industrial standards due to their excellent proton conductivity and high chemical stability. However, high cost, poor strength, shrinkage at high temperatures, and use of fluorinated chemicals hinder their widespread use. Therefore, there is an urgent need to develop membranes that can be alternatives to existing membranes without compromising the cost and environmental impact. Leveraging their porosity, properties, low cost, and thermal and chemical stabilities, clay-based membranes could be a new alternative for new-generation materials for such applications.

Our research presents a novel pathway for developing flexible and durable hybrid clay membranes by modifying them with zwitterions. The ionic conductivity of the membranes, measured using electrochemical impendence spectroscopy in a non-aqueous electrolyte solution, was found to be in the range of 10^{-4} S/cm, which is comparable to the ionic conductivities of related membranes used in electrochemical energy storage devices; this is a significant new development considering clays are insulators. Our study exhibits a new avenue to engineer highly efficient ion-conducting membranes with high thermal stability (300 °C) that can provide an efficient and recycle-free approach to developing a new generation of separators from sustainable sources for energy applications, especially for battery technology.

3:15pm **2D+EM+QS-ThA-5 Unveiling Composition-Structure Relationships for the Discovery of Novel High-Entropy 2D Materials Using the Mixed Enthalpy-Entropy Descriptor***, **Dibyendu Dey,*** University of Central Florida*; O. Ogunbiyi,* University of Missouri*; B. Ball,* University of Central Florida*; L. Liang, M. Zachman,* Oak Ridge National Laboratory*; Y. Yang,* University of Missouri*; L. Yu,* University of Central Florida

High-entropy two-dimensional materials (HE-2DMs) represent an emerging class of materials that show promise for numerous functional applications. These materials inherit the distinctive features of conventional 2D materials, such as reduced dimensionality, exceptional flexibility, and a large surface-to-volume ratio, while introducing a high configurational entropy of mixing to the system. Despite their immense potential, the experimental realm of HE-2DMs has thus far been limited to a few materials, leaving the complex interplay between their composition, structure, and synthesizability largely unexplored. In this work, by utilizing the Mixed Enthalpy Entropy Descriptor (MEED) [**1**], the material space of high-entropy 2D chalcogenides, including Group IV (Ti, Zr, Hf), Group V (V, Nb, Ta), and Group VI (Cr, Mo, W) metals in their 2H, 1T, and 1T' phases, has been systematically explored. MEED uniquely encapsulates the chemical and structural attributes critical for synthesizing HE-2DMs in their diverse polymorphs, demonstrating capabilities beyond any existing descriptor. Guided by MEED predictions, several top-candidate high-entropy tellurides and selenides, which exhibit extraordinary potential for applications in flexible electronic devices and advanced batteries, have been synthesized.

Acknowledgments: This work is supported by the US Department of Energy (DOE) Basic Energy Sciences (BES) under Award Number DE-SC0021127.

Reference:

1. Dibyendu Dey, Liangbo Liang, Liping Yu, Journal of the American Chemical Society 146, 5142 (2024).

3:30pm **2D+EM+QS-ThA-6 Antenna-Coupled Magic-Angle-Twist-Graphene Josephson Junction Millimeter Wave Detector***, **David Castro,*** University of Central Florida

We designed a sensitive detector of THz and mm waves using an antenna-coupled magic-angle-twist-graphene Josephson junctions. Magic angle twisted bilayer graphene superconducts at a transition temperature of ~2K. We can create a lateral Josephson junction by selectively gating different sections of a single sheet of magic angle graphene. The detection mechanism in our design is based on the change in maximum zero-voltage DC current in response to an applied AC signal at the junction. We expect it to be faster than bolometric detection mechanisms while maintaining high sensitivity. We determined that the bowtie antenna would work best for this device by using finite element electrodynamic simulations. We estimated the responsivity, noise-equivalent-power, and the prospects for single-photon detection. This detector device can be used in the future for sensing applications and quantum information systems.

Acknowledgments

This work was supported by U. S. Army OSD Phase II STTR contract W911NF23C0027 and bymatching funds from the Florida High Technology Corridor (I-4) Program.

3:45pm **2D+EM+QS-ThA-7 Antenna-Coupled Graphene Josephson Junction THz/mm-wave Detector***, **Rachid Ben Khallouq,*** University of Central Florida

We will discuss design, manufacturing processes, response characteristics, and tolerance to twist-angle variations of antenna-coupled Josephson-junction detectors fabricated from magic angle graphene tailored for detecting mm-wave and THz radiation. We find that Josephson junctions realized in magic angle graphene exhibit exceptionally high dynamic resistance at the peak zero-voltage current. When a small microwave voltage is applied across the junction, it induces a change in the voltage-current correlation, resulting in a notable DC output voltage. External radiation can energize a suitable antenna, generating the required AC voltage across the junction. These detectors operate via a non-thermal mechanism, offering the potential for both speed and sensitivity. They display a bolometric response, with an estimated temperature coefficient of resistance of 300%/K. We will show different designs and detection mechanisms and compare them to other technologies.

This work was supported by U. S. Army OSD Phase II STTR contract W911NF23C0027 and bymatching funds from the Florida High Technology Corridor (I-4) Program.

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