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FOREWORD

On behalf of the Organising and the International Scientific Committees we take great pleasure in welcoming you to Abu Dhabi (UAE) for the 1st edition of the Innovative & Industrial 2D/Advanced Materials Summit & Expo (I2DM2024). This cutting-edge International Summit will bring together world leaders, prominent researchers, and industry visionaries to explore and unlock the boundless potential of Advanced Materials.

I2DM2024 Highlights:

- Expected attendance: 275 participants in-person
- 60 Plenary, Keynote & Invited Speakers
- Nearly 60 oral contributions
- 14 Exhibitors
- 5 Parallel Workshops covering the whole value chain of "Advanced Materials innovation"
- Rounds tables to engage with industry leaders, potential partners, and investors to build valuable connections
- Industrial Forum to get an updated understanding of Advanced Materials based technologies from worldwide industries
- B2B forum (Brokerage event) to encourage companies, universities, investors, and research centers to foster technical cooperation in the Advanced Materials sector

We are also indebted to the following Scientific Institutions, Companies and Government Agencies for their help and/or financial support:
Graphene Composites, Intratomics, Technology Innovation Institute (TII), Constructor Tech, Strata, Sanad, Levidian, XPANCEO, Graphmatech, Abu Dhabi Convention and Exhibition Bureau and Khalifa University of Science and Technology.

We also would like to thank all the exhibitors, speakers and participants that join us in-person this year.

We truly hope that I2DM2024 serves as an international platform for communication between science and business.

Hope to see you again in the next edition of the Innovative & Industrial 2D/Advanced Materials Summit & Expo (I2DM2025) in Abu Dhabi (UAE).

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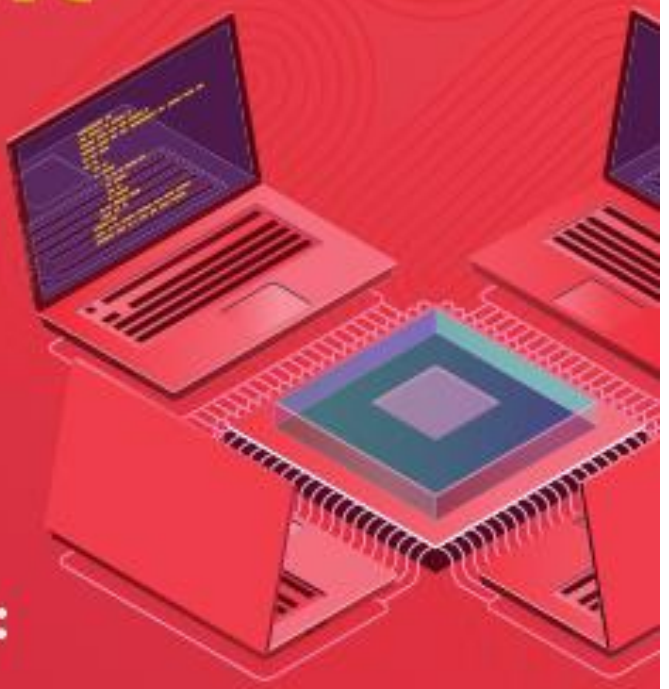

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www.phantomsnet.net

Molecular Matter under 2D Confinement

Andre Geim
University of Manchester, UK
Andre.K.Geim@manchester.ac.uk

It is now possible to create angstrom-scale channels that can be viewed as if one or a few atomic planes are pulled out of a bulk crystal leaving behind a two-dimensional space. I shall overview our experiments on this subject, which covers the properties of gases, liquids and ions under the extreme confinement.

High Precision Electrohydrodynamic Printing and Application to 2D Materials

Doyoung Byun

Department of Mechanical Engineering, Sungkyunkwan University, Suwon-Si, Gyeonggi-do, Republic of Korea.

ENJET Co. LTD, Suwon-Si, Gyeonggi-do, Republic of Korea.

dybyun@skku.edu

Abstract

Printing techniques, particularly inkjet methods, offer promising solutions for high-resolution manufacturing due to their additive nature, design flexibility, compatibility with large-area substrates, and cost-effectiveness. However, conventional inkjet printing, which relies on thermal or acoustic droplet ejection, is limited to a resolution of ~20–30 μm, constrained by droplet size and placement errors. While lithographic-based techniques can assist in creating high-resolution features, they require additional processing steps.

In contrast, electrohydrodynamic (EHD) printing uses electric fields to drive fluid flow, enabling sub-micron precision and patterning at scales below 1 μm. This technique allows for intricate geometries and is particularly well-suited for high-resolution electronics applications, such as the printing of electrodes and complex circuits. EHD printing surpasses the resolution limitations of conventional techniques without necessitating additional patterning steps, representing a new frontier in advanced manufacturing.

EHD printing is currently used to create high-precision patterns from 2D materials and metals, including silver, graphene, transition metal dichalcogenides (TMDs), MXenes, and van der Waals heterostructures. By optimizing key parameters such as applied voltage, nozzle geometry, substrate interaction, and ink rheology, nanoscale features with high uniformity and minimal defects can be achieved. Ongoing research demonstrates its potential for next-generation flexible electronics, sensors, and energy storage devices.

Moreover, the performance of EHD-printed 2D material-based devices—such as field-effect transistors (FETs), photodetectors, and supercapacitors—has been demonstrated, highlighting the superior device performance achievable through precise material deposition. This positions EHD printing as a versatile and scalable method for advanced 2D material systems, driving innovation in nanotechnology and flexible electronics.

3D printing functional nanoporous membranes and separation materials

Ludovic F. DUMEE, Hari Balakrishnan, Laura Carvalho, Robel Tekle, Hassan Arafat (Arial 10)
Khalifa University, Research and Innovation Center on 2D Nanomaterials (RIC2D), Abu Dhabi, United Arab Emirates
Ludovic.dumee@ku.ac.ae

Abstract

Over the past 20 years, 3D printing technologies have emerged as innovative tools to generate macro-porous materials, with potential in complex structures impossible to otherwise develop by traditional manufacturing. More recently, advanced composite materials have been developed at the mili and micro scale following progress in new polymers and resins formulations as well as greater resolution control for both Fused Deposition Modelling and Dynamic Light Polymerisation. Breaching the micron-scale barrier, to generate nano-porous materials has however remained to date a major challenge, due to either rheological limitations or minimum printable pixel size achievable. New strategies arising from polymer monoliths development have however emerged to generate ultra-porous materials, with macron-sized thicknesses and yet nanoscale pores. Our team has developed innovative strategies based on advanced resins formulations to print nano-porous membranes, and nano-textured catalysts as well as adsorbents. In this presentation, the feasibility to develop complex 3D membrane architectures as well as functional 2D nanomaterials composites with this novel process at scale will be demonstrated for a range of chemistries and applications. Nanocomposite structures with excellent nano-load distributions and incorporation into porous polymeric matrixes are critical to achieving scale of production and roll-to-roll 3DP functional films production will also be demonstrated. In this presentation, the development of nanoporous membranes with near isoporous structures with pores ranging from as low as 10 nm and up to hundreds of nanometers will be demonstrated. Functional complex 3D structures, showcasing the potential of various ranges of nanomaterials directly into the membranes will be showcased with nanosheets and nanoparticles to generate photo-catalytic and electrocatalytic membrane reactor systems, allowing for simultaneous filtration across the pores and reactions to occur at the membrane surface. The scalability of the approach will also be demonstrated to produce at scale (few meters long) consistent membranes by 3D printing.

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Twintronics of van der Waals ferroelectrics

Vladimir Falko
National Graphene Institute, University of Manchester, Booth St East, M13 9PL, UK
vladimir.falko@manchester.ac.uk

Over the recent years, several studies have established ferroelectric properties of rhombohedral transition-metal dichalcogenides (TMD), both grown as bulk crystals and assembled into twisted bilayers and multilayers [1-5]. For bilayers assembled from monolayer TMD crystals with parallel orientation of unit cells, lattice reconstruction (characteristic for small-angle twisted bilayers [6,7]) results in the out-of-plane polarised ferroelectric domains and networks of domain walls, switchable by mutual sliding of the monolayers, prompted by an out-of-plane electric field [3], manifested by the hysteretic field-effect transistor [4] and tunneling FET [8] operations, and readable optically by the linear Stark shift of the interlayer excitons [9].

In bulk 3R-TMD crystals, groups of layers with the same stacking order appear as three-dimensional twins separated by planes of twin boundaries. Here, we propose [10] the formation of two-dimensional (2D) electron/hole gases at twin boundaries, analyse their stable density in photo-doped structures, which appears to be in the range of $n^{*}\sim 8\times10^{12}cm^{-2}$ for electrons at both intrinsic mirror twin boundaries in bulk crystals and twisted twin boundaries in structures assembled from two thin mono-domain films. We also predict 'magic' values of twist angles between the assembled twins, for which the commensurability between the accumulated carrier density, n^{*}, and moiré pattern would promote the formation of a strongly correlated state of electrons, such as a Wigner crystal.

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Figures

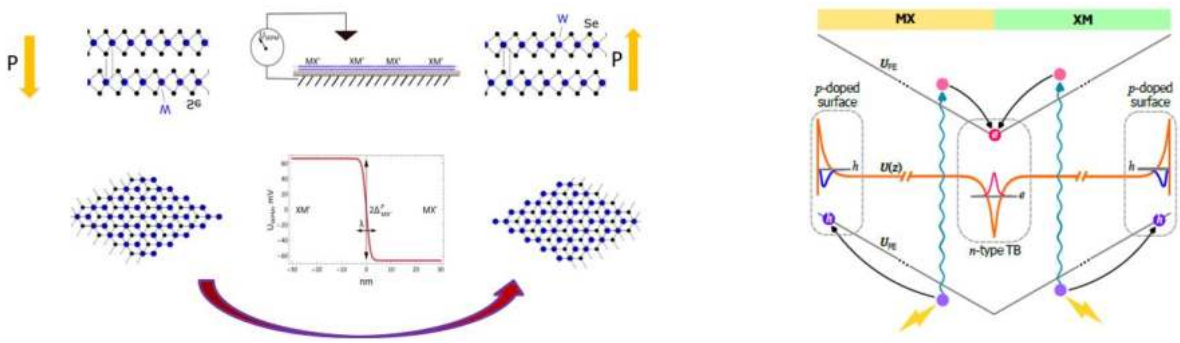

Figure 1: Left: interfacial ferroelectric polarisation, switchable by sliding. Right: electron accumulation at the planes of twin boundaries (internal or twistronic) in thin films of rhombohedral transition metal dichalcogenides.

Organic 2D Membranes in Emerging Energy Devices

Xinliang Feng
[a] *Max Planck Institute of Microstructure Physics*
[b] *Technische Universitaet Dresden*
Xinliang.feng@tu-dresden.de

In the pursuit of sustainable energy solutions, the advancement of novel materials that enhance performance while minimizing environmental impact is of paramount importance. This is particularly true with regard to the development of membrane technologies. Significant efforts have been made to go beyond the conventional polymer membranes. Consequently, the 2D membranes with a laminar transport mechanism offer distinctive prospects due to their well-defined ion transport channels. Nevertheless, the transport pathway of laminar transport would remain relatively lengthy and predominantly influenced by the sheet size and the presence of defects or grain boundaries in the 2D materials with their stacked structures.
In this lecture, we will focus on organic 2D membranes as a novel type of membranes, with a particular focus on their potential for the development of innovative energy devices. These materials are distinguished by their molecular thinness and extensive lateral dimensions, which afford precise control over structural features such as pore size, thickness, stacking structures, and functional group positioning. Two-dimensional polymer thin films represent the most significant category of organic 2D membranes. We will commence with the presentation of the bottom-up synthesis methods, which employ on-water surface chemistry to program the supramolecular assembly of monomers on the water surface. This is the crucial step in guiding the subsequent 2D polymerization and formation of crystalline 2D framework structures. Specific attention will be devoted to the role of these membranes in energy storage and conversion devices, including batteries and osmotic power generators. In this context, the unique and selective ion transport properties of organic 2D membranes towards various metal and proton ions will be particularly discussed, underscoring their potential to transform energy device technology.

Scalable Synthesis of MXenes

Yury Gogotsi
A.J. Drexel Nanomaterials Institute, and Department of Materials Science and Engineering, Drexel University, Philadelphia, PA 19104, USA
Gogotsi@drexel.edu

2D carbides, nitrides, and carbonitrides of early transition metals known as MXenes are among the few nanomaterials that have jumped into the limelight not only because of their exotic structure, an infinite number of possible compositions, or attractive properties but also because of numerous practical applications [1]. The family of MXenes has been expanding rapidly since the discovery of Ti_3C_2 at Drexel University in 2011. This presentation will describe the state of the art in manufacturing those new 2D materials and their delamination into single-layer 2D flakes and assembly into films [2-4]. The most common published processes for MXene synthesis include:

- Aqueous and non-aqueous HF etching of MAX phases, M_2A_2X and other layered precursors
- Aqueous HCl/HF, HCl-LiF (NaF or other fluoride silts), or NH_4HF_2
- Electrochemical etching in aqueous fluoride or chloride solutions
- Alkali etching (autoclave assisted)
- Supercritical CO_2 solution etching
- Halogen etching of MAX phases (solution or high-temperature gas)
- Molten salt etching of MAX (elevated temperatures of over 600°C)
- CVD synthesis from metal chlorides and methane
- Topochemical transformation of 2D oxides, transition metal chalcogenides, or graphene/graphite

The synthesis method largely determines the surface chemistry of the material. The versatile chemistry of the MXene family renders their properties tunable for a large variety of energy-related, electronic, optical, biomedical, and other applications. In particular, the applications of MXenes in electrochemical energy storage and harvesting, electrocatalytic water splitting and water purification/desalination are promising [1]. However, MXene antennas, sensors, actuators, epidermal and implantable electronics as well as coatings for EMI shielding and thermal regulation are equally attractive.

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Multifunctional 2D Composites for the Energy Transition

Ian Kinloch,
University of Manchester, National Graphene Institute and Henry Royce Institute, Manchester, UK
Ian.kinloch@manchester.ac.uk

The energy transition requires a new generation of materials to deliver high performance at low weight. This transition is made more difficult with traditional performance materials such as fluoropolymers becoming restricted due to environmental concerns and challenges in the environmental cost of producing and recycling materials. The exceptional combination of mechanical, electrical, barrier and thermal properties of 2D materials make them ideal to address these challenges, with composites being used to translate their properties to the bulk scale [1,2].

Herein, we will explore the fundamental design rules for 2D material composites using a combination of ideal experimental systems and simulation to understand the role of flake size, surface chemistry, dispersion etc. We will also show how 2D materials can work in harmony with conventional filler materials (e.g. glass fibre, carbon black etc) to enhanced properties [3] and how these properties are effect by recycling. The translation of these rules to produce advanced composite materials will be exemplified using electrical and thermal conductivity in thermosets and thermoplastics, EMI shielding [4], thermoelectric [5], hydrogen barrier properties for gas cylinders [6], new fluorine-free elastomeric and ultra-high molecular weight polymeric seals [7], and low friction metal surfaces [8,9].

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Two-dimensional Materials: Films and Lattices

Abdallah Hamouda, Baosong Li, Abdullah Solayman, Kishor Shingare, **Kin Liao**
Khalifa University, Abu Dhabi UAE

Kin.liao@ku.ac.ae

Two-dimensional (2D) materials, such as graphene, are thin-layered materials consisting of a single or a few layers of atoms. 2D materials are attractive for their potentially diverse applications in key technological areas due to their unique properties in terms of electrostatic efficiency, mechanical strength, tunable electronic structure, and optical transparency. Isolation/synthesis of graphene from its precursor some twenty years ago has opened the door for the discovery and exploration of other emerging 2D materials; more than 2,000 of them that can be easily exfoliated have been discovered or synthesized to date, and yet their physical and chemical properties are largely unexplored. In this talk, we focus on studying the mechanical properties of thin films of $Ti_3C_2T_x$ MXene where *Ti* is titanium, *C* is carbon, and *T* represents a terminal group. Effect of fabrication technique, size (thickness), strain rate, as well as annealing temperature on the mechanical behavior of MXene thin film will be reported. In addition, we will also report the durability of MXene composite film under moisture environment for the purpose of effective electromagnetic interference (EMI) shielding. Subsequently, we have fabricated lattices made of 2D materials and their mechanical and thermal behavior will be discussed.

Harnessing Molecular Transport through 2D Material Membranes: Precision and Potential Applications

Prof Rahul Raveendran Nair
National Graphene Institute and Department of Chemical Engineering, University of Manchester, Manchester, UK
rahul@manchester.ac.uk

Abstract: Permeation through nanometre-pore materials has been attracting unwavering interest due to fundamental differences in governing mechanisms at macroscopic and molecular scales, the importance of water permeation in living systems, and relevance for filtration and separation techniques. Latest advances in the fabrication of artificial channels and membranes using two-dimensional (2D) materials have enabled the prospect of understanding the nanoscale and sub-nm scale permeation behaviour of water and ions extensively. In particular, several laminate membranes made up of 2D materials show unique permeation properties such as ultrafast permeation of water and molecular sieving. In my talk, I will discuss our recent results on controlling molecular transport through various 2D materials-based membranes by an external parameter and will discuss the prospect of developing next-generation intelligent membranes based on 2D materials.

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Targeted multi-scale dispersion of 2D materials in advanced composites

Prasad Potluri
Northwest Composites Centre & Graphene Engineering Innovation Centre (GEIC)
Department of Materials, University of Manchester, UK
Prasad.potluri@manchester.ac.uk

Abstract

This presentation looks at the manufacturing strategies for incorporating 2D materials at multiple length scales in fibre reinforced polymer composites. While coating natural fibres with GNP or GO improved tensile modulus and strength [1], similar improvements are not expected for aerospace grade carbon fibres. Here the objective is to improve interlaminar, intra-laminar fracture toughness, damage tolerance, fatigue performance as well as novel ways to heal/repair damage. Incorporating relatively small amounts (0.5%) of GNP/GO incorporated in bulk resin through 3-roll milling and subsequent prepregging improved fracture toughness[2], spray coating more than 0.2% [3] resulted in agglomeration and reduction in fatigue properties. However, nanoscale particles my be introduced without agglomeration up to 10% weight fraction of the resin resulting in 3-4 fold increase in fatigue life [4]. In this work, thermoplastic fibres, dissolvable and non-dissolvable have been utilised in delivering 2D materials at significantly higher concentrations in specific locations of interest. Non-dissolvable thermoplastic fibres in the form of comingled [5] or micro-wrapped [6] have shown the potential of healing/damage repair and impact damage tolerance. Nonwoven interleaves demonstrated improved mode I and Mode II fracture toughness[7,8]. Previously, dissolvable fibres [9] such as phenoxy have demonstrated some improvement in fracture toughness. Here, we use dissolvable fibres and electrospun veils to deliver highly dispersed graphene [10] in the regions of interest in a composite laminate.

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Artificial Intelligence for realistic modelling of electronic, thermal, optical and transport properties in **trillion atoms scale models** in complex forms of 2D Materials-based composites and amorphous compounds

Stephan Roche
ICREA Institució Catalana de Recerca i Estudis Avancats, 08010 Barcelona, Spain
Catalan Institute of Nanoscience and Nanotechnology (ICN2), CSIC and BIST stephan.roche@icn2.cat

Abstract

Artificial Intelligence-based techniques have become critical to accelerate the innovation processes from material growth to characterization and properties prediction. Particularly challenging is the modelling of disordered (amorphous) materials, complex interfaces and random assemblies of (2D) materials which are mainly used today in applications.

In that perspective, complex forms of (reduced) graphene oxides and related composites as well as amorphous materials such as boron nitride (aBN) and “amorphous graphene” (aG) have recently become prominent materials for many different applications, notably due to their good properties such as thermal stability, mechanical properties, insulating behaviour, and ultralow dielectric constant in aBN (<2). Moreover, amorphous films are more suitable to large area deposition compared to clean hBN or graphene since they can be grown at low temperatures (about 400 ºC) and on various substrates [1-3]. However, their properties strongly depend on the nature and degree of disorder, which needs a well-defined metrics for benchmarking different materials. Having such metrics in place will allow to tune the properties and performance of these films during the fabrication for desired applications. In this context, revealing the relationship between fabrication strategies and the material properties of the film is also crucial.

Capturing the key features of the amorphous nature of materials requires theoretical characterization to understand how material properties change with the microstructure. Since simulations of amorphous materials need large structural models, density functional theory (DFT) is not a suitable tool despite the high accuracy it offers. On the other hand, molecular dynamics (MD) simulations with empirical interatomic potentials require much less computational cost; however, they can turn out to be not accurate enough to correctly describe the local environment of amorphous materials. Machine learning-driven interatomic potentials (ML-IP) can describe the local environment with a similar accuracy to DFT and at a much lower cost [4,5]. Here, we introduce Gaussian approximation potentials (GAP) for atomistic simulations of aBN incorporating different contaminators and doping materials, which are trained on a large dataset of atomic structures generated by DFT calculations [6-8]. We will present a systematic analysis to screen out possible realistic morphologies as a function of growth parameters, such as temperature, quenching rate, and the presence of a dopant, and their corresponding material properties using GAP-driven MD simulations. The extensive simulations of a large quantity of possible structures presented here can guide experimental research and provide trends of scaling behaviour as a function of experimentally controllable parameters. The impact of amorphousness on dielectric properties will be also discussed for aBN and aG in the light of recent breakthroughs and claims [9,10].

We also present AI-driven computational workflows that could revolutionize advanced materials design and engineering, in which the automated building of structural and electronic models and their implementation into our in-house linear scaling computational algorithms (www.lsquant.org) enables the simulation of electronic, optical, transport properties in disordered models of materials containing up to the trillion atoms scale while keeping the accuracy of ab-initio approaches. These workflows will be designed to boost the innovation in a variety of technologies and applications in concertation and partnerships with industries.

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Driving Sustainability: Advances in Waste Management for Green Graphene Synthesis and Lightweight Thermoplastic Manufacturing

Assoc. Prof. Dr. Burcu Saner Okan[1]
[1]*Sabanci University Composite Technologies Center of Excellence and Integrated Manufacturing Technologies Research and Application Center (SU-IMC), Teknopark İstanbul, 34906 Pendik, Istanbul, Turkey*
burcu.saner@sabanciuniv.edu

Recycling studies in the waste tires, waste plastics, and waste carbon fiber reinforced composites industries play a crucial role in advancing sustainable waste management practices, reducing environmental impact, and fostering a circular economy mindset. Instead of traditional recycling processes, it is possible to produce high value-added carbon nanomaterials by using a rich hydrocarbon source in plastics and rubbery materials which are also primary source for graphene. Also, sustainable green graphene enhanced compounds can be produced by gathering different waste sources and providing suitable compatibilization with sizing solutions and functionalized additives in compounding process. In addition, stringent regulations in the automotive sector mandate a minimum of 25% recycled materials, including 25% post-consumer waste, in compositions, aiming for net-zero emissions. At this point, upcycling is a significant concept to bring an end to the life cycle of materials and open various new application routes for graphene production and its sustainable plastic materials. The present work provides an insight into the importance of green synthesis methods in graphene nanomaterials synthesis by combining recycling and upcycling technologies. It is observed that different plastic wastes based on their aromaticity and alifaticity and thermoset wastes and biomass can lead to the formation of different dimensional graphene structures such as 2D plates/sheets and 3D spheres. The produced graphene materials are used for the design of lightweight composite structures for automotive and plastic industry by reducing adverse environmental impacts and adopting energy-efficient manufacturing technologies. Furthermore, responsible management of carbon fiber waste through recycling and reuse initiatives is imperative for sustaining the carbon fiber industry and mitigating its environmental footprint. The widespread use of carbon fiber reinforced composites (CFRP) and the anticipated growth in consumption have led to substantial CFRP waste accumulation. Through the development of graphene derived from waste, compound formulations are devised using recycled polymer sources (e.g., PP and PA), natural fibers (such as hemp and flax), and recycled carbon fibers, aiming to replace glass fiber reinforced plastic in commodity products. Additionally, Life Cycle Assessment studies integrate into raw materials and parts, fostering circular economy models. Consequently, this multidisciplinary work ensures significant innovation potential of graphene in the field of thermoplastic-based composites and overcomes the needs by addressing greenhouse gas emissions with sustainable designs.

2D Materials Enhanced Composites: Shaping the Future of Aerospace Structures

Rehan Umer
Department of Aerospace Engineering and RIC2D, Khalifa University, Abu Dhabi, UAE
rehan.umer@ku.ac.ae

2D materials are revolutionizing the development of advanced composites by enhancing their multifunctionality and performance, paving the way for the next generation of aerospace structures. These enhancements include improved mechanical properties, energy storage capabilities, EMI shielding, and real-time sensing [1, 2]. In addition to traditional applications, 2D materials are now being explored in the manufacturing of high-performance hydrogen storage tanks, where their interaction with fibers and matrices plays a crucial role in increasing strength, durability, and performance under extreme conditions, including cryogenic environments essential for hydrogen storage. This presentation will explore how 2D materials, such as graphene, can transform aerospace structures and components. A comprehensive roadmap will be presented that shows how graphene-enhanced composites are central to the "factory of the future". The interaction between graphene with both thermoset and thermoplastic matrices, as well as its interaction with different reinforcements will be examined to showcase how these composites optimize mechanical properties, particularly for aerospace and hydrogen storage applications.

Furthermore, we will discuss the integration of graphene-based smart sensors into composites, allowing for real-time structural health monitoring during manufacturing and in-service use. These sensors bridge the gap between physical aerospace structures and cyber-physical systems, generating data that can drive intelligent, adaptive manufacturing processes [3, 4]. While graphene offers immense potential as an interface between physical components and digital technologies, several technical challenges remain. The presentation will address these challenges and outline future opportunities for integrating graphene-based sensing networks with digital twin technologies, improving production efficiency, and reducing material defects.

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Multiscale computational modeling for accelerating the understanding and performance of 2D materials for energy applications

Lourdes F. Vega[1,2], Daniel Bahamon[1,2], Yuting Li[1,2], Nirpendra Singh[1,3], Marcelo Lozada-Hidalgo[1,4]
[1] Research and Innovation Center for graphene and 2D-materials (RIC2D), Khalifa University of Science and Technology, Abu Dhabi, UAE.
[2] Research and Innovation Center on CO_2 and Hydrogen (RICH Center), Chemical and Petroleum Engineering Department, Khalifa University, Abu Dhabi, UAE
[3] Department of Physics, Khalifa University of Science and Technology, Abu Dhabi, UAE
[4] Department of Physics and Astronomy and National Graphene Institute, The University of Manchester, Manchester, UK.

lourdes.vega@ku.ac.ae

Computational techniques and theoretical models play a key role in establishing the structure–property relationships necessary for understanding and designing materials with novel properties and enhanced performance. These methods range from ab-initio molecular dynamics simulations (AIMD) to density functional theory (DFT), reactive molecular dynamics (ReaxFF MD), classical molecular simulations (MS), kinetic models (KM), coarse-grain models (CG) and process design and optimization (PDO). The increase in computational power together with advanced methods development for calculating properties of materials at different scales has put computational modeling at the forefront of accelerating the materials discovery and design, being an essential tool for this purpose. In recent years, machine learning (ML) combined with AIMD or DFT has gained significant attention in materials design, offering high accuracy with reduced computational costs. The application of these modeling tools combined with advanced experimental techniques is particularly relevant for graphene and 2D materials, as there are several hundreds of 2D materials potential candidates for different applications still to be explored.

In this presentation we will focus on some selected applications of 2D materials related to sustainable energy. Among the different technologies available for reducing greenhouse emissions, green (or low carbon) hydrogen and carbon capture, utilization, and storage (CCUS) have been recently identified by the International Energy Agency as two key technologies to decarbonize the energy and industrial sectors, expected to contribute to 30% to achieving net zero emissions by 2050 [1]. After a general introduction on the need of development efficient materials for energy and the basics on computational modeling, the presentation will focus on the use of combined advanced experimental techniques with computational modeling (and ML) for understanding and improving the performance of 2D materials for selected applications: (1) the development of new proton conducting 2D materials [2] for fuel cells, understanding the effect intense electric fields and nano-scale ripples to increase their catalytic activity [3], where hundreds of materials are explored with the use of ML. This work is done in collaboration with the group of Prof. Sir A. Geim and Dr. M. Lozada-Hidalgo at the University of Manchester through RIC2D, (2) improving the performance and mechanical stability of hybrid adsorbent materials for CO_2 capture, combining graphene oxide (GO) with metal organic frameworks (MOFs) [4] and (3) 2D catalytic materials for CO_2 reduction. We will show how the integration of AIMD and ML not only accelerates the discovery of high-performance proton-conducting membranes but also provides a deeper understanding of the fundamental mechanisms underlying proton permeation in 2D materials. For the case of materials for CO_2 capture, understanding the role of GO through molecular simulations allows optimizing the hybrid composition to improve their performance at the process conditions. Finally, high-throughput screening of 2D materials and their modified versions (doped or functionalized) combining DFT with ML let to identify promising candidates for CO_2 reduction to chemicals and fuels, experimentally validated when possible.

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Chitosan/MXene/GO Catalytic Nanocomposite membrane for Removing Dye and Heavy metals

Linda Zou, Chao Yu

Department of Civil Infrastructure and Environment Engineering and Research & Innovation Center for Graphene and 2D Materials (RIC2D), Khalifa University of Science and Technology, Abu Dhabi, PO Box 127788, United Arab Emirates
linda.zou@ku.ac.ae

Abstract (Arial 10)

2D materials MXene and graphene oxide (GO) were employed in developing chitosan-based catalytic nanocomposite membranes for the removal of dye molecules and heavy metals from textile industry wastewater. Owing to the existing of defect sites, the incorporated MXene induced the decomposition of hydrogen peroxide (H_2O_2), the generation of reactive oxygen species, which oxidize methylene blue (MB) and reduce cobalt (Co^{2+}) and copper (Cu^{2+}) ions. The fabricated chitosan/MXene/GO (CMG) membrane in this research exhibited high removal efficiencies of 96%, 78% and 76% for dye, cobalt ions and copper ions, which were 4, 3.9 and 4 times higher than that of neat membrane, respectively. Similar results of 95% were also observed in total organic matter (TOC) removal for both concentrations of dye. The CMG membrane also showed superior fouling resistance, which effectively prevented the attachment of bovine serum albumin (BSA) on the membrane surface in accelerated fouling experiment, with much less flux reduction than the neat membrane indicating its remarkable anti-fouling performance that ascribed from the catalytic activity of MXene. The achievements provided a new insight for using nano-additives enhanced membrane technology to efficiently remove hazardous contaminants such as dye and heavy metals from industrial effluent.

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Figures

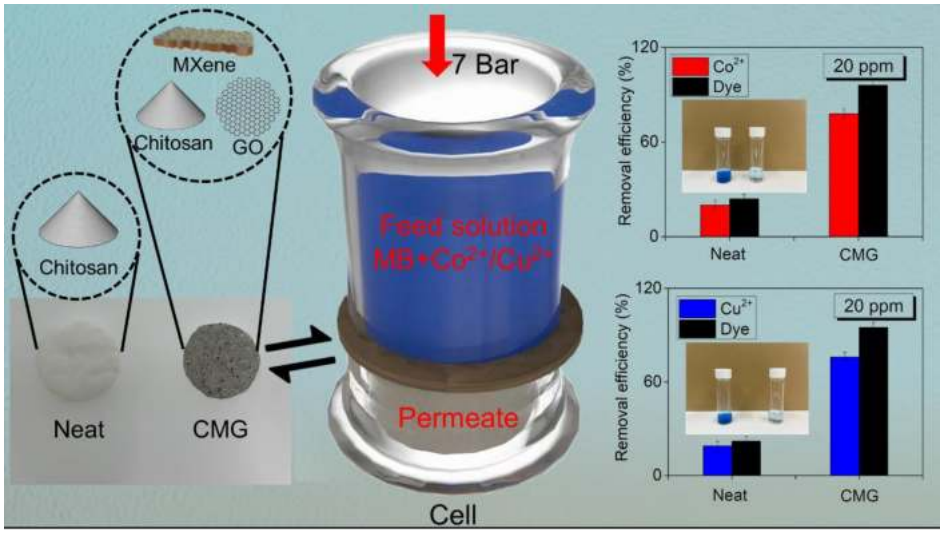

Figure 1: Simultaneous removal of dye chemical and heavy metals by Chitosan/MXene/GO catalytic nanocomposite membrane.

Multifunctional Properties of 3D Printed Graphene/MXene based Architected Cellular Materials

Rashid K. Abu Al-Rub, Juveiriah Ashraf, Somayya Taha, Jing Fu, Abdullah Solayman, Kin Liao
Advanced Digital & Additive Manufacturing (ADAM) Group, Department of Mechanical & Nuclear Engineering, Khalifa University, Abu Dhabi, UAE
rashid.abualrub@ku.ac.ae

Abstract
The mathematically well-known triply periodic minimal surfaces (TPMS) have unique topological characteristics making them ideal for creating metamaterials and structural systems with excellent multifunctionality [1], especially fabricated out of 2D materials such as graphene and MXene. In this work, we present a scalable fabrication method of ultralightweight standalone TPMS-based architected cellular materials out of graphene/MXene using 3D printed sacrificial scaffolds [2,3]. The fabrication method includes graphene/MXene coating of the TPMS scaffolds via a hydrothermal process, followed by drying and thermal etching of the scaffold. Various characterization techniques are used to assess the quality of the standalone graphene/MXene cellular materials. Also, the thermo-electro-mechanical properties of these cellular materials as a function of the graphene/MXene concentration and cell topology are evaluated. Furthermore, their performance in various applications is assessed. Some of these demonstrations are in collaboration with industry such as Dassault Aviation. This true academia-industry collaboration will be emphasized in this talk, which is yielding fruitful applications of these novel types of architected metamaterials made of various 2D materials.

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Figures

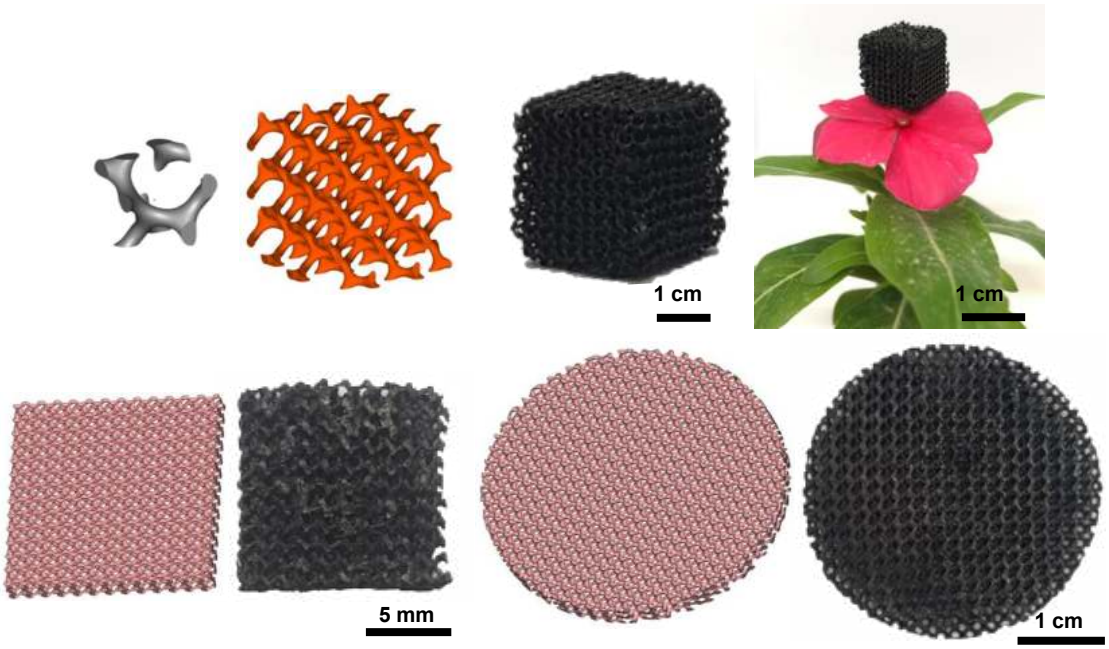

Figure 1: Designed and fabricated TPMS-based graphene architected cellular materials.

Graphene-enabled stimulated Raman microscope for oncology

Giulio Cerullo[1,2], Matteo Negro[2]
1 Dipartimento di Fisica, Politecnico di Milano, Piazza L. da Vinci 32, 20133 Milano, Italy
2 Cambridge Raman Imaging Srl, Via Durando 39, 20158 Milano, Italy giulio.cerullo@polimi.it

Stimulated Raman scattering (SRS) microscopy is a powerful nonlinear optical technique for chemical identification of (bio)-molecules based on their intrinsic vibrational spectrum, which allows high-speed label-free imaging of cells and tissues [1]. However, despite its promise as a disruptive label-free imaging and diagnostic tool, SRS microscopy still suffers from several limitations, which prevent its massive uptake in the biomedical arena and confine it to applications in specialized optics laboratories. The laser sources required for generation of the synchronized pump/Stokes pulses are exceedingly complex, bulky and expensive. Furthermore, SRS microscopes typically work at one or a few vibrational frequencies, providing limited biochemical information. In this work, exploiting the unique optical properties of graphene and other 2D materials [2], we drastically simplify the architecture of the laser system used for SRS microscopy, reducing its footprint and cost and enhancing its reliability. Furthermore, we implement broadband SRS microscopy [3], measuring the SRS signal over a wide spectrum of frequencies simultaneously and thus combining the molecular information of spontaneous Raman microscopy with the imaging speed of a coherent process. Our broadband SRS microscope has the following unique characteristics, which cannot be found in any other commercial instrument: i) label-free imaging; ii) living cell imaging; iii) high (μs pixel dwell time) acquisition speed, enabling the observation of cellular dynamics by time-lapse imaging or fast scanning of human biopsies. All this is achieved in a compact, low-cost, hands-free product design. Our broadband SRS microscope thus combines information on the morphology and on the biomolecular composition of cells, without altering their natural state with exogenous molecules or invasive interventions. As such, it is expected to revolutionize the study of the cellular origin of diseases and of cancer immunotherapy. Furthermore, our microscope allows high resolution, high speed measurement of the vibrational spectra of large areas of unstained tissue samples, providing at the same time morphological and biomolecular data and allowing label-free histopathology and accurate tumour diagnosis (Figure 1).

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Figures

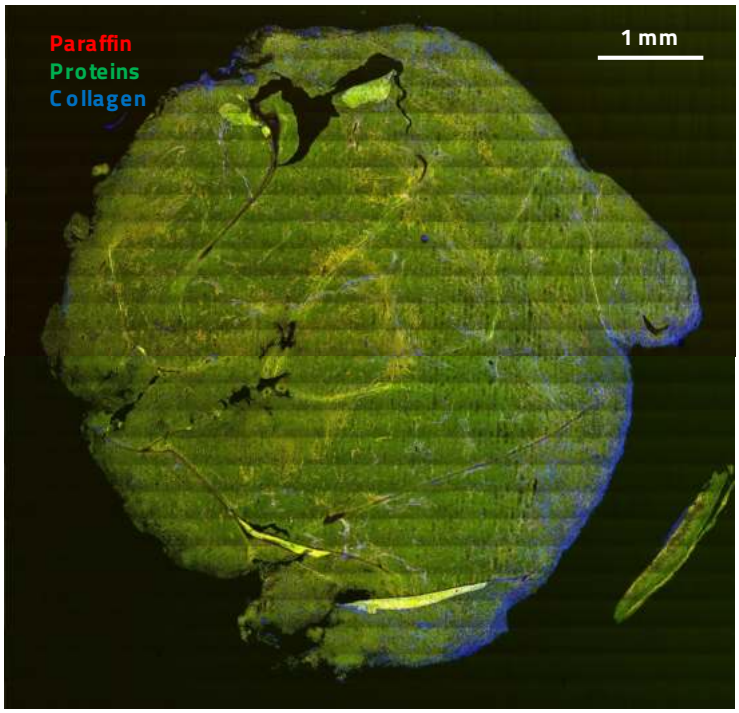

Figure 1: SRS image of a 10-μm-thick human tumor tissue sample (size: 6650 x 6910 μm) following formalin fixing/paraffin embedding and dewaxing.

Evolution in Inherent Vibration-Suppressive Materials

Dr Stephen Devine, Sandy Chen
Graphene Composites Ltd, NETPark Incubator, Thomas Wright Way, Sedgefield, TS21 3FD, United Kingdom
Steve.devine@graphenecomposites.com

Abstract

From Aerospace through to Healthcare and Manufacturing, the need to control and/or supress vibration across a wide range of products and markets is a critical requirement. Whether it is protecting delicate electronics from excess vibration on a satellite launch or controlling supersonic shock waves in ballistic armour, the use of the right combination of material allows this control while maintain other properties such as strength. This study shows how graphene composites has developed materials for extreme vibration suppression in ballistic events and how technology transfer can be achieved to utilise these materials in other market areas. Combining polymers into a composite structure can wield strong, lightweight materials with excellent vibration dampening characteristics without compromising tensile and flexural properties.

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Figures

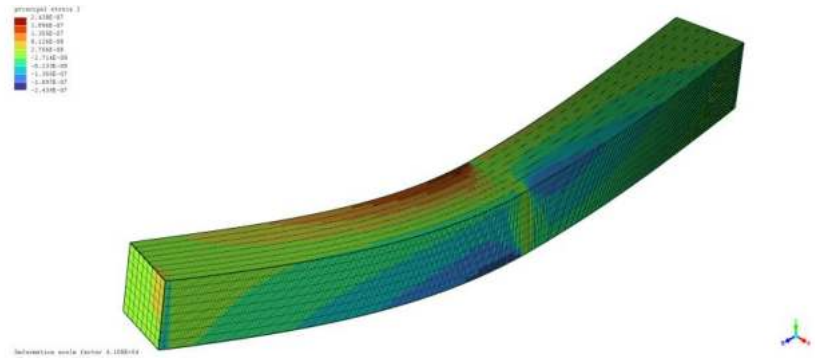

Figure 1: Simulation of strain in composite bar

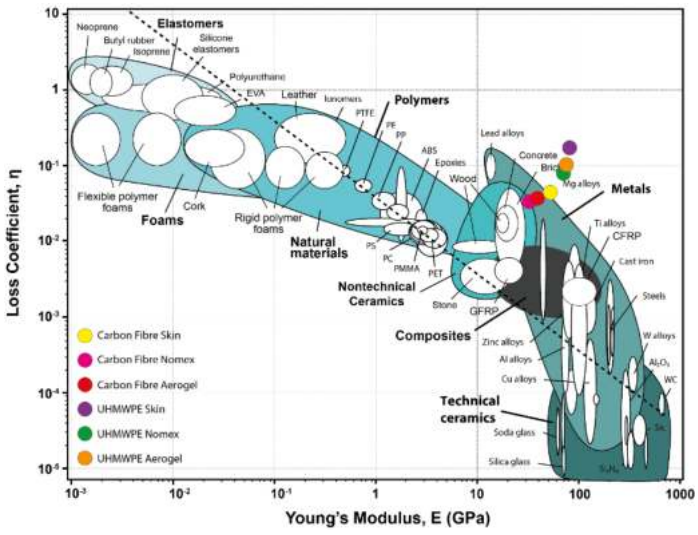

Figure 2: Ashby Chart relating to loss coefficients of GC structural materials [1]

Graphene composites: enabling innovative applications in the aerospace and automotive industries

Costas Galiotis
Institute of Chemical Engineering Sciences, Foundation for Research and Technology-Hellas, Stadiou Str, Patras, Greece
Department of Chemical Engineering, University of Patras, Patras, Greece
c.galiotis@iceht.forth.gr

Abstract
The design of lightweight vehicles is crucial for enhancing fuel efficiency and achieving improved performance while minimizing negative environmental impacts. In order to lower fuel consumption and meet the CO_2 emission targets set by EU regulations, the automotive and aerospace sectors have been increasingly interested in the production of lightweight components and the replacement of metal parts with composite structures. In this context, graphene emerges as the next-gen solution to improve vehicle functionality, reduce production costs for manufacturers and decrease fuel consumption for end users.
In this talk, two case studies of innovative applications of graphene-based composites in the automotive and aerospace sectors are discussed: i) the graphene-enhanced Dallara Stradale car and ii) graphene-based ice protection systems.
Graphene-related materials (GRMs) have been introduced into CFRP panels in the Dallara Stradale car with the aim to enhance fracture toughness, damping, impact, strength and stiffness of specific exterior and interior components. Specifically selected GRM grades were mixed with resin in view of the production of modified CFRP prepregs. The initial selection of materials was followed by the production of prepregs and the fabrication of model panels, which were also subjected to a predefined testing campaign, prior to the fabrication of the final parts to be mounted on the modified Dallara Stradale test car. The efforts were integrated by the assembly of the protype vehicle, followed by a set of large-scale testing and evaluation of the new materials, mounted on the car. The Dallara Stradale prototype exhibited a paramount fire resistivity behaviour, an increase of 23% in the thermal conduction properties, an impressive enhancement in the attenuation of vibrations by 55%, combined with an improvement of 15% in stiffness and bending resistance.
Accumulation of ice on the external surfaces of the aircraft (e.g. wings and propellers) can be extremely dangerous, and graphene-based de-icing systems can offer a low-weight, highly efficient and flexible solution. Graphene-polymer nanolaminates have been recently demonstrated to be highly efficient and responsive heaters [1]. These composites consisting of continuous layers of graphene alternated to thin films of high-performance polymers, present not only a significant enhancement of mechanical and electrical properties but, very interestingly, show impressive Joule heating efficiency. In fact, upon the application of an electrical potential, they can reach temperatures higher than 250 °C, with heating rates up to 325 °C/s. The produced heaters show a very uniform distribution of the temperature even when bend and are characterized by low power consumptions and high areal power densities, and can be introduced as de-icing elements in aircrafts.

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Patenting and Commercialization of Graphene Materials and Application Technologies: A Challenging Journey of 22 Years (2002-2024)

Bor Z Jang, Co-founder and CEO
Global Graphene Group (Angstron Materials, Inc.), 1240 McCook Ave., Dayton, OH 45404 USA
Bor.Jang@G3-AM.com

Abstract

Dr. Jang has done some significant work in the graphene technology space as reflected by the following key technology milestones: (a) Dr. Jang's team filed world's first patent application on graphene as a new material in 2002 [1] and multiple patent applications in June and August 2004 [2,3]; (b) gave a technical presentation on electronic behavior of graphene at the American Physical Society annual meeting in 03/2004 [4]; (it may be respectfully noted that Drs. K. S. Novoselov and A. Geim published their truly remarkable paper in *Science* in October 2004 [5]); (c) established Angstron Materials, Inc. (AMI) in 2007 and scaled up the production of graphene oxide in 2013; (d) invented the supercritical fluid exfoliation process in 2006 [6], liquid phase exfoliation (ultrasonication) process for graphene and other 2D materials in 2007 [7], and electrochemical exfoliation in 2007 [8]; and (e) invented graphene-based supercapacitors in 2006 [9], graphene-protected battery electrode materials (e.g., graphene-encapsulated Si) in 2007 [10], and graphene-based thermal films (thermal management materials) also in 2007 [11]. With this rich experience in graphene technology development and commercialization, Dr. Jang will offer some personal perspectives on the rapidly emerging graphene industry, emphasizing the opportunities and challenges in commercializing graphene materials and products. The technical and commercial challenges experienced by graphene producers will be high-lighted. The needs of graphene industry for truly cost-effective graphene production processes and commercially competitive products will be discussed in this presentation. Truly breakthrough graphene production and application technologies are essential to the emergence of an economically viable graphene industry. For instance, a significant challenge is the notion that graphene is a unique material that requires different processes to bring out the most desirable characteristics for a particular application. In other words, different processes are required to produce different types of graphene materials for different applications in different market sectors. There are also technical, economical, and regulatory issues that must be addressed in order for the large-scale production of affordable graphene materials to be fully realized. This will be followed by a discussion of some of the potential and realized applications of graphene materials, including thermal management, supercapacitors, batteries, and functional composites.

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Terahertz Spectroscopy for Electrical Characterization of 2D Materials

Peter Bøggild[1], Peter Uhd-Jepsen[2]
[1]DTU Physics and [2]DTU Electro, Technical University of Denmark, 2800 Kgs. Lyngby, Denmark
pbog@dtu.dk

Over the past decade, we demonstrated terahertz spectroscopy to be an efficient tool for fast, nondestructive electrical characterization of graphene on various substrates [1-2], including silicon, sapphire, and polymers. Key parameters such as conductivity, carrier density, carrier mobility, and uniformity can be extracted across wafer-scale graphene, and a metrology standard for THz-TDS graphene was recently published through the International Electrotechnical Commission [3]. Several important questions arise: can THz quality control (QC) be applied to roll-2-roll production systems? How reliable and robust is THz-QC and does it work equally well on all substrates? Will THz-QC be useful for process development? What can we learn about the uniformity and grain structure of 2D films [4]? With the increasing interest and progress in large-scale manufacturing of other 2D materials, such as transition metal dichalcogenides, how will THz-TDS contribute to scientific research and quality control of these materials? In this talk I will discuss the state-of-the-art and recent progress in THz-based quality control (THz-QC) and address possibilities, problems, and open questions related to this emerging technology, and show results on R2R inline THz-QC, large-scale mapping of TMD films [5], graphene micro and nanoribbon gratings, and nanoscale conductivity measurements on graphene with THz scattering SNOM [6].

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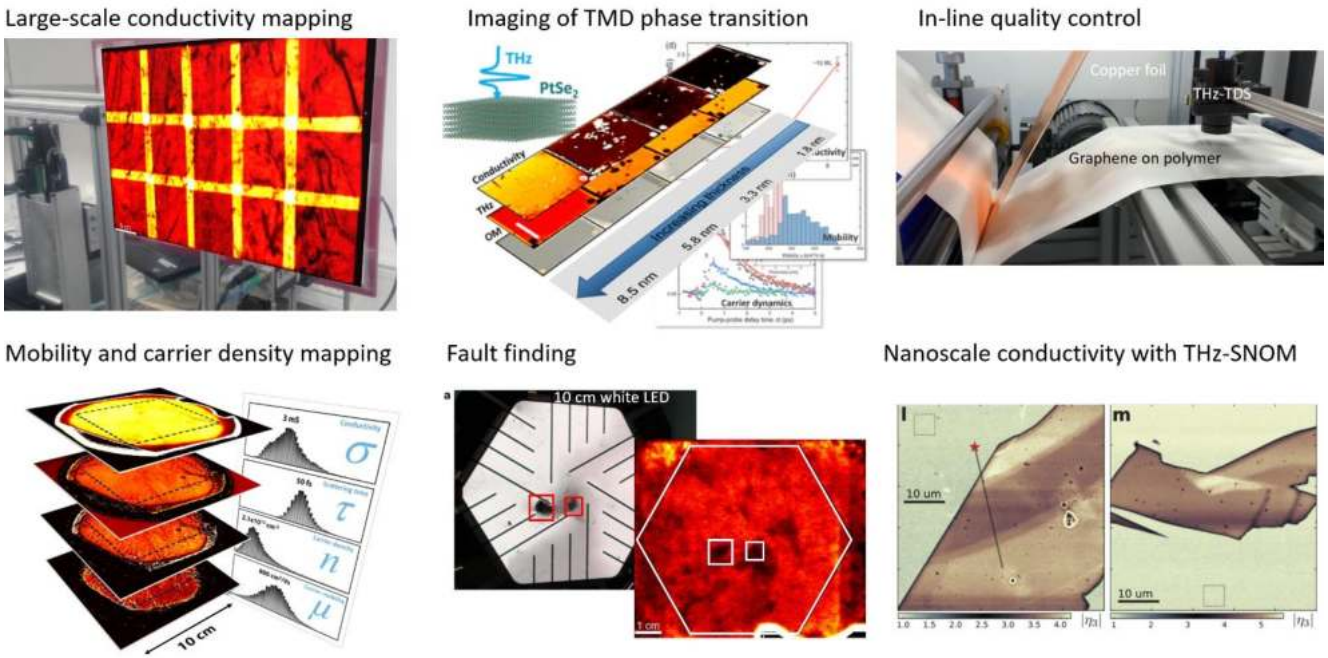

Figure 1: The talk will cover different examples of THz-TDS used for quality control, R&D and research.

Giant Optical Anisotropy in van der Waals Materials: Perspectives and Challenges

Volkov V.S.[1], Ermolaev G.A.[1], Grudinin D.V.[1], Vyshnevyy A.A.[1], Mazitov A.B.[1], Tselikov G.I.[1], Kruglov I.A.[1], Arsenin A.V.1, Novoselov K.S.[2]
[1]*Emerging Technologies Research Center, XPANCEO, Dubai, UAE*
[2]*Department of Materials Science and Engineering, National University of Singapore, Singapore*
vsv@xpanceo.com

Abstract

Materials with high optical anisotropy are of great importance in technology and science [1]. Recently, one of the largest birefringences in the visible and near-infrared intervals up to 0.8 was reported in quasi-one-dimensional crystal $BaTiS_3$ [2]. However, anisotropic nanophotonics requires an optical anisotropy of about 1.5 to fully exploit the advantages of anisotropic properties [3, 4]. Inspired by this challenge, we focused on two-dimensional materials and their bulk counterpart – van der Waals (vdW) materials.

Our findings showed that their fundamental difference between interlayer strong covalent bonding and interlayer weak van der Waals interaction leads to unprecedented high birefringence with values exceeding 1.5 in the infrared and 3.0 in the visible spectral intervals (for example, see optical constants of MoS_2 in Figure 1). Thus, our studies enable a new field of vdW anisotropic nanophotonics. In detail, we managed to achieve unmatched lateral dimensions for van der Waals-based waveguides with only several tens of nanometers footprint. In other words, it gives a unique opportunity to place around 10000 waveguides on an mm-scale photonic chip. These characteristics make us a step closer to electronic integrated circuits. Hence, vdW-based photonic integrated circuits can become a decisive platform for an electronic-to-photonic replacement to increase computer data processing. The idea behind the use of vdW materials has four advantages. First, vdW materials have larger optical bandgap in comparison with conventional high refractive index materials (TiO_2, GaP, Si, Ge, and many others) and, therefore, smaller operation wavelength without dissipative losses. Secondly, vdW materials have one of the largest refractive indices among known materials. Thirdly, the record-breaking optical anisotropy of vdW gives an additional degree of freedom for the design optimization of integrated photonic elements.

Finally, vdW materials have dangling bonds-free surfaces and atomically sharp edges after the lithography process, which results in minimum scattering losses in photonic waveguides and high-intensity nonlinear properties in addition to superior linear response. From a broader perspective, we would like to note that these vdW features are also beneficial for countless optical devices (resonators, dielectric mirrors, waveplates, and many others) beyond on-chip integration.

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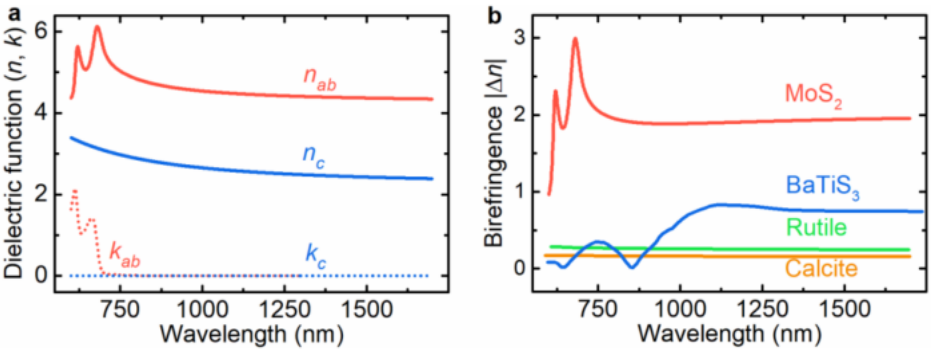

Figure 1: a. Optical constants of MoS_2. **b.** Birefringence of MoS_2 in comparison with other anisotropic materials.

Extraordinarily transparent compact metallic metamaterials

Xiaofei Xiao
Technology Innovation Institute, Masdar City, Abu Dhabi, United Arab Emirates
xiaofei.xiao@tii.ae

Metals are highly opaque, yet we show numerically and experimentally that densely packed arrays of metallic nanoparticles can be more transparent to infrared radiation than dielectrics such as germanium, even for arrays that are over 75% metal by volume. Despite strong interactions between the metallic particles, these arrays form effective dielectrics that are virtually dispersion-free, making possible the design of optical components that are achromatic over ultra-broadband ranges of wavelengths from a few microns up to millimetres or more. Furthermore, the local refractive indices may be tuned by altering the size, shape, and spacing of the nanoparticles, allowing the design of gradient-index lenses that guide and focus light on the microscale (see figure a). The electric field is also strongly concentrated in the gaps between the metallic nanoparticles, and the simultaneous focusing and squeezing of the electric field produces strong 'doubly-enhanced' hotspots (see figure b) which could boost measurements made using infrared spectroscopy and other non-linear processes over a broad range of frequencies, with minimal heat production.

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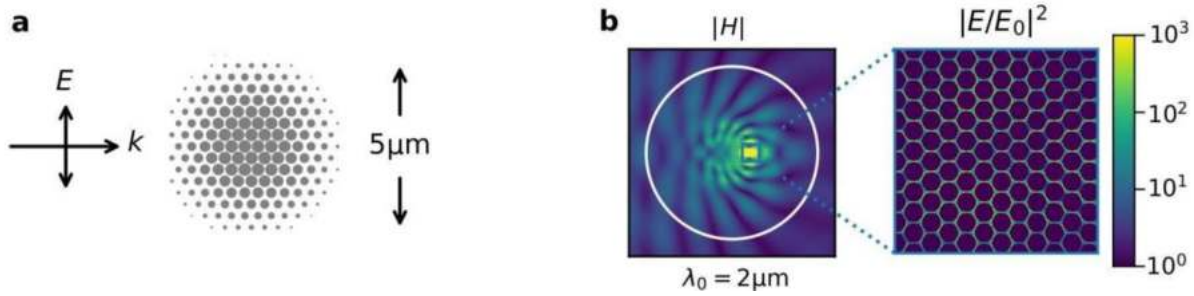

Figure 1: (a) Schematic of a 'concentrator' gradient-index lens composed of gold nanocylinders on a triangular lattice with 50nm site-to-site separation (b) Magnetic near-fields and broadband 'doubly-enhanced' electric field hotspots

Laser Induced Graphene: A New Paradigm

Yarjan Abdul Samad, Rami Elkaffas, Shanavas Shajahan, Dhinesh Babu Velusamy
Khalifa University of Science & Technology, Abu Dhabi, UAE
Yarjan.abdulsamad@ku.ac.ae

As graphene and related materials increasingly integrate into various industries [1, 2], the necessity to produce high-quality graphene sheets on a large scale becomes crucial [3]. Here, we present a unique approach for large scale production of graphene through laser-assisted graphite expansion followed by ultrasonic exfoliation. The present method utilizes laser technology to significantly expand graphite, achieving an expansion rate of 800 mL/g with a remarkably low energy consumption of just two watts per second. The graphene samples exhibited high quality (ID/IG) ~ 0.13 and few layers with a (I2D/IG) ~ 0.52. Through filtration technique, free-standing films with different thicknesses (11-69 µm) were successfully prepared, reaching significant electrical conductivity up to (~ 1707 S/cm). Graphene film with a 11 µm thickness achieve the highest absolute effectiveness (SSE/t) of ~ 58666 dB cm^2 g^{-1}, surpassing most current graphene and MXene films, which typically present values in the range of 10000 to 40000 dB cm^2 g^{-1}.

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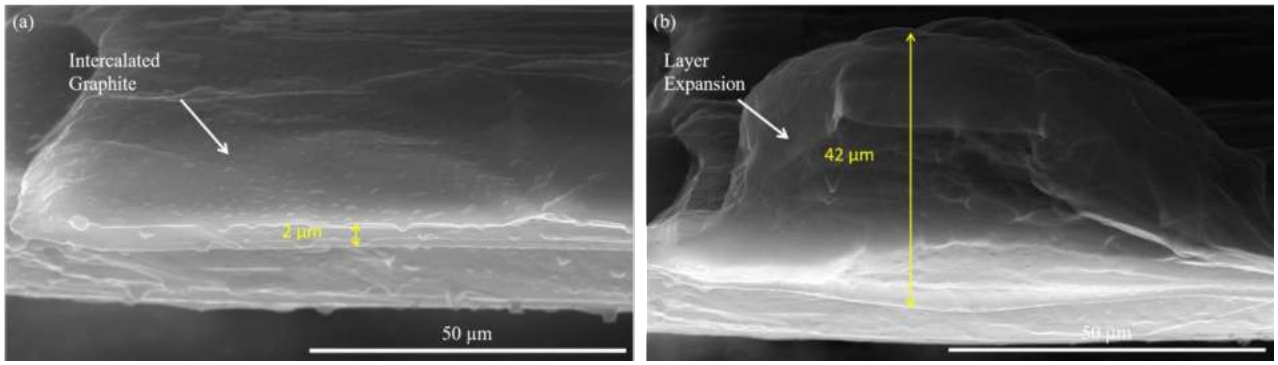

Figure 1: a) SEM of Intercalated Graphite, (b) *In Situ* Expansion of Intercalated Graphite in SEM

Robust collaboration between design, process, production and commercial teams : a key element to successfully scale-up advanced materials

Alban Chesneau
Carbon Waters, France
alban.chesneau@carbon-waters.com

Context: Based on a unique technology, Carbon Waters develops, produces and markets performance additives for paints, polymers and composites based on 2D materials. Our products enable major advances in the fields of transport, renewable energies, energy storage and construction. Our experience has shown that the successful industrialization and commercialization of advanced materials, and in particular 2D materials, is a complex process requiring close collaboration between Research and Development (R&D), Production and Marketing. This presentation, based on concrete examples, highlights the specific challenges and the solutions implemented to deliver maximum added value for our customers.

Relationship between Material Typology and Obtained Properties: Material typology, including chemical composition, microstructure and manufacturing processes, directly influences final properties, such as mechanical strength, conductivity or durability.Understanding and mastering this relationship is crucial to developing materials that meet technical specifications while being suitable for industrial production processes.This understanding requires ongoing collaboration between R&D, which designs the materials, and Production, which manufactures them on a large scale.

Variability in the production of advanced materials: The high variability of materials within production batches is widely observed throughout the 2D materials industry.Even modest deviations in material quality can seriously compromise the quality of the final product, and explains why so many manufacturers are still reluctant to use this type of material. For a company specializing in 2D materials, the main challenge is to limit the variability of batch quality rather than the quantity produced. To achieve this, it is essential for R&D to work closely with production to optimize manufacturing processes and reduce these variations, as well as to set up a quality control system that guarantees uniform quality in line with strict market standards.

Design for customer needs: The commercial success of advanced materials obviously depends on their ability to meet specific customer needs.However, these specific needs are still often unknown, and the materials produced are not easily usable or do not generate the added value expected by users.At Carbon Waters, the marketing department works closely with R&D from the earliest stages of development to ensure that materials are designed with identified requirements in mind. This customer-centric approach enables us to create tailor-made solutions, increasing the chances of adoption by end-users.

Case studies and solutions developed by Carbon Waters: Case studies will illustrate how effective collaboration has overcome these challenges. These examples show that ongoing dialogue between R&D, Production and Marketing is essential to ensure successful industrialization and commercialization.

Conclusion: The industrialization of advanced materials cannot be successful without close collaboration between R&D, Production and Marketing. Reducing variability, designing materials according to type, and responding to customer needs are key steps in ensuring product quality, performance and commercial success. This integrated approach within an appropriate organization is essential to maintain a competitive edge in the advanced materials sector.

Additive manufacturing of ceramics from precursors

Paolo Colombo
Department of Industrial Engineering, University of Padova, Padova, Italy
Department of Materials Science and Engineering, Pennsylvania State University, USA
Department of Mechanical Engineering, University College London, UK
paolo.colombo@unipd.it

Additive manufacturing of ceramics is somewhat limited by their high melting temperatures and the processing issues related to handling of feedstocks containing a large volume of particles. Processing slurry-based feedstocks, in fact, poses several challenges: a high amount of powder is required to promote densification and results in high viscosity, scattering and sedimentation phenomena in vat photopolymerization processes, as well as clogging problems at the nozzle for extrusion-based processes.
Some of these issues can be solved or mitigated when using all liquid, precursor-based feedstocks. Our research activities have therefore focused on the use of preceramic polymers as well as sol-gel solutions as feedstock for the production of ceramic components by additive manufacturing. Despite the many advantages related to their liquid nature, there are also some challenges related to the reactivity of sol-gel systems and to the high amount of solvent usually present, while preceramic polymers are limited in the range of compositions available.
Additive manufacturing of geopolymer solutions or powders has also been investigated, as precursors for different components of interest for absorption, catalysis or high temperature applications.
In this talk, our strategies for producing high quality ceramic components using a variety of precursor feedstocks will be presented. Different additive manufacturing techniques were used to fabricate components ranging in size from the sub-micron to the tens of centimeters, including direct ink writing, digital light processing, two photon polymerization, robotic arm manufacturing and volumetric additive manufacturing.

Can We Produce a Carbon-Negative Material Made of Carbon?

Dr Ugo Sassi
Levidian Nanosystems Ltd, Cambridge, United Kingdom
ugo.sassi@levidian.com

Our planet is warming. As the global temperature keeps rising, we are experiencing more frequent and severe weather events, such as heavy rainfall, flooding, droughts, and heatwaves.

The increase of greenhouse gas concentrations in Earth's atmosphere has a direct effect on the rise of global temperatures. Among various greenhouse gases, the International Energy Agency (IEA) shows that anthropogenic methane (CH_4) emissions account for approximately 30% of global warming [1]. Therefore, driving methane emissions reductions across all scales in the next few years will be a critical factor in our journey to fight climate change.

Here, I will present Levidian's LOOP technology (figure 1), a system designed to decarbonise carbon-intensive industrial processes, transforming decarbonisation from a cost into a source of revenue [2]. LOOP converts methane into two valuable products: hydrogen and graphene - a super-material with high commercial value, that can be used to enhance the intrinsic characteristics of products in several industries.

The LOOP process is one of the most sustainable production techniques for graphene. Indeed, when biomethane is used as an input gas and renewable energy is deployed to electrically power the LOOP, the resulting graphene carbon footprint could even be negative.

Levidian graphene's unique characteristics will be presented, as well as its impact on batteries performance.

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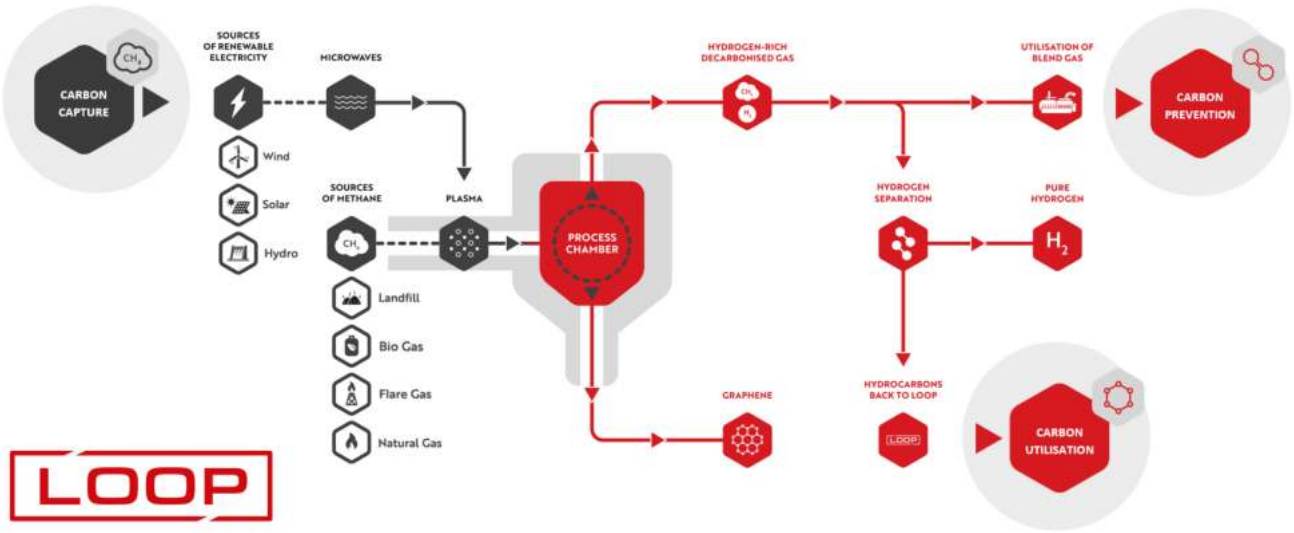

Figure 1: LOOP technology decarbonising via 3 mechanisms: carbon capture, carbon prevention and carbon utilisation.

Emerging Two-Dimensional Materials *via* Wet- chemistry: Application in Energy and Electronics

Ali Shaygan Nia and Xinliang Feng

Max Planck Institute for Microstructure Physics, Department of Synthetic Materials and Functional Devices, Halle, Germany
Chair for Molecular Functional Materials, Center for Advancing Electronics Dresden (cfaed) Technische Universität Dresden, Dresden, Germany

ali.shaygan_nia@mpi-halle.mpg.de

2D layered materials (2DLM), including van der Walls heterostructures (vdWHs), intercalated compounds, and superlattices, are important building blocks for the next generation of energy devices as well as (opto-)electronic, spintronic, and quantum devices due to their remarkable chemical and physical properties. To this end, scalable synthesis of 2DLM with high purity and specific functionalities is key to advancing fundamental studies toward applications. In this context, we use wet chemistry methods, in particular **electrochemical intercalation and exfoliation**, to synthesize 2DLM. Another key feature of wet chemistry is the **solution processability** of the developed 2DLM, which enables scalable device fabrication using different printing technologies such as inkjet and 3D printing.

Among different synthetic protocols, electrochemical exfoliation[1] of layered materials is a very promising approach that offers high yield, excellent efficiency, low cost, simple instrumentation, and excellent up-scalability. Remarkably, playing with electrochemical parameters enables functionalization and tunable material properties and increases the material diversities from graphene to a broad spectrum of 2D semiconductors[2], 2D magnets, etc.

"In this talk, I will take you through our journey, starting from the early stages of developing electrochemical exfoliation techniques for graphene and other 2D materials to their upscaling and diverse applications in electronics and energy storage. This journey ultimately led to the creation **two spin-off companies**: one focused on the "**production of 2D materials"** and the other dedicated to developing "**aqueous batteries,"** specifically zinc-based batteries.

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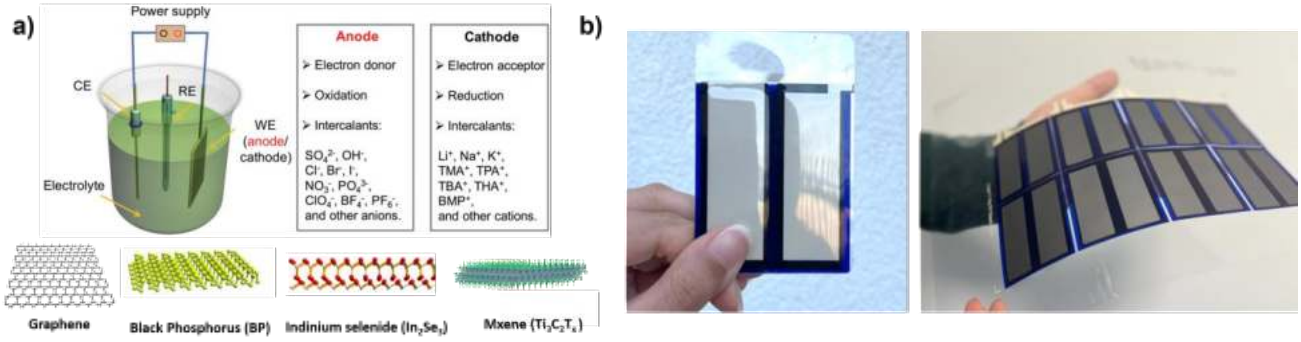

Figure 1: a) Electrochemical exfoliation process to produce 2D materials **b)** Graphene-based printed battery prototypes

New 2D dielectrics and magnets for electronic applications

Zdenek Sofer
Dept. of Inorganic Chemistry, University of Chemistry and Technology Prague, Technicka 5, 166 28 Prague 6, Czech Republic Organization
zdenek.sofer@vscht.cz

This presentation will explore recent advancements in the development of high-quality, low-defect 2D magnetic materials. Beyond the well-known classes of transition metal halides and chalcogenides, we will introduce the rapidly expanding category of mixed halogen-chalcogenides. Chromium sulfo-bromide, a key material in this family with an FeOCl structure, exhibits A-type antiferromagnetic ordering at low temperatures. Through exfoliation and defect engineering, this material can transition into a ferromagnetic state. We will discuss the chemistry of CrSBr, including doping and functionalization—both covalent and non-covalent—and its impact on magnetic and optical properties, highlighting potential applications in electronic devices. Additionally, the talk will cover 2D dielectric materials and doping of 2D semiconductors (Figure 1), which play a critical role in device fabrication, showcasing the development and applications of novel high-k 2D dielectrics and large-scale crystal growth of hexagonal boron nitride at atmospheric pressure using diverse metal fluxes [1].

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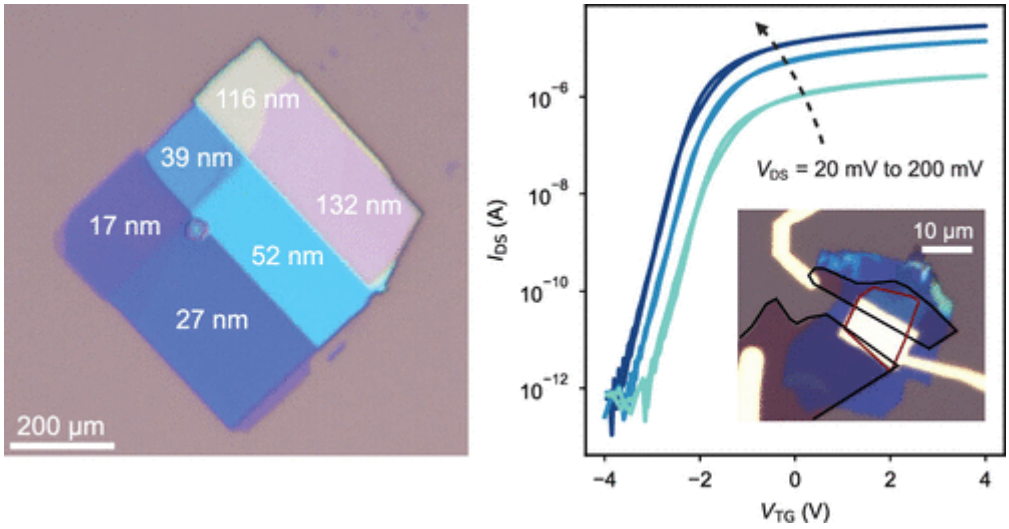

Figure 1: Exfoliated LaOBr layered dielectric and its transistor characteristic in combination with graphene.

Graphene-based MEMS devices and route to manufacturing

Aravind Vijayaraghavan
University of Manchester, Oxford Road, Manchester, UK
aravind@manchester.ac.uk

Graphene is the novel atomically-thin carbon layer with superlative properties that are ideal for MEMS applications – a combination of extremely high stiffness and breaking strength, high elasticity, and extremely low mass [1]. I will present our results on the development of the graphene-polymer heterostructure MEMS membrane which demonstrated a viable solution to the challenge of large-area defect free graphene MEMS device fabrication with high yield and excellent device performance [2]. Latest results will include extending the previous demonstrated 'strained transfer' technique for producing uniaxially pre-tensioned graphene membranes [3,4] to a biaxially pre-tensioned membrane which provides further significant improvement in performance. The deflection performance of the graphene membrane and the resulting capacitance changes are modelled and verified by a von-Karman finite element solver [5]. We have recently shown that the graphene MEMS membrane can be integrated into commercial multi-user MEMS processes. We will demonstrate pressure sensors and capacitive micromachined ultrasound transducers (CMUTs) based on graphene-polymer heterostructure MEMS membranes integrated with chips fabricated on the PiezoMUMPs and PolyMUMPs platforms. The pressure sensors offer a combination of very high sensitivity and wide operating pressure range while the CMUTs are novel in being able to operate at near-zero DC bias, in the frequency range of 1 – 10 MHz, which is commensurate with medical ultrasound and non-destructive testing applications. The combination of these significant and novel advances means that graphene MEMS devices can now be fabricated based on commercial MEMS platforms, allowing for vastly increased device complexities and yield and a route to large-scale manufacturing and commercial implementation.

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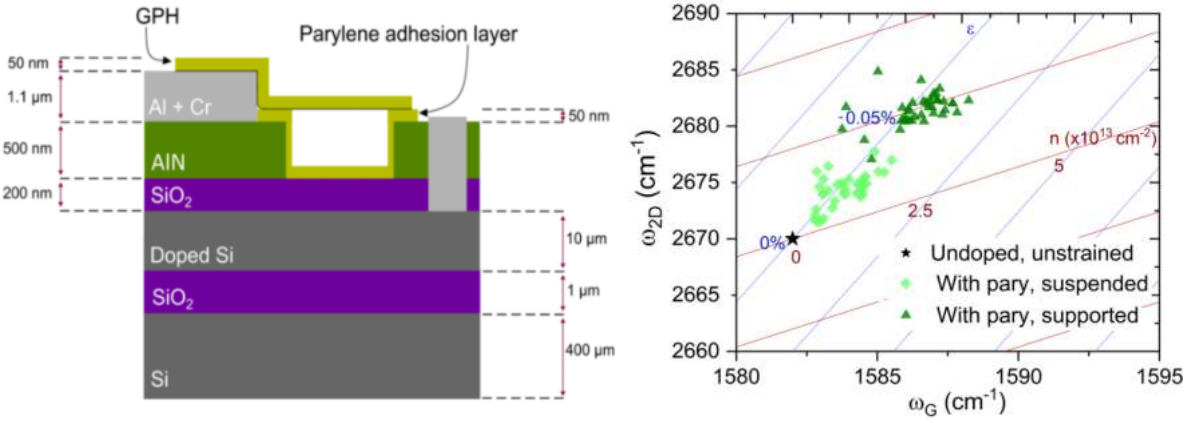

Figure 1: (a) Schematic cross-section of a graphene-parylene heterostructure membrane integrated on a PiezoMUMPs architecture substrate. (b) Statistical Raman peak-shift analysis to confirm biaxial pre-tension in the graphene membrane.

5-min charging technology

Yury Alaverdyan
Nyobolt, UK
Yury.Alaverdyan@nyobolt.com

85 percent of our energy in manufacturing and transportation comes from burning fossil fuels. Transportation itself accounts for almost two thirds of the oil used worldwide. According to recent estimations, we have 40 years of oil and 50 years of gas left before we run out. We need all the technological developments imaginable to make sure that we reach 100% renewable energy by 2050. Besides, combustion of fossil fuels leads to toxic exhausts, and nearly 1.2 million people die each year due to air pollution, especially in urban areas. Decarbonization of manufacturing and transportation has become time-critical, and quick technological advances are urgently needed. One of the most effective ways is a combination of renewable energy, electrification and battery storage technology. However, in order to be widely adopted, such battery systems must be fast-charging, convenient, cheap and efficient.
After 5 years' development in the anode materials' chemistry, unique cell design and scale-up method, Nyobolt has finally created the battery system capable of charging a vehicle under 5min, achieving up to 25,000 cycles without significant degradation. Our technology unlocked the potential for electrification in commercial robotics by increasing uptime 3 times. High-power and heavy-duty vehicles and tools powered by Nyobolt batteries benefit from nearly degradation-free charge-discharge cycles. In June 2024, our prototype sports car's battery packs has achieved exceptional charging rate of 5.5kWh/min (equivalent to 330kW of rapid charging) in the first on-road driving and charging test, adding ~40km per minute. This demonstrated topping up a vehicle from 10% to 80% in only 4min 37sec.
The anode technologies developed by Nyobolt are based on niobium tungsten oxide (NWO) chemistry and graphite-dominant species. NWO suits high cycle life applications, while the graphite-dominant batteries benefit from higher energy density, lower cost and weight, while maintaining good power and cycle life characteristics.

Figures

Decarbonizing the Fossil Fuel Sector Through High-Temperature Materials for Solid Oxide Fuel Cells

Mohammad Ali Haider[a,b]
[a]*Indian Institute of Technology Delhi - Abu Dhabi, Khalifa City, Abu Dhabi, UAE*
[b]*Renewable Energy and Chemicals Lab, Department of Chemical Engineering, Indian Institute of Technology Delhi, Hauz Khas, New Delhi-110016,* haider@iitdabudhabi.ac.ae, www.reclab.in

Abstract

Global fossil fuel CO_2 emissions total approximately 35 gigatons per year, with around half originating from coal. Achieving net-zero emissions necessitates significant reductions, requiring disruptive technologies such as zero-emission coal and third-generation power systems. This transition relies on the development of innovative catalyst materials for effective fuel utilization and CO_2 reduction. Towards this, high-temperature solid oxide fuel cells (SOFCs) offer several advantages, facilitating efficient energy production and CO_2 reduction through reversible operation. However, advancing effective electrode materials for zero-emission coal or SOFC-integrated power systems presents a significant technological bottleneck **[1-2]**. To tackle these material design challenges, we adopt a combined experimental and theoretical approach, analysing the rate-limiting processes in the materials **[3]**. We propose rational tailoring of the electrode material through nanostructuring approaches, which could lead to breakthroughs in SOFC electrode design **[2]**.

Inorganic perovskite materials are touted as the next generation of electrode materials for energy conversion in high temperature electrolyzers and SOFCs owing to its significantly high electronic and ionic conductivity. In search of a suitable composition of the perovskite material, several combinations of cations are proposed to design the perovskite, which can match the desired conductivity and stability in the high temperature electrochemical device (electrolyzes or a fuel cell). Herein a bottom-up approach in designing the composition of cations and dopants is presented to come up with a rationale to discover new materials for oxygen reduction reaction in SOFCs. More specifically, material stability in oxidizing environment is probed to design high performance electrodes wherein mechanistic elucidations of the rate-limiting processes is leading to the rational electrode design. For example, in a geometrically well-defined experiment, cation segregation to the surface is observed to limit the SOFC performance. This acts as a stumbling block in the commercial success of the SOFCs. Following which, strategies are proposed to control cation segregation at the molecular level, which may significantly improve the electrochemical performance. This is elucidated in nanostructured fabrication of the electrode material as a thin film **[3]** or a nanoparticle **[2].**

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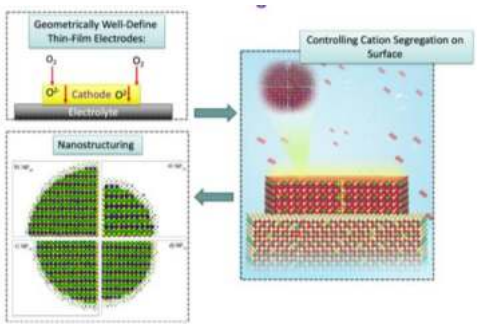

Figure 1: Mechanistic and rational design of high-temperature materials for solid oxide cells.

Biosketch: Prof. M. Ali Haider is working as a Vice Provost Research and External Engagement at the Indian Institute of Technology Delhi- Abu Dhabi. He holds an M.S. and PhD in Chemical Engineering from the University of Virginia, as well as a B.Tech. from the Indian Institute of Technology (IIT) Guwahati. Prof. Haider serves as an Editorial Advisory Board member for the journal ACS Sustainable Chemistry & Engineering. In 2023, he visited the Catalysis Research Center, Technical University Munich, as an Alexander von Humboldt fellow. The Royal Society of Chemistry has recognized his research contributions on various occasions, designating him as the 'Emerging Investigator' in the Reaction Chemistry & Engineering journal, a 'Highly Cited Author' in the Green Chemistry journal, and as part of the 'Editor's Choice Collection' in the Journal of Materials Chemistry A. He was a visiting fellow at the Catalysis Center for Energy Innovation at the University of Delaware, supported by the 'Bioenergy-Award for Cutting Edge Research' sponsored by the Indo–US Science and Technology Forum. For his research work in utilizing high-performance computing (HPC) to solve problems related to sustainability and climate change, Hewlett Packard Enterprise and Intel have bestowed upon him the 'Dr. A.P.J Abdul Kalam HPC Award for R&D in HPC Application'. He is a member of The National Academy of Sciences, India (NASI) and the Indian National Young Academy of Sciences (INYAS), actively engaging in delivering motivational and popular science lectures on sustainability, climate change, nanoscale catalysis, and renewable energy.

Chemical Sensing with Graphene Liquid-Gate Transistors

Pedro Alpuim[1,2], Mafalda Abrantes[1,2], Tiago Pereira[1], Telma Domingues[1,2], Bruno M. Costa[3], João Mouro[1], Luís Jacinto[4], Jérôme Borme[1]
[1]*International Iberian Nanotechnology Laboratory, Braga, Portugal*
[2]*Centro de Física das Universidades do Minho e Porto, Universidade do Minho, Braga, Portugal*
[3]*Instituto de Investigação em Ciências da Vida e da Saúde, Escola de Medicina, Universidade do Minho, Braga, Portugal*
[4]*Experimental Biology Unit, Department of Biomedicine, Faculty of Medicine, University of Porto, Porto, Portugal*
pedro.alpuim@inl.int

Abstract
Biosensing with graphene transistors, with their promising potential, is a significant area of research. Their inherent 2D nature, high carrier field-effect mobility and ambipolar transport, chemical inertness and robustness, and the possibility of surface functionalization make them a compelling choice. The sensing principle – local gating by analyte molecules whenever they attach to the graphene channel – modulates its Fermi energy, causing a shift in the transistor transfer curve, typically detected by measuring the point of minimum conductance [1]. I will show the attomolar detection of single-stranded DNA containing a mutation occurring in brain tumor cells and the results on neurotransmitter detection using a short-strand dopamine-specific DNA aptamer [2]. I'll present DC and AC configurations for the graphene chip interrogation and signal acquisition. Finally, liquid-gate transistors often suffer from electrical instability due to the interaction of their charge carriers with the defects in the surrounding insulator layers [3]. Here, we present a complete model for the observed transfer curve drift based on the electron capture and emission rates from and to the SiO_x defect bands. Once understood, this effect can be controlled, effectively removing the drift in most practical situations.

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Figures

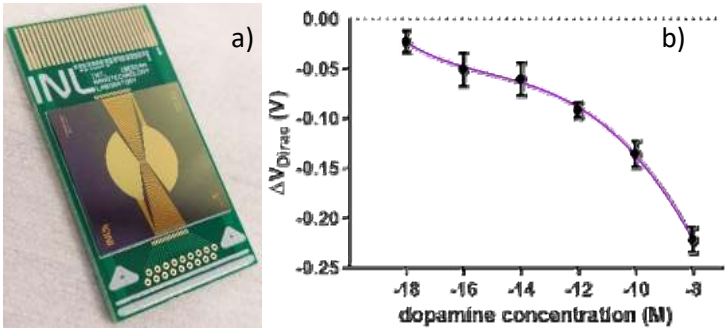

Figure 1: a) Graphene 32-transistor transparent chip for b) dopamine detection in animal model brain homogenates.

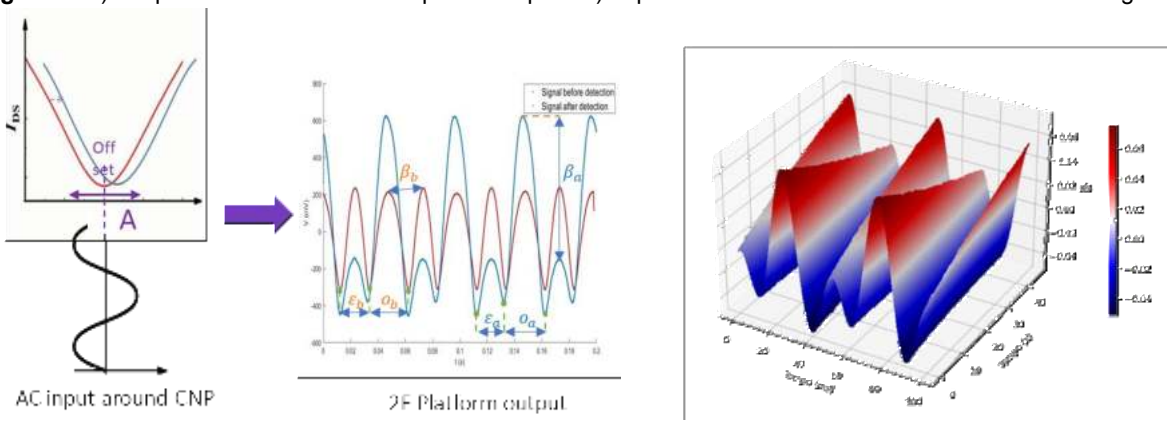

Figure 2: Dopamine detection in an opto-evoked animal model in AC f/2f mode: the transistor polarized at the CNP is a frequency doubler. The signal is the distortion in the 2f output as local gating shifts the polarization away from CNP.

Nano-Characterization of Nanomaterials Using Electron Microscopy

Dalaver H. Anjum, Mohamed E. Daoud, Zeyad M Abdulhamid, Yarjan Abdulsamad, and Kyriaki Polychronopoulou
Khalifa University, P. O. Box 127788, Abu Dhabi, United Arab Emirates
Dalaver.anjum@ku.ac.ae

The concept of nanotechnology was introduced by 20th-century celebrated Physicist Richard P. Feynman, who proposed using 1 nm^3 size clusters as “computer bits” [1, 2]. He noted the inadequate spatial resolution of the transmission electron microscope (TEM), which could not meet the challenges of imaging and characterizing the objects down to single nanometer-size clusters. Understandably, Feynman argued that the spatial resolution of TEM instruments should be improved [2]. Albeit unrelated, there have been consistent efforts to improve the resolution and capability of TEM instruments. In this regard, the significant developments introduced into TEM Instrumentation include spherical aberration correctors, high throughput X-ray dispersive spectroscopy (EDS) detectors, counting mode electron energy loss spectrometers (EELS), and pixelated array direct electron detectors [3, 4]. With the help of such correctors, contemporary TEMs routinely provide atomic-scale imaging and elemental and chemical analyses of samples [5]. For instance, a TEM's four-dimensional scanning transmission electron microscopy (4DSTEM) mode allows quantifying the microscale residual stresses in the range of tens of nanometers (Figure 1). Similarly, STEM-EDS mode can investigate the morphological and chemical properties of nanocomposites synthesized by combining nanoparticles (NPs) with 2D materials (Figure 2). Additional examples of nanoscale analysis of 2D materials with a TEM can also be noted.

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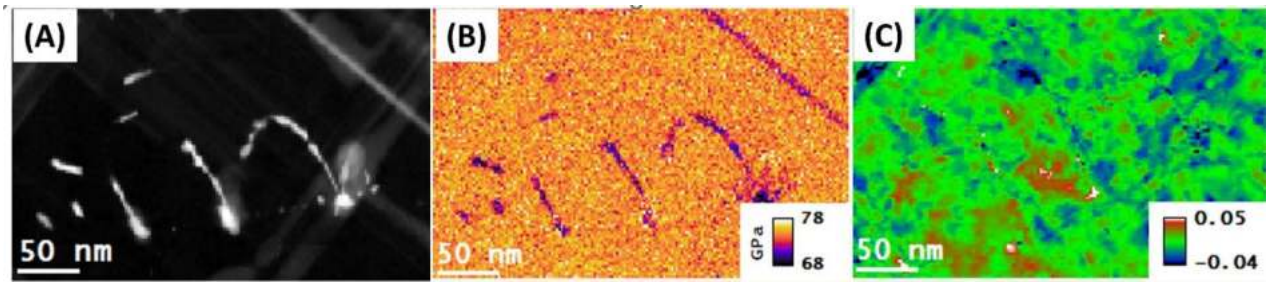

Figure 1: Nanoscale mapping of mechanical properties of Al2024 alloy. (A) DF-STEM Image. (B) Young’s modulus map was generated at a 3 nm pixel size using the STEM-VEELS mode of a TEM. (C) The strain map was also generated at a 3 nm pixel size using the 4DSTEM mode of TEM.

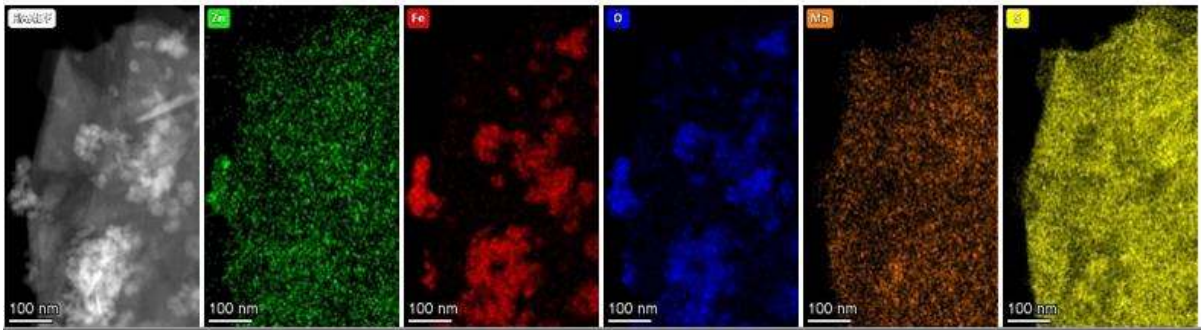

Figure 2: Morphological and elemental analysis of zinc-ferrite and molybdenum disulfide nanocomposite carried out using STEM-EELS mode of a TEM.

2D Material Membranes for Nanofiltration Applications

Mark A. Bissett
Molymem Ltd, Manchester, UK
Department of Materials, University of Manchester, Manchester, UK

Mark@Molymem.com
Mark.Bissett@Manchester.ac.uk

2D nanomaterials are becoming more and more popular within academia for applications in separation technology and recently we have seen them begin to transition from the lab into industry. Our company, Molymem Limited, is a University of Manchester spin-out which is commercialising our patented technology based on the 2D nanomaterial molybdenum disulphide (MoS_2). This material is used to form a coating consisting of a laminar structure of these 2D layers on top of porous supporting layers, and allows for an improvement in performance for efficient ionic rejection and nanofiltration applications in the water treatment industry. We can control the rejection and flux through chemical functionalisation of this coating as well as the use of composites of different 2D materials, allowing for a high degree of tunability. In this talk, I will give a technical background of our technology, and put it in context of the progress in the wider academic field on the use of 2D materials for filtration I will discuss some recent case studies which demonstrate the applicability of this technology to tackle real world problems, as well as discuss future directions we may see these 2D materials get adopted in the near future.

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Figures

Figure 1: Photograph showing an MoS_2 coated ceramic tubular membrane (Left). Photograph showing pilot scale testing facility using Molymem membranes. (Right)

Graphene industrial application towards decarbonization

Sivasambu Bohm & Benjamin Sarkozy
Industry Fellow at Imperial College London
& Graph-Nova

Lianhua_Bohm@outlook.com

Removal of 100 to 1,000 gigatonnes of CO2 this century may be needed to achieve deep decarbonization and avoid exceeding the 1.5°C climate target. Graphene materials and nanotechnology is playing key role. Graphene has found its use in numerous industrial applications due to its unique properties. While its impermeable and conductive nature can replace currently used anticorrosive toxic pigments in coating systems, graphene can be an important component as a next-generation additive for many industrial applications (1). Graphene, a sheet of carbon atoms bound together in a honeycomb lattice pattern, is hugely recognized as a “wonder material” due to the myriad of astonishing attributes it holds. It is a potent conductor of electrical and thermal energy, extremely lightweight chemically inert, and flexible with a large surface area. It is also considered eco-friendly and sustainable, with unlimited possibilities for numerous applications.
The current bottlenecks in using graphene & graphene oxide are the availability of cost-effective, high-quality materials from graphite and their effective incorporation into the product matrices.

On overcoming these factors, graphene may attract significant demands in terms of volume consumption. Graphene can be produced on industrial scales and cost-effective top-down routes such as chemical, electrochemical, and/or high-pressure mechanical exfoliation. Graphene depending on end applications can be chemically tuned and modified via functionalisation so that easy incorporation into product matrices is possible. This talks able to discuss and Graphene advanced production methods and their impact on the quality of graphene produced in terms of energy input and quality. Graphene with an average thickness below five layers were produced by few methods with varied defects. Graphene additive role in Graphene Inks and Li-ion batteries, Anti corrosion coating for automotive, PEM Fuel cells as well discussed and commercial development electric floor heating of construction applications.

Keywords: Graphene, Few Layer Graphene, Graphene industrial scale up production, Inks and coatings, Graphite, PEM Fuel cells, Li-Ion Battery additives.

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High dimensional analysis for 2D material interactions with the immune system

Lucia Gemma Delogu[1,2]
1. *Department of Biological Sciences, Khalifa University of Science and Technology, Abu Dhabi, UAE*
2. *Department of Biomedical Science, University of Padua, Padua, Italy*
lucia.delogu@ku.ac.ae

Deepening our understanding of immune cell behavior is vital for creating safe, effective treatments, particularly as immune cell therapy, also known as cellular immunotherapy or cell-based immunotherapy, represents a groundbreaking approach in the treatment of various diseases, including cancer. Transition metal carbides and nitrides (MXenes)[1], a novel family of 2D nanomaterials, show promise as advanced trackers for immune cells, key for precise diagnostics and therapies.[2–4] Traditional cell labeling methods have stagnated due to limited chemical options, impeding progress in applied medicine. Moreover, these methods are incompatible with single-cell mass cytometry by time-of-flight (CyTOF), a globally adopted technology that improves classical flow cytometry. We propose an innovative solution utilizing MXenes to overcome these challenges. Our method, Label-free sINgle-cell tracKing of 2D matErials by mass cytometry (LINKED), leverages a novel, biocompatible, multiplexed, label-free detection approach via CyTOF and Mass Ion Beam Imaging by Time-of-Flight (MIBI-TOF).[2] Our approach overcomes chemical limitations and integrates seamlessly with CyTOF, allowing for nanomaterial detection and simultaneous measurement of diverse immune cell and tissue features. I will share how the linked approach[2] can be applied to other 2D materials [5] and micro e nanoplastics[6]. Moreover, I will show how our work[2] promises to advance immunological research significantly, offering refined cell labeling and tracking techniques crucial for the advancement of translational medicine (*unpublished data*).

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MXenes for Interface Engineering in Halide Perovskite Photovoltaic

Aldo Di Carlo
CRM-ISM, Istituto di Struttura della Materia-CNR, via del Fosso del Cavaliere 100, 00133 Rome (Italy)
CHOSE-University of Rome Tor Vergata, via del Politecnico 1, 00133 Rome (Italy)
Aldo.dicarlo@uniroma2.it

Perovskite solar cells (PSCs) have emerged as one of the most promising next-generation photovoltaic (PV) technologies due to their high efficiencies and simple solution-based fabrication processes, comparable to conventional PV systems. Interface engineering plays a critical role in multi-layered PSCs by controlling many properties of the overall system. We previously demonstrated that graphene and other 2D materials, such as MoS_2, can effectively tune interface properties and improve cell efficiency.[1,2] In this talk I will present the discuss about the $Ti_3C_2T_x$ and other MXenes with different surface terminations (T_x) as an effective strategy to modulate the work function (WF) of both the perovskite absorber and the electron transport layer (ETL), thus optimizing the perovskite/ETL interface and enhancing cell performance and stability.

Using ultraviolet photoemission spectroscopy and Density Functional Theory (DFT) calculations, we demonstrate that incorporating $Ti_3C_2T_x$ into halide perovskite and ETL enables WF tuning without altering other electronic properties. We establish a nonlinear correlation between the terminal group composition and the resulting WF for both standalone MXenes and MXene/perovskite composites. Our results [3] show that the dipole moment induced by $Ti_3C_2T_x$ at the perovskite/ETL interface can modify the band alignment between these layers, leading to significant performance improvements. Specifically, MXene-modified PSCs in a direct (nip) configuration show a 26% increase in power conversion efficiency (PCE) and reduced hysteresis compared to reference cells. Similarly, for the inverted (pin) configuration using a NiO/perovskite+MXenes/PCBM stack, comparable enhancements were observed.[4] Specifically, using MXenes on the n-side of a pin cell structure (NiO/perovskite/C60/BCP/Cu) significantly enhances cell stability, achieving T90 > 2000 h under continuous light soaking at Maximum Power Point in ambient conditions and T80 > 1000 h under thermal stress at 85 °C.[5]

I will also show as MXenes combined with other 2D materials can be effectively used in perovskite/silicon tandem cell [6], modules and panels paving the way for possible industrialization of the MXene-Perovskite PV.

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Towards a new generation of antiviral tools. Hyperbranched polylysine nanopolimers and photoactive carbon dots as effective antivirals

Plinio Innocenzi
Department of Biomedical Sciences. Laboratory of Materials Science and Nanotecnology (LMNT). University of Sassari. Viale San Pietro, 43/B. Italy *Contact:* plinio@uniss.it

The coronavirus pandemic (COVID-19) has shown that different approaches must be put in place to confront viral infections. There is strong need for treatment options and a strong request for other effective, safe, and broad-spectrum antiviral systems in light of future emergent pandemics. In our laboratory we have developed two different nanotools as innovative antivirals based on carbon dots. The first example is a polymeric nanomaterial derived from L-lysine, with an antiviral activity against SARS-CoV-2 associated with a good safety profile in vitro. Nanoparticles of hyperbranched polylysine, synthesized by L-lysine thermal polymerization and catalyzed by boric acid, effectively inhibit the SARS-CoV-2 replication. The virucidal activity is associated with the charge and dimension of the nanomaterial, favouring the electrostatic interaction with the viral surface being only slightly larger than the virion dimensions.

Carbon dots (C-dots) are a type of nanomaterial that can produce reactive oxygen species (ROS) when photoactivated. These ROS can disrupt the structure of viruses, making C-dots a promising candidate for biocidal applications. Additionally, C-dots exhibit oxidant-antioxidant properties that can be used for antibacterial, wound healing, and antiviral purposes. Pro-oxidant C-dots have been developed via microwave synthesis using an amino acid, glycine, and 1,5-diaminonaphtaleneas precursors. The C-dots shown to contain radical centers whose intensity increases upon illumination by UV and also visible light. They also show the capability of generating singlet oxygen through energy transfer to oxygen molecules when irradiated. The C-dots exhibit effective virucidal activity and have been tested in vitro using two different variants of SARS-CoV-2. Antiviral C-dots have been finally used to functionalize a model surface, inducing a strong virucidal activity against the SARS-CoV-2 coronavirus with both ultraviolet (UV) and visible (VL) light. Controlled activation of C-dots can produce ROS on demand, ensuring their safe and effective use. With the development of photoactivated C-dots, effective disinfectants for enveloped viruses and antiviral surfaces are expected to emerge.

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Figures

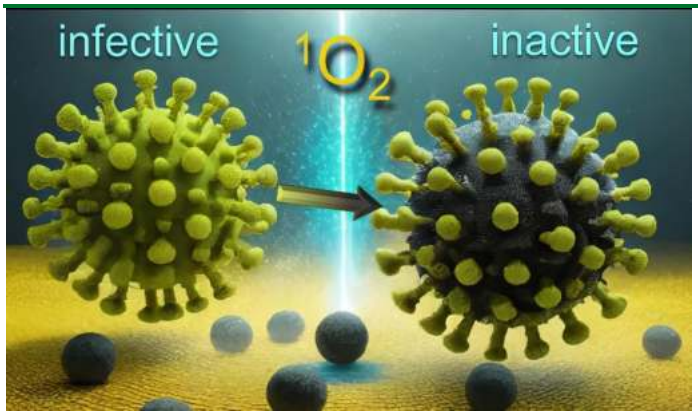

Figure 1: Singlet oxygen produced by C-dots is able to inactivate SARS-CoV-2 virions

Observing various Moiré pattern on two-dimensional (2D) materials by advanced Atomic Force Microscopy (AFM) based imaging techniques

Chris Jung
Park Systems Corp. South Korea

The observation of moiré patterns in two-dimensional (2D) materials has become a focal point in materials science due to the unique electronic and mechanical properties these patterns can induce. Advanced Atomic Force Microscopy (AFM) based imaging techniques, including Conductive AFM (C-AFM), Piezoresponse Force Microscopy (PFM), Lateral Force Microscopy (LFM), and Torsional Resonance Mode AFM (TFM), provide high-resolution insights into these moiré patterns. These techniques enable the detailed characterization of surface topography, electronic properties, and mechanical behavior at the nanoscale. By utilizing these advanced AFM methods, researchers can visualize and manipulate the moiré superlattices formed in 2D heterostructures, such as graphene on hexagonal boron nitride (hBN) or transition metal dichalcogenides (TMDs). The findings reveal that the moiré patterns significantly influence the local electronic states, leading to phenomena such as flat bands and correlated insulating states. This research not only enhances our understanding of 2D materials but also opens up new possibilities for designing novel electronic devices with tailored properties

Plasma Jet Printing and in Situ oxidation of Mxene surfaces

Satheesh Krishnamurthy
Advanced Technology Institute, Surrey Ion Beam Centre, University of Surrey, Guildford, UK
Contact s.krishnamurthy@surrey.ac.uk

We developed an innovative approach to print TiO_2-Ti_2C MXene heterostructures with promising applications in photocatalysis. Leveraging a low-powered atmospheric pressure plasma jet (APPJ) for in situ oxidation of Ti_2C MXene provides a controlled and energy-efficient route to forming TiO_2 layers with tailored electronic and structural properties. The in-situ oxidation method using APPJ promotes the formation of defect-rich TiO_2 on the Ti_2C substrate, which can enhance photocatalytic performance due to improved light absorption and charge separation. The creation of vacancies and mixed oxidation states of Ti and C likely contributes to a broadening of the absorption spectrum and facilitates electron mobility, crucial for efficient photocatalysis. The introduction of vacancies and the variation in valence states of titanium and carbon enhances the electronic density of states near the Fermi level. This modification may improve the MXenes catalytic efficiency by reducing electron-hole recombination rates and enabling more effective charge transfer.

The use of APPJ not only enables in situ oxidation but also offers flexibility for surface functionalization, which is advantageous for tailoring the photocatalytic properties to specific applications. Additionally, APPJ's potential in printing and depositing these materials on diverse substrates can open new avenues in device integration and scalability. These TiO_2-Ti_2C MXene heterostructure shows promise for thin-film photocatalytic electrodes, which could be useful in environmental and energy-related applications, such as wastewater treatment and hydrogen production. Its deployment versatility could also extend to other photocatalytic and optoelectronic uses.

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From Lab to Field: Overcoming Challenges in Perovskite Photovoltaics Commercialization through 2D Interface Engineering

Emmanuel Kymakis
Department of Electrical & Computer Engineering, Hellenic Mediterranean University, Heraklion, Crete, Greece.
kymakis@hmu.gr

Perovskite photovoltaics (PePV) have emerged as a highly promising alternative energy solution over the past decade. Their potential for high efficiency makes them suitable for both large-scale solar farms and low-power applications, such as Internet of Things (IoT) devices. The power conversion efficiency (PCE) of PePVs has now surpassed 26%, approaching the performance of the most efficient crystalline silicon solar cells. Despite these impressive PCE, translating this performance to large-area photovoltaic (PV) panels in real-world outdoor settings remains a significant challenge. One of the critical hurdles is interface engineering, which is essential for the effective commercialization of PePVs technology. This involves the use of solution-processable two-dimensional (2D) materials, such as graphene and transition metal dichalcogenides, to enhance the interfaces within the solar cells. These 2D materials play a crucial role in protecting the perovskite layer from environmental factors like oxygen, moisture, and metal ion migration. Additionally, they improve charge dynamics at the interfaces, which is vital for maintaining high efficiency and stability.
The potential and challenges of PePVs have been demonstrated through extensive field testing. For instance, at a solar farm on the HMU campus in Crete, five square meters of perovskite PV panels were installed, and their energy output was continuously monitored using custom-built maximum power point trackers. Over eight months (T80 of 5,832 hours), the energy output experienced a 20% decline, despite initially surpassing 260 W at its peak. The primary causes of this degradation were identified as high temperatures, solar irradiance, moisture, and oxygen infiltration due to lamination failure. Distinctive light-soaking behaviors were also observed, which affected the power output and revealed the progression of optical defects over time. These behaviors are crucial to understand as they impact the long-term performance and stability of PSCs.To enhance the performance, durability, and stability of PSCs in real-world environments, advanced characterization techniques are being deployed alongside conventional methods. Continuous I-V tracing, for example, enables real-time monitoring of current-voltage characteristics over extended periods. This provides valuable insights into the operational stability and dynamic behavior of PSCs, especially under fluctuating environmental conditions. Therefore, optimizing the optical configuration, including the orientation and inclination of modules during installation, is essential to maximize energy output. This is particularly important in climates with substantial temperature fluctuations. Understanding phenomena such as light-soaking and analyzing temperature dependence coefficients are crucial for predicting the long-term stability of PSCs. In conclusion, while PSCs hold great promise for the future of solar energy, significant challenges remain in translating their high efficiency to large-scale applications. Through continued research and field testing, particularly in interface engineering and advanced characterization techniques, we can better understand and overcome these challenges, paving the way for the effective commercialization of PePVs technology.

Advancing Memory Technologies with 2D Materials

Ammar Nayfeh
RIC2D / Khalifa University, UAE
ammar.nayfeh@ku.ac.ae

Two-dimensional (2D) materials, offer exceptional mechanical strength, atomic-scale thickness, with good conductivity allowing for miniaturization of nonvolatile memory while enhancing performance. In this talk, an exploration of research conducted on several prominent 2D materials, including graphene, molybdenum disulfide (MoS2), covalent organic frameworks (COF) and conjugated microporous polymers (CMP) is highlighted. Using the state of art equipment at Khalifa University housed in the United Arab Emirates (UAE) and the regions first cleanroom fabrication facility that allows for growth and fabrication of advanced 2D materials. The talk addresses current challenges faced in growth, synthesis, and design of 2D materials for memory technologies. These materials provide avenues for engineering novel memory applications, such as high-performance, flexible electronics, and next-generation wearables. The use of 2D nanomaterials could allow for development of next generation memory devices. Moreover, 2D materials are poised to transform the landscape of memory with a potential to form the cornerstone of an entirely new class of memory technologies.

Upcycling and recycling of commercial water filters using graphene derivatives

Vincenzo Palermo[a,b], Lidia Lancellotti,[a] Sara Khaliha, [a] Francesca, Tunioli, [a] Antonio Bianchi,[a] Cristian Bettini, [a] Alessandro Kovtun,[a] Massimo Gazzano,[a] Tainah Dorina Marforio,[c] Zhen Yuan Xia[b], Matteo Calvaresi,[c] Chiara Zanardi,[a,d] Manuela Melucci.[a]

[a]*Institute for Organic Synthesis and Photoreactivity, National Research Council (ISOF-CNR), Bologna (BO), Italy*
[b]*Department of Industrial and Materials Science, Chalmers University of Technology, Gothenburg, Sweden*
[c]*Department of Chemistry 'G. Ciamician', Alma Mater Studiorum University of Bologna, Italy*
[d]*Department of Molecular Sciences and Nanosystems, Ca' Foscari University of Venice, Italy*

palermo@isof.cnr.it

Commercial water filters use often hollow fibers (HF) made of polymers, typically polyethersulfone (PES), for microfiltration. Each filter typically includes hundreds of sub-millimeter diameter fibers (e.g. 300 μm) with nanometric pores that define the module cut-off (ca. 150 nm). The feed solution flows inside the fiber, and purified water exits through the lateral pores.
Graphene oxide (GO) has gained attention as a leading material for creating advanced membranes for water filtration and desalinization. These can be made by filtering GO nanosheets in water on porous substrates, resulting in organized membranes with nanochannels. However, GO-based membranes have been limited to lab use due to difficulties in producing larger, uniform filters necessary for real-world applications like water purification.
In past years we demonstrated the possibility to use together commercial filters and nano-materials, coating PES fibers with GO to obtain a composite bilayer membrane.[1-3] This membrane retains the microfiltration properties of PES-HF while also enabling the adsorption of small ions and molecules. This year, we used the same approach to recycle scraps deriving from industrial production of commercial filters.[4] Hollow fibers were cut in small granular particles and upcycled as sorbents of several classes of emerging and standard water contaminants, such as drugs, heavy metal ions, and a mixture of per- and poly-fluoroalkyl substances (PFASs). The millimetric sized granules outperformed granular activated carbon (GAC), the industrial sorbent benchmark, in the adsorption of lead, diclofenac, and PFOA from tap water.

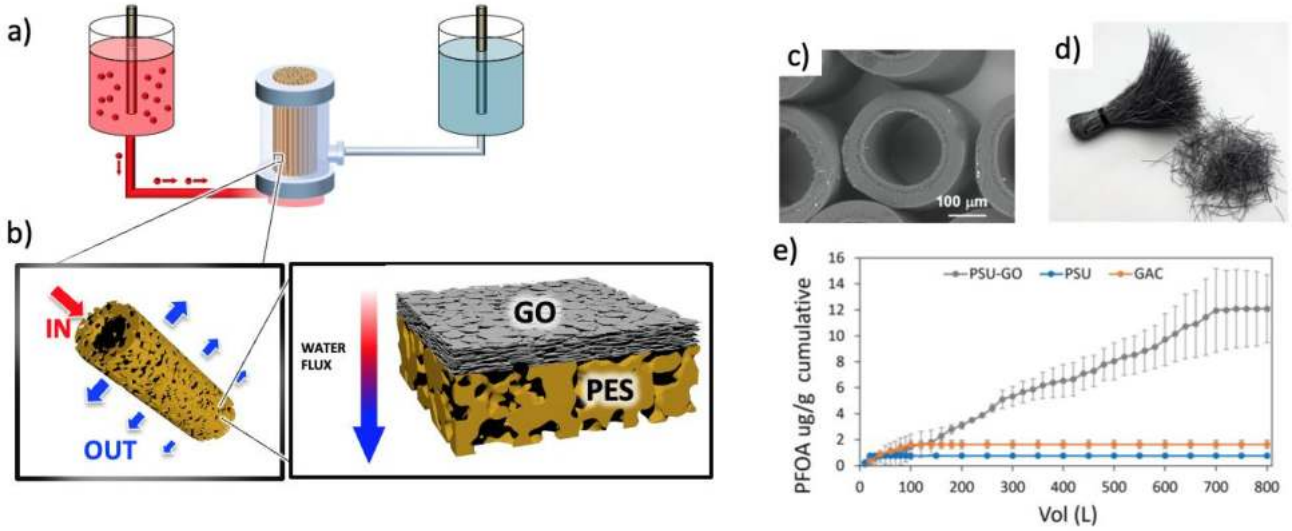

Figure 1: a) cartoon showing hollow fiber filtration. c,d) SEM and photo of typical hollow fibers. e) Cumulative performance of removing perfluorooctanoic acid pollution from water upon filtration of >800 L, as compared to Benchmark.

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Organic (nano)bioelectronics for point of care diagnostics

Anna-Maria Pappa
Khalifa University, UAE
anna.pappa@ku.ac.ae

The development of micro-electronic devices that bridge the gap between the rigidity of traditional electronics with the soft mechanics of biological systems is highly desirable. The emergence of highly conjugated polymers with interesting electronic and optical properties, opened up exciting directions in biomedical research including point-of-care diagnostics. With the ultimate goal of fully integrated wearable sensors combined with IoT, and that of autonomous at-home diagnostic tests, polymer electronics have been heavily explored the past decade resulting in novel device configurations. Multiplexing capability, ability to adopt to complex performance requirements in biological fluids, sensitivity, stability, literal flexibility and compatibility with large-area processes are only some of the merits of conjugated polymers for point of care diagnostics. This talk will summarize our recent efforts on developing (nano)biosensors for health monitoring, harnessing the ease and versatility in processability of polymers with the high surface to volume ratio of 2D structures/ materials, with direct applications in point-of-care diagnostics.

Tailoring Ni-based catalysts for Dry Reforming of Methane and Hydrogen Production: The Forefront of Sustainable Energy

Aseel G.S Hussien, Eswar P. Komarala, **Kyriaki Polychronopoulou**
Department of Mechanical Engineering, Khalifa University of Science and Technology, Main Campus, P.O. Box 127788, Abu Dhabi, United Arab Emirates
Center for Catalysis and Separations, Khalifa University of Science and Technology, P.O. Box 127788, Abu Dhabi, United Arab Emirates
kyriaki.polychrono@ku.ac.ae

Dry reforming of methane (DRM) is an endothermic catalytic process that converts greenhouse gases (GHGs) into clean hydrogen (H_2) fuel and synthesis gas (syngas, CO/H_2), positioning it as a key player in sustainable energy solutions. The syngas produced can be utilized for fuel production and high-value chemicals. Despite its potential in mitigating global warming, DRM has not yet been industrialized due to economic challenges.

$CH_4 + CO_2 \leftrightarrow 2\ CO + 2\ H_2$; $\triangle H+$ (298 K) = + 247.3 kJ mol^{-1} (Eq. 1)

In this keynote talk, I will present the main challenges facing DRM and highlight the crucial role of catalyst design in developing robust and stable catalysts to enhance reaction performance and stability. Additionally, I will explore advanced methodologies for catalyst evaluation, particularly transient isotopic isothermal experiments (TIIE), which is powerful tool for understanding catalytic mechanisms.

The economic viability of Ni-based catalysts has spurred numerous studies on these systems for DRM. However, high operating temperatures and competing side reactions, such as methane decomposition and CO disproportionation, lead to sintering of active sites and carbon deposition on the catalyst surface. Factors such as metal-support interaction, preparation methods, porosity, and metal dispersion significantly influence catalyst performance.

Various catalyst carriers namely doped ceria and SBA-15, alongside unsupported metal-organic frameworks (MOFs) are discussed in details. Doping ceria with other trivalent rare-earth metals (La+3) increases lattice oxygen mobility and basicity which improved coke resistance. The improved stability and carbon inhibition were correlated to the liable oxygen that gasified the carbon formed during the reaction. In another study, SBA-15 was used to combine the benefits of doped ceria and mesoporosity. The high surface area of SBA-15 was used to improve the interaction between Ni active sites and CeLa10Cu promotor and confinement of the Ni in its channels (dispersion). Whereas, in the case of coalesced Ni- and La-MOFs, negligible carbon formation and high CH4 conversion rates under DRM conditions at 800 °C were used. The use of terephthalic acid (BDC) as an organic linker achieved strong metal-support interactions (SMSI) and produced highly active and stable catalysts towards DRM reaction.

In conclusion, while DRM holds significant promise for the future of hydrogen energy, challenges remain for its commercialization. Through continued research and advanced characterization techniques, we can deepen our understanding and overcome these hurdles, paving the way for the effective commercialization of the DRM process.

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The role of advanced materials in the future of Space Exploration

Carlo Saverio Iorio
Université Libre de Bruxelles
carlo.iorio@ulb.be

Advanced materials play a critical role in shaping the future of space exploration, offering solutions to challenges like extreme temperatures, high radiation, and limited resources. Innovations in materials science, including lightweight composites, radiation-resistant polymers, and self-healing materials, enhance the safety, durability, and efficiency of spacecraft and habitats. These materials enable longer missions, more resilient structures, and greater sustainability in deep-space environments. As space exploration pushes further into unknown territories, the development and deployment of advanced materials will be key to supporting human presence and scientific discovery beyond Earth's orbit.

Facile nanomaterial coated 3D printed spacer architectures for effective scaling control in membrane systems

Navya Thomas[1,2], Mahendra Kumar[1], Giovanni Palmisano[1], Rashid Abu AlRub[1], Reham Nuaimi[1], Emad Alhseinat[1], Reza Rowshan[3], Hassan Arafat[1]
[1]*Technology Innovation Institute, Abu Dhabi, United Arab Emirates*
[2]*Khalifa University, Abu Dhabi, United Arab Emirates*
[3]*New York University - Abu Dhabi Campus, Abu Dhabi, United Arab Emirates*
Navya.Thomas@tii.ae

In recent explorations of membrane-based desalination, innovative spacer designs and surface modifications are emerging as powerful tools to combat scaling, a persistent challenge in water treatment [1]. This study investigates the potential of 3D-printed, highly engineered spacers with advanced 2D nanomaterial coatings to enhance flux performance and mitigate scaling in membrane distillation (MD) systems. By utilizing 3D printing, we can create custom-designed spacer architectures that optimize flow within membrane channels, achieving both high flux rates and lower pressure drops. These uniquely structured spacers enhance flux by up to 50% compared to conventional mesh designs in MD process [2]. Further enhancing their effectiveness, we modified the surface chemistry of these 3D-printed spacers with nanomaterial coatings, including graphene, graphene oxide, reduced graphene oxide, and fluorinated silica nanoparticles. These coatings adjust surface properties such as wettability and free energy, introducing functional groups that alter spacer interactions with scalants. Coatings with graphene and fluorinated silica nanoparticles, in particular, create a micro-rough, hydrophobic surface texture with reduced surface energy, thus weakening the attachment of scalants at membrane-spacer contact points and lowering membrane scaling. The nanomaterial-coated spacer demonstrated a 74% reduction in scalant attachment compared to the uncoated spacer [3]. The integration of flow-optimized design and surface engineering showcases the role of nanomaterial coatings in enhancing performance, demonstrating how a spacer-centric approach can complement traditional membrane-focused strategies in desalination applications.

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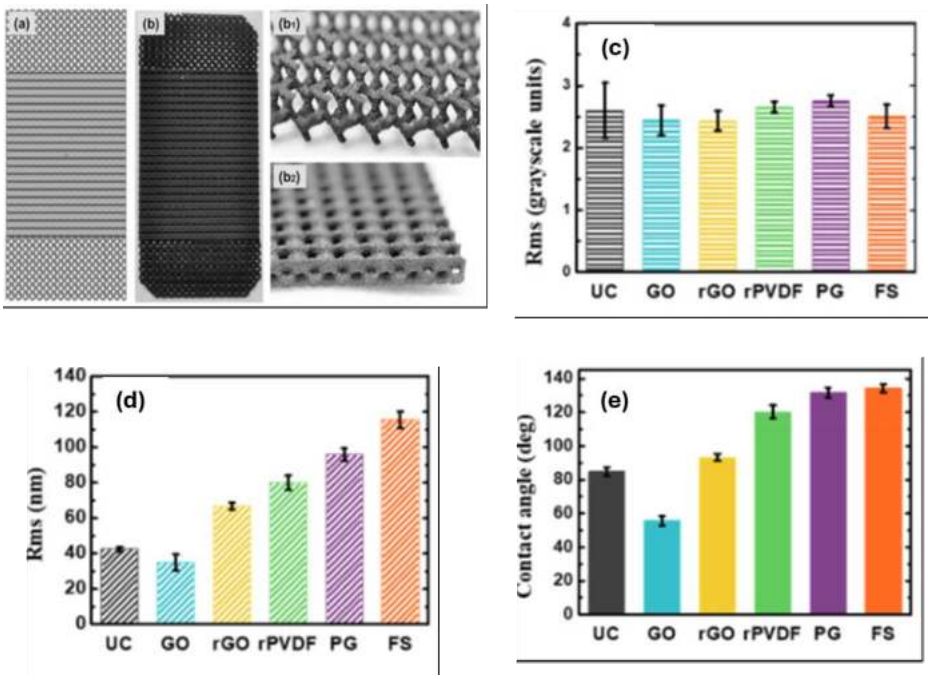

Figure 1: (a) Orthographic CAD drawing, (b) photographic image of the hybrid (Gyr-tCLP) 3D printed TPMS spacer, zoomed photographic images of (b1) Gyroid and (b2) tCLP architectures; comparison of the (c) macro-roughness, (d) micro-roughness, (e) contact angle measurements of nanomaterial coated and uncoated surfaces (UC – uncoated, GO – graphene oxide, rGO – reduced graphene oxide, PG – pristine graphene, FS – fluorinated silica).

Harnessing 2D Materials and Artificial Intelligence (AI) for Breakthroughs in Atmospheric Water Harvesting for Sustainable Water Solutions

Samar N. Abd Elwadood, Ludovic F. Dumée, Georgios Karanikolos, Samuel S. Mao.
Khalifa University, Department of Chemical Engineering, Abu Dhabi, United Arab Emirates
Research and Innovation Center on 2D Nanomaterials RIC2D
Center for Membranes and Advanced Water Technology CMAT
Samar.abdelwadood@ku.ac.ae

Water vapor is abundantly available in the atmosphere, making atmospheric water harvesting (AWH) technologies a promising solution for sustainable water production. We present novel composite networks, combining 2D graphene-based nanosheets within a polymeric matrix, which demonstrate exceptional water capture capabilities, with an intake of up to 7.15 g of water per gram of sorbent. The inclusion of graphene nanosheets enables desorption through natural sunlight, raising the temperature of the material by 71 °C within 20 minutes and yielding 3.36 liters of water per kilogram of sorbent per cycle. Additionally, the potential of metal-organic frameworks (MOFs) for AWH is explored, leveraging a machine learning (ML) approach to identify top-performing MOFs for water adsorption. By analyzing their structure, framework chemistry, and operational conditions, the ML models predict water adsorption properties, facilitating the screening of approximately 100,000 MOFs. This combination of experimental and data-driven methodologies underscores the potential of AWH technologies to sustainably and efficiently harvest water from atmospheric sources, while also offering new insights into the use of advanced materials like MOFs and composite hydrogels.

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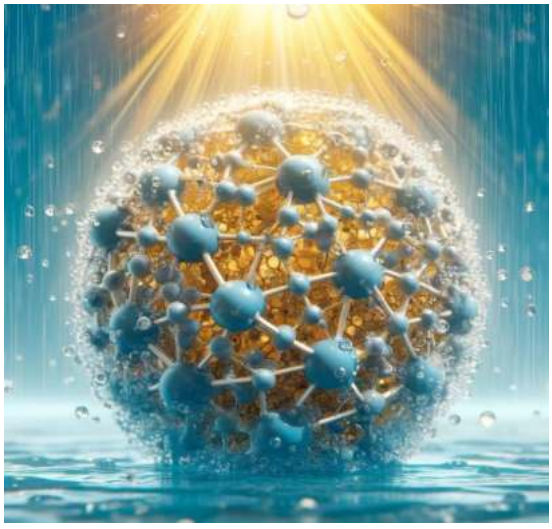

Figure 1: A novel network sorbent for AWH integrating 2D graphene-based nanosheets optimally assembled within a polymeric matrix.

Investigation of Electrochemical, Morphological, Rheological and Mechanical Properties of Nano-layered Graphene / Zinc Nanoparticles Incorporated Cold Galvanizing Compound at Reduced Pigment Volume Concentration

Dr. Muhammad Abid
Marjan Polymer Industries, Lahore 54000. Pakistan
info@marjanpolymer.com

The ultimate goal of this research was to produce a cold galvanizing compound (CGC) at reduced pigment volume concentration (PVC) to protect metallic structures from corrosion. The influence of the partial replacement of Zn dust by nano-layered graphene (NGr) and Zn metal nanoparticles on the electrochemical, morphological, rheological, and mechanical properties of CGC was investigated. EIS was used to explore the electrochemical nature of coatings. The EIS results revealed that the partial replacement of Zn by NGr and Zn nanoparticles enhanced the cathodic protection at reduced PVC (4:1) by improving the electrical contact between the Zn particles and the metal substrate. The Tafel scan was conducted to support the cathodic behaviour of the coatings. The sample formulated solely with Zn at PVC 4:1 was found to be dominated in physical barrier characteristics over cathodic protection. By increasing the concentration of NGr in the formulation, the corrosion potential shifted towards a more negative side. The coating with 1.5% NGr showed the highest galvanic action at reduced PVC. FE-SEM confirmed the interconnected network of conducting particles. The coating without NGr and Zn nanoparticles at PVC 4:1 showed significant gaps between the Zn dust particles. The novelty was evidenced when micrographs showed the consistent distribution of NGr and Zn nanoparticles all over the surface, which acted as a bridge between spherical Zn particles and provided cathodic protection at a reduced PVC. The layered structure of graphene also improved the physical shielding effect of the coatings, which limited the diffusion of electrolytes and corrosion products (oxides/hydroxides) into the coatings, which was reflected by the salt spray test. The rheological properties of coatings showed good liquid/fluid properties. All the coatings showed excellent adhesion but had different strength values. A real-time scratch resistance assessment showed all the coatings had good scratch resistance.

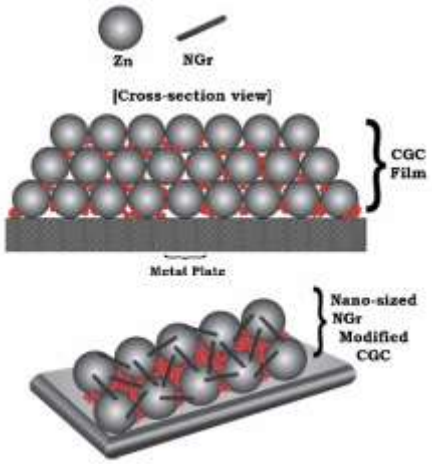

Figure 1: Structural Diagram Showing the Distribution and Function of Nano-Layered Graphene (NGr) and Zinc (Zn) Nanoparticles in Cold Galvanizing Compound (CGC) for Corrosion Protection

Functional PDA-coated MXene-Based Membranes for Targeted Antibiotic Purification in Hospital Effluents

Aya Fadl Aboukhater [1,2], Mahendra Kumar[1,2], and Shadi W. Hasan[1,2]

[1]*Research and Innovation Center in Graphene and 2D Materials (RIC-2D), Khalifa University, Abu Dhabi, UAE*

[2]*Center for Membrane and Advanced Water Technology, Khalifa University, Abu Dhabi, UAE*

Aya.aboukhater@gmail.com

Abstract

Two-dimensional (2D) lamellar membranes, particularly those incorporating mixed matrix MXene-based surfaces, have earned significant interest in water purification applications. Despite this interest, many 2D mixed matrix membranes face substantial challenges, including high instability, elevated internal resistance, low selectivity, and inadequate anti-fouling properties. This study introduces a novel approach to address these drawbacks by fabricating highly stable and charge-tunable modified MXene membranes. The membranes exhibit over 98% separation capabilities for various pharmaceuticals (tetracycline, and sulfamethoxazole) and demonstrate notable anti-fouling performance. The fabrication process involves the creation of high-performance MXene membranes with stable and tunable lamellar nanochannels through facile self-assembly. This process utilizes negatively charged 2D MXene ($Ti_3C_2T_x$) nanosheets. Importantly, the MXene's charge tunability is achieved through a one-step missile step-inspired sieve base addition reaction during functionalization. Various characterization techniques, including XRD, FT-IR, Raman, TGA, XPS, Zeta-potential, SEM, and SEM-EDS, were employed to confirm the successful synthesis and gain insights into the physical and chemical properties of the nanomaterials and membranes. The impact of increasing functionalized MXene loading was investigated at levels of 0.5wt%, 1wt%, and up to 6wt%. Membrane stability, tested over one month, revealed enhanced stability in membranes containing functionalized MXene compared to unmodified MXene.

Figures

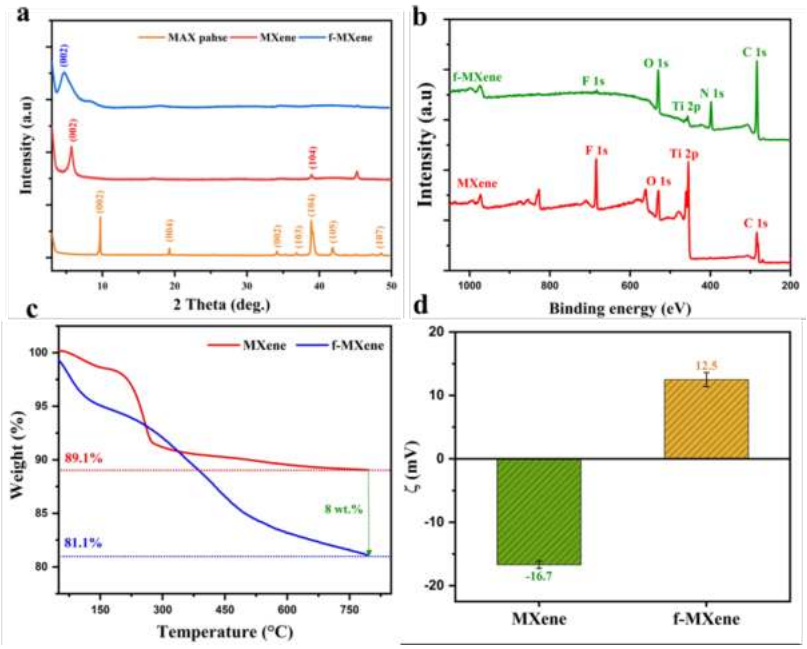

Figure 1: Characterization of MXene and f-MXene nanocomposites (a) XRD spectra; (b) XPS survey; (c) TGA data and (d) zeta potential (ζ; mV).

Self-dewatering Polyacrylic Acid-Alginate-Graphene Oxide hydrogel as an osmotic drawing agent in groundwater fertigation

Ahmed Mamdouh Aboulella [a,b], Adetunji Alabi [a,b], Maryam R. Al Shehhi [a], Linda Zou [a,b,*]
[a] *Department of Civil and Environmental Engineering, Khalifa University, PO Box 127788, Abu Dhabi, United Arab Emirates*
[b] *The Research & Innovation Center for Graphene and 2D Materials (RIC-2D), Khalifa University, PO Box 127788, Abu Dhabi, United Arab Emirates*
linda.zou@ku.ac.ae

Abstract (Arial 10)
Here, we report a graphene oxide-based hydrogel (which is a follow-up from Alabi et al. [1], [2]) used as an osmotic drawing agent for groundwater fertigation. In this work, a PAG hydrogel was fabricated from polyacrylic acid (PAA), sodium alginate (SA), and graphene oxide (GO) and showed a high swelling ratio of 25.8. For comparison, another PA hydrogel was prepared without GO nanosheets. Then, the hydrogels were characterized using SEM, EDX, AFM, FTIR, Raman, and the swelling ratio test. The characterization techniques indicated the successful synthesis of the hydrogels. Afterward, the two hydrogels were tested using DI water feed for water production. The PAG hydrogel showed higher water production at 26 ± 1 mL compared to 15 ± 1 mL for the PA hydrogel. In addition, self-dewatering of hydrogel was achieved in this setup. No external energy source was required. Instead, the dewatering relied solely on the weight of the feed and the testing cell to exert mechanical compression on the hydrogel, allowing it to release the entrapped water within the hydrogel, while not causing damage to the hydrogel's structure, and its absorption capacities. Afterward, the PAG hydrogel with higher water production than PA was selected to carry out the FO fertigation treatment of groundwater. Before the water test, the hydrogel was soaked in KCl solution, allowing KCl to infiltrate the hydrogel's structure and enhance the hydrogel's osmotic pressure. The PAG hydrogel showed a high water draw for DI water, and GW feeds at 56.5 ± 1.5 mL, and 26.5 ± 3.5 mL, corresponding to 4.80 ± 0.12 L/m² h, and 2.3 ± 0.31 L/m² h respectively. Moreover, the product water as a diluted fertilizer solution achieved a concentration equivalent to 0.14 M KCl, suitable for irrigation application. The results of this study contributed towards a more sustainable FO process by identifying a new hydrogel material as a drawing agent, which not only achieved self-dewatering to release entrapped water but also effectively diluted the fertilizer KCl for fertigation application. Some of the future work on this hydrogel could be to investigate the impacts of different operating conditions (e.g., feed pH, feed temperature) on the performance of the FO process.

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Figures

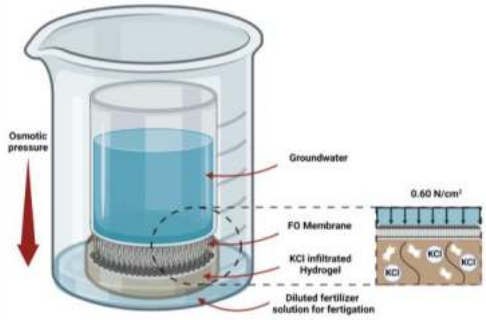

Figure 1: The testing setup of the hydrogels for fertigation

pH-dependent water permeability switching and its memory in MoS_2 membranes

Amritroop Achari
C. Hu, P. Rowe, H. Xiao, S. Suran, Z. Li, K. Huang, C. Chi, C. T. Cherian, V. Sreepal, P. D. Bentley, A. Pratt, N. Zhang, K. S. Novoselov, A. Michaelides, R. R. Nair
National Graphene Institute, University of Manchester, Manchester, M13 9PL, UK
amritroop.achari@manchester.ac.uk

In recent years, 2D material-based membranes have attracted significant attention for their potential applications in various fields, such as water desalination, gas separation etc. So far, most of the developments have been focused on improving efficient separation processes for industrial applications. However, in the last few years, there has been some effort toward making next-generation intelligent membranes. Intelligent translocation of molecules is one of the vital roles of biological membranes. Mimicking such systems can help us develop smart membranes, which can autonomously change their permeation depending on the external environment and would play a pivotal role in intelligent technologies for tomorrow.

In this talk, I shall discuss about our recent work, where we developed MoS_2 membranes that show phase responsive transport of water molecules and prove that only 1T' phase of MoS_2 is water permeable. We demonstrate the memory effects and stimuli responsive transport through such 1T´ MoS_2 membranes by executing water and ion permeation that follow a pH-dependent hysteresis with a permeation rate that switches by a few orders of magnitude. We further illustrate the potential application of this phenomenon in autonomous wound infection monitoring and pH-dependent nanofiltration.[1]

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Growth, characterization and perspectives of applications of novel 2D carbon-based materials

Simona Achilli[1], Guido Fratesi[1], Nicola Manini [1], Giovanni Onida[1], Andi Rabia[2], Andrea Li Bassi[2], Francesco Tumino[2], Alessio Orbelli Biroli[4], Alberto Bossi[3], Valeria Russo[2], Nicolò Bassi[2], Wei Xu[5], Carlo S. Casari[2]
[1]*Dept. of Physics, Università degli Studi di Milano, Via Celoria 16,20133 Milano (Italy)*
[2]*Dept. of Energy, Politecnico di Milano,via Ponzio 34/3 – 20133, Milano (Italy)*
[3] *Istituto di Scienze e Tecnologie Chimiche "G. Natta" del CNR (CNR-SCITEC), SmartMatLab Centre, Via Golgi 19, 20133 Milano (Italy)*
[4]*Dipartimento di Chimica, Università di Pavia, via Taramelli 12 - 27100 Pavia, (Italy)*
[5] *Interdisciplinary Materials Research Center, College of Materials Science and Engineering, Tongji University, Shanghai 201804, (P. R. China)*

simona.achilli@unimi.it

Novel 2D carbon-based materials, as graphynes and graphdiynes, formed by atoms with both sp- and sp2-hybridization [1], display interesting structure-properties relationship that make them suitable for different applications, including nanoelectronics, catalysis, photo-conversion and water splitting [2]. Exploiting a bottom-up on-surface synthesis approach, based on temperature-driven assembly of molecular precursors, it is possible to design different π-conjugated networks with tailored structural, electronic and optical properties [3]. In view of their applications is of fundamental importance to understand how the structure and the growth conditions affects the final properties and define protocols for the fabrication of extended 2D layers and for their controlled manipulation.

After a brief overview of the technological relevance of these 2D materials, we present a multidisciplinary characterization of hybrid sp- sp^{2-} 2D systems obtained by on-surface synthesis of brominated molecular precursors on metal surfaces. By combining *ab initio* theoretical calculations and different experimental techniques, such as Scanning Tunneling Spectroscopy and Microscopy (STS and STM), Raman spectroscopy and Angle-Resolved Photoemission (ARPES) we are able to give a thorough description of nanoscale 2D networks [4-9]. In particular we analyze the evolution of the structural, electronic and vibrational properties during the different stages of the formation, passing from the as deposited metallorganic network to pure sp-/ sp^2- nanostructures upon annealing, and we show the effect of the substrate coupling on their electronic properties.

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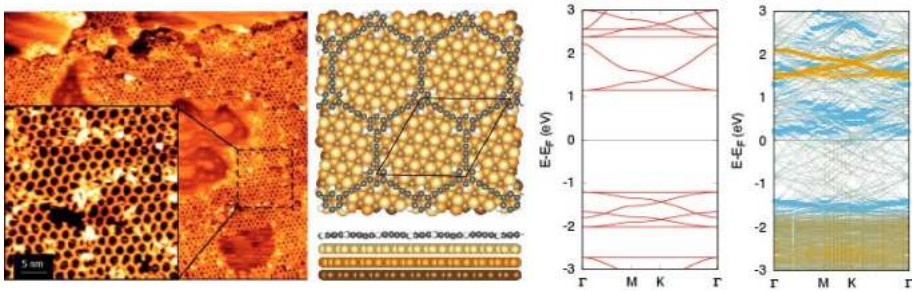

Figure 1: STM image and theoretical model of h-GDY/Au(111). On the left: calculated bandstructure of the freestanding and supported network.

Ultrathin graphene-based membrane with precise molecular sieving and ultrafast solvent permeation

R. Al Busaidi[1], Q. Yang[2], Y. Su[2] , C. Chi[2], C. T. Cherian[2], K. Huang[2], V. G. Kravets[2] , F. C. Wang[3] , J. C. Zhang[4] , A. Pratt[4] , A. N. Grigorenko[2] , F. Guinea[2,3], A. K. Geim[2] and R. R. Nair[2]
Physics department, college of science, Sultan Qaboos University, Muscat, Oman
[2]Membrane group, school of Chemical Engineering and Analytical Science & National Graphene Institute, University of Manchester, Manchester, UK
3Chinese Academy of Sciences Key Laboratory of Mechanical Behavior and Design of Materials, Department of Modern Mechanics, University of Science and Technology of China, Hefei, Anhui 230027, China
rahmaalb@squ.edu.om

Graphene oxide (GO) membranes continue to attract intense interest due to their unique molecular separation properties combined with rapid permeability. The membranes are limited to aqueous solutions due to their apparent impermeability to organic solvents, which has not yet been fully explained. Here, we report efficient and fast filtration of organic solvents through GO laminates containing smooth two-dimensional (2D) capillaries made from large (10–20 μm) flakes. Without modification of sieving characteristics, these membranes can be made exceptionally thin, down to ∼10 nm, resulting in fast water and organic solvent permeation. We attribute organic solvent permeation and sieving properties to randomly distributed pinholes connected by 1 nm graphene channels. Organic solvent permeation rates decay exponentially with membrane thickness, but water continues to permeate quickly, in agreement with previous reports[1-4]. The potential of ultrathin GO laminates for organic solvent nanofiltration is demonstrated by showing >99.9% rejection of small molecular weight organic dyes dissolved in methanol. GO membranes have enormous potential for purification and filtration technologies as a result of our research

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Electrical, Optical, and Structural Characterization of Molybdenum Trioxide (MoO3) Nano Rods Particles

Saleh Saeed Saleh AlDarmaki, Ayman Rezk, Shanavas Shajahan, Rami Elkaffas, Yarjan Abdulsamad, Ammar Nayfeh

Khalifa University, Abu Dhabi, UAE

100064472@ku.ac.ae

Molybdenum trioxide (MoO_3) is a promising material for semiconductor devices due to its unique electrical and optical properties [1], making it suitable for memristive and charge-trapping applications in non-volatile memory and neuromorphic computing [2]. This study focuses on the deposition of MoO_3 films via spin coating, characterizing their electrical, optical, and structural properties, and integrating them into a charge-trapping device [3]. MoO_3 crystals were dissolved in isopropyl alcohol (IPA) at concentrations of 1g/L, 5g/L, and 10g/L, with the solution sonicated using a sonicator bath for 90 minutes, to ensure uniform dispersion and homogeneity. The deposition was conducted by spin coating speeds between 1200-2000 rpm, on silicon substrates of size 1.5x1.5 cm^2 and a solution volume of 10uL per layer. Structural and morphological analysis using SEM, and AFM revealed clustering in higher concentration solutions, which was mitigated by centrifuging at 5000 rpm for 30 minutes. Depositing the centrifuged solution exhibited a mean thickness value of 20nm, which represents a 2D layer of MoO3 [4]. Optical and electrical characterization confirmed a distinct absorption edge at 350 nm, a direct bandgap of approximately 3.2 eV for the deposited samples, and 3.6eV for the MoO_3 solution [5]. A high carrier mobility was also recorded averaging 1.8 × 10^3 $cm^2/V{\cdot}s$. MoO_3 was also integrated into charge-trapping devices with Aluminum Oxide (Al_2O_3) layers sandwiching the MoO_3 layer on a highly doped silicon base, demonstrating promising I-V characteristics [6]. These findings showcase MoO_3's potential for future semiconductor applications, with further optimization planned to enhance material deposition and device performance.

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Figures

Figure 1: Microscope Image of Orthorhombic Crystals structures of MoO_3 (α-MoO_3)

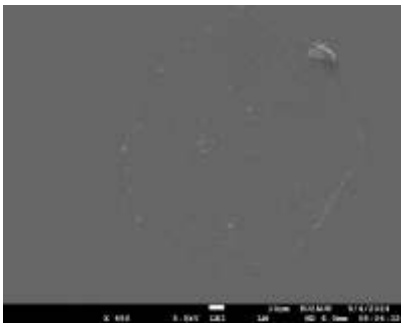

Figure 2: SEM image of Centrifuged MoO_3 deposited on silicon

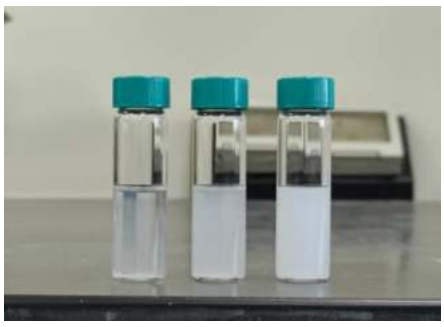

Figure 3: MoO_3 solution concentrations of 1g/L, 5g/L, and 10g/L (left to right)

Efficient membrane-based Direct Air Capture (m-DAC) technology using Graphene Oxide/Pebax based Mixed Matrix Membranes

Omnya Al-Yafiee* [a,b], Priyanka Kumari [a,b], Georgios N Karanikolos[c], Ludovic F. Dumée [a,b]
[a] *Khalifa University, Department of Chemical and Petrochemical Engineering, Sas Al Nakhl Campus, Abu Dhabi, United Arab Emirates*
[b] *Research and Innovation Center on 2D nanomaterials (RIC2D), Khalifa University, Sas Al Nakhl Campus, Abu Dhabi, United Arab Emirates*
[c] *Department of Chemical Engineering, University of Patras, 26504 Patras, Greece*
*Contact@ Speaker's email: 100062559@ku.ac.ae

The increasing concentration of carbon dioxide (CO_2) in the atmosphere is a significant driver of global warming and climate change, necessitating effective strategies to capture and reduce CO_2 emissions, even from dilute sources. This paper investigates advanced membrane-based technologies for capturing CO_2 from air. Traditional carbon capture methods, such as amine-based absorption, are effective but come with significant drawbacks, including high energy consumption, increased costs, and substantial water usage. Membrane gas separation offers a promising alternative due to its process simplicity, and lower energy demands [1]. Hence, this research explores the development of highly selective and permeable polymeric asymmetric membranes for capturing CO_2 from low concentration sources. The membranes were synthesized by forming Pebax -MH1657 films, which were incorporated with Graphene Oxide (GO) to improve permeability and selectivity, on a macroporous support made of poly(sulfone) (PSF) to provide the mechanical support necessary for the active layer to stand. Further amine functionalization to the GO was also investigated to study the impact of amine group attachment to the matrix in the performance, and two types of amines were used, Primary amine (NH_3) and Polyethylenimine (PEI). Chemical, physical, and morphological analysis to investigate the nature and compatibility of produced membranes to the desired application were done. As well as Pure gas and mixed gas (10% v/v CO_2 and 0.04% v/v CO_2 content in N_2) permeance tests were performed to study the performance of the membranes by obtaining the permeance and selectivity of the membranes at different loadings of GO in the matrix. The MMMs prepared in this research were able to achieve, under DAC condition, selectivity and permeability of 68 and 21.27 GPU with the A-GO MMM (0.3 wt.% loading), and 56and 16.9GPU with the PEI-GO MMM for the same loading. The findings demonstrate the potential of membrane technology in efficiently capturing CO_2 from dilute sources, paving the way for more sustainable and cost-effective solutions to mitigate climate change.

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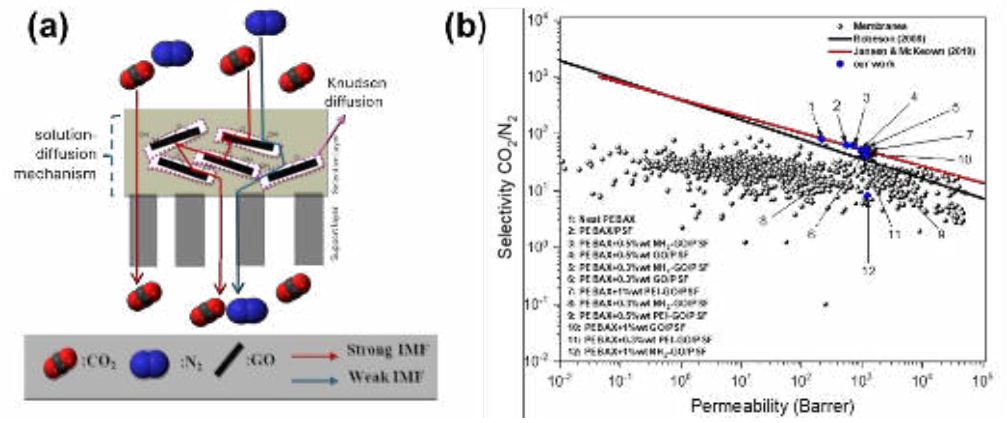

Figure 1: (a) The GO-based Mixed matrix membrane MMMs structure and diffusion mechanisms expected to occur, (b) Pure Gas permeation results :The ideal selectivity plotted against Permeability in Barrer; the white dots represent data from literature [2].

Nanocomposite Ion Exchange Membranes Based on Modified Graphene Oxide for Desalination

Adetunji Alabi [a,b], Linda Zou [a,b]
[a] *Department of Civil and Environmental Engineering, Khalifa University, PO Box 127788, Abu Dhabi, United Arab Emirates*
[b] *The Research & Innovation Center for Graphene and 2D Materials (RIC-2D), Khalifa University, PO Box 127788, Abu Dhabi, United Arab Emirates*
adetunji.alabi@ku.ac.ae; linda.zou@ku.ac.ae

There have been considerable research efforts to produce ion exchange membranes (IEMs) with desirable properties for electromembrane processes such as electrodialysis desalination. IEMs have received considerable interest owing to their critical role in electromembrane processes [1]. An approach gaining much attention is via the incorporation of graphene-based nanomaterials in the polymeric matrix of IEMs to create nanocomposite IEMs [2]. This is due to the electrical conductivity, mechanical strength and specific surface area of graphene [3]. We present a strategy that successfully uses graphene-based nanosheets as the only source of electrochemical properties in nanocomposite IEMs. Here, modified graphene-based nanomaterials were incorporated into an uncharged polymeric matrix to create nanocomposite IEMs for electrodialysis desalination. A newly developed mold-casting technique was used to fabricate the nanocomposite IEMs with high content of modified graphene-based nanomaterials as the source of ion exchange capabilities. The fabricated nanocomposite IEMs demonstrated favorable properties and performances including comparable current efficiency and salt removal during electrodialysis experiments.

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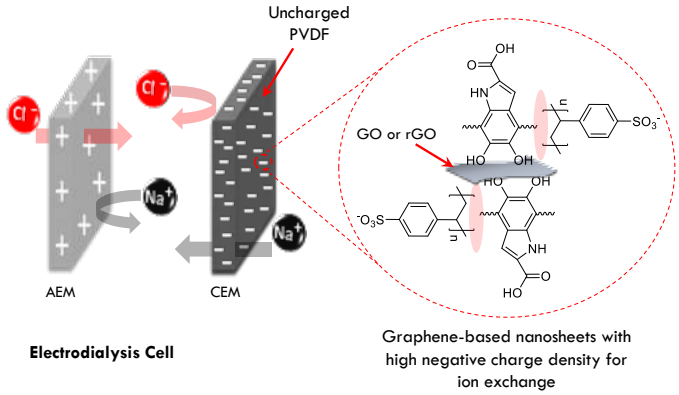

Figure 1: Electrodialysis cell and components of the fabricated nanocomposite IEMs.

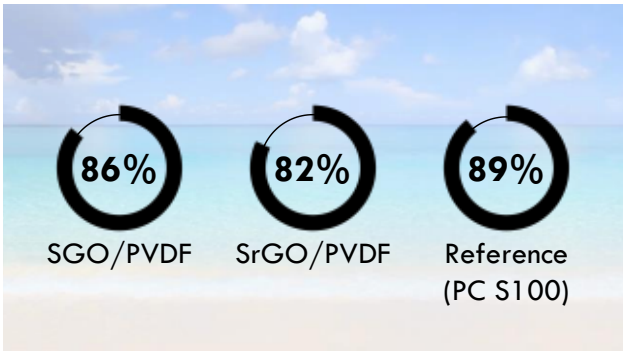

Figure 2: Salt removal of the fabricated nanocomposite IEMs and reference IEM during the electrodialysis test

Use of spinel ferrite oxides and rGO composite electrode in capacitive deionization for Copper (II) removal

Rahat Alam[a], Muhammad Faheem[a], Ahmed Al Hajaj[b], Linda Zou[a]
[a]*Department of Civil Infrastructure and Environment Engineering, Khalifa University of Science and Technology, P.O. Box 127788, Abu Dhabi, United Arab Emirates*
[b]*Department of Civil Infrastructure and Environment Engineering, Khalifa University of Science and Technology, P.O. Box 127788, Abu Dhabi, United Arab Emirates*
100060837@ku.ac.ae

Abstract

Copper ions are a hazardous component in wastewater, which can be effectively removed using capacitive deionization (CDI). Nanosized spinel ferrite oxide crystals are promising for enhancing copper ion adsorption through lattice-based intercalation. In this study, two nanocomposite electrodes, $NiFe_2O_4$/rGO (NFO/rGO) and $CoFe_2O_4$/rGO (CFO/rGO), are synthesized via a hydrothermal method. The rGO nanosheets are intertwined with the dense structures of NFO and CFO crystals, forming a scaffold that increases specific surface area, conductivity, and adsorption capacity. The synthesized materials are characterized using SEM, EDS, TEM, XRD, BET, and XPS techniques. The hybrid pseudocapacitive nanocomposites, NFO/rGO and CFO/rGO, exhibited electrochemical capacitances of 125.15 F g^{-1} and 186.08 F g^{-1}, respectively, at 10 mVs^{-1}. CDI experiments demonstrated that the nanocomposites NFO/rGO and CFO/rGO have high copper ion removal capacities of 132.42 mg g^{-1} and 137.00 mg g^{-1}, respectively, outperforming previously reported electrodes. A thorough quantitative electrochemical analysis revealed the adsorption mechanism and their percentage contributions. Out of both electrodes, CFO/rGO possesses better crystallinity, smaller crystal size, and narrower pore size, leading to a higher surface area, more active sites for Cu^{2+} adsorption, and improved diffusion kinetics. Both nanocomposite electrodes show excellent regeneration and stability over multiple cycles. The outstanding adsorption performance is attributed to the nanosized spinel's channels and narrow pore size distribution in the NFO/rGO and CFO/rGO nanocomposites, which facilitate efficient ion intercalation/deintercalation. This study underscores the potential of high-performance ion-intercalating spinel ferrite oxide electrodes for heavy metal removal from wastewater.

Figures

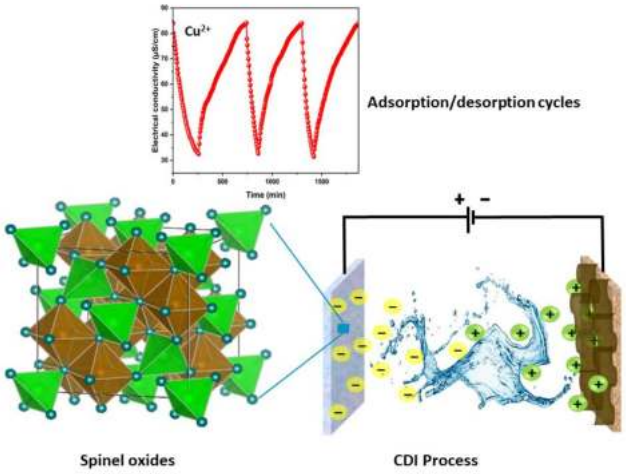

Figure 1: Adsorption process in capacitive deionization

Environmentally Stable MXene Inks for Electrohydrodynamic Jet Printing of Micro-Electronics

Shahzaib Ali [a], Faisal Shahzad [c], Hassan A. Arafat [c, *], Dae-Hyun Cho [d, *], Doyoung Byun [a,b, *]

[a] *Department of Mechanical Engineering, Sungkyunkwan University (SKKU), 2066 Seobu-ro, Jangan-gu, Suwon-si, Gyeonggi-do 16419, Republic of Korea.*
[b] *Department of Display Engineering, Sungkyunkwan University (SKKU), Suwon 16419, Republic of Korea*
[c] *Research and Innovation Center for Graphene and 2D Materials (RIC2D), Khalifa University, Abu Dhabi, 127788, United Arab Emirates.*
[d] *Department of Mechatronics Engineering & Department of Energy System Engineering, Gyeongsang National University, 501 Jinju-daero, Jinju-si, Gyeongsangnam-do, Republic of Korea*

Contact: shahzaibali@g.skku.edu

Inkjet printing, a non-contact, direct patterning technique that forms designs by ejecting ink droplets, has gained significant attention in the fabrication of electronic devices requiring diverse pattern geometries. Electrohydrodynamic (EHD) jet printing, a more advanced variant of this technology, enables the deposition of high-viscosity inks exceeding several hundred cP, which is beyond the capabilities of conventional inkjet methods. This advancement allows for the formation of intricate, high-resolution patterns that are difficult to achieve otherwise. While photolithography remains the dominant patterning method in electronic device manufacturing, it requires multiple steps—such as coating, exposure, development, and subsequent drying or curing processes leading to extended production times and increased costs.

In contrast, inkjet printing simplifies the workflow, involving only the printing and post-processing stages, which significantly accelerates production and reduces costs. This method also eliminates the need for photoresist and developer, using only the necessary amount of material, making it both economically and environmentally sustainable. In this study, we optimized MXene ink, known for its exceptional conductivity and volumetric capacitance, for use in EHD jet printing. Given MXene's known vulnerability to oxidation under ambient conditions, we carefully evaluated its oxidation resistance. Additionally, we characterized the conductivity and pattern resolution of the printed electrodes to confirm their suitability for high-performance electronic applications.

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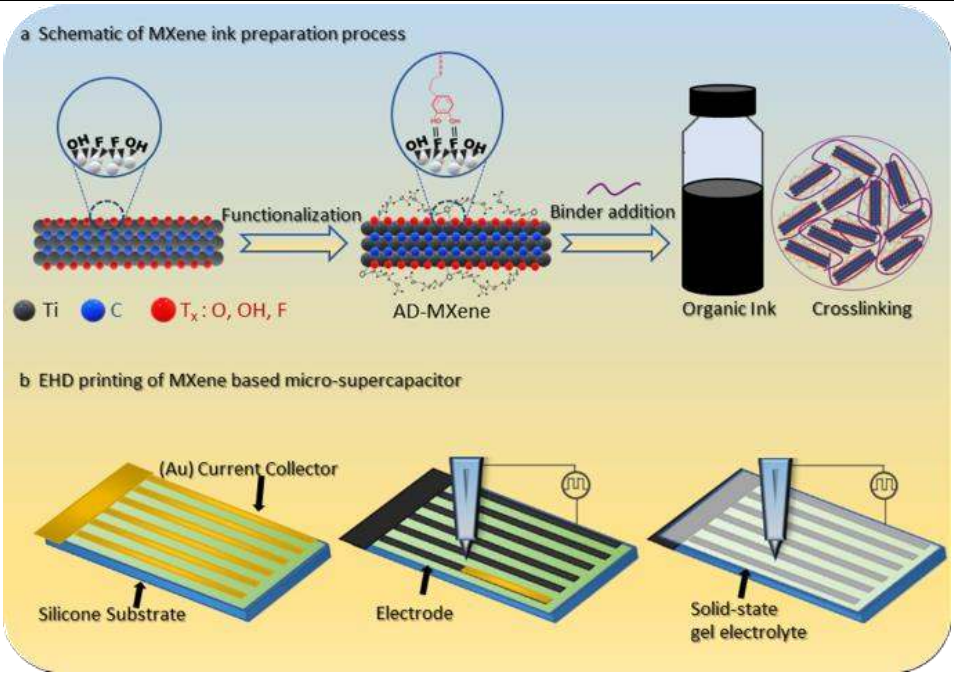

Figure 1: Schematic illustration of (a) environmentally stable MXene ink synthesis, and (b) EHD jet printing of micro electronic devices.

Electrostatic Modulation of Interdot Tunnelling in Bilayer Graphene Quantum Dots

Hassan Allami, Daniel Miravet, Pawel Hawrylak
Department of Physics, University of Ottawa, ON K1N 6N5, Ottawa, Canada
hassan.allami@gmail.com

We investigate two gate-defined quantum dots in bilayer graphene, where a tunable gate-induced electric field controls the bulk gap. The design also allows for the manipulation of the confining potential and the dots' filling through tunable finger-gates and a back-gate [1]. Using an atomistic model, we demonstrate that varying the electric field modulates interdot tunnelling. Our results show that the tunnelling oscillates as the electric field changes and, in typical cases, can be tuned to nearly zero, similar to the bonding-antibonding tunnelling quench observed in InAs quantum dot molecules [2]. This effect occurs in the tunnelling between orbitals of the same valleys in the two dots and should be observable in transport experiments. Additionally, we present an analytical model to explain how the external electric field modulates tunnelling by controlling the interference pattern in the overlap of the corresponding wavefunctions.

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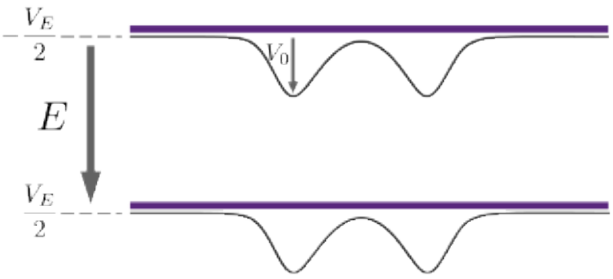

Figure 1: Schematic side view of the system, with the thick purple lines representing the graphene layers. The thin black curves under each layer represent the electric potential profile with a tunable depth V_0. A tunable bias V_E generates an electric field between the layers, opening a gap between the valence and conduction states.

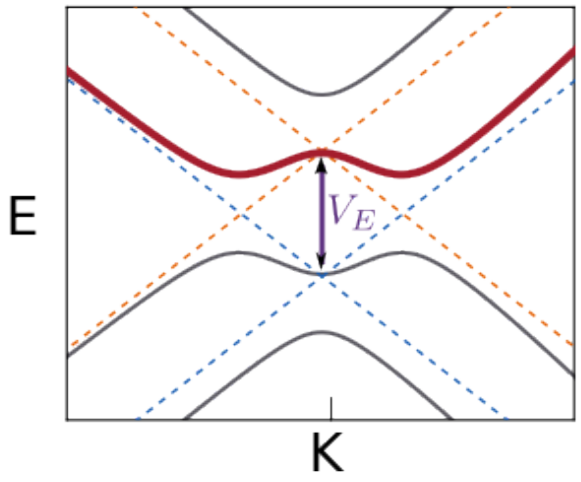

Figure 2: Schematic of the bulk band structure near the K point, illustrating how the interlayer electric field opens a gap and creates a Mexican hat shape in the lower conduction band (thick red curve).

Scalable Liquid Phase Exfoliation of Layered and 2D Materials

Mariam Badawi, Muhammad Faizan, Yarjan Abdul Samad, Imran Afgan
Khalifa University, Shakhbout Bin Sultan St, Abu Dhabi, UAE
100063763@ku.ac.ae

Liquid phase exfoliation (LPE) methods are becoming increasingly significant in the exfoliation of graphene and other 2D materials due to their easiness and high production rates compared to other mechanical or chemical methods [1]. Inks produced by LPE are required in a wide range of applications including but not limited to flexible electronics [2], conductive coatings, and composite materials. The scalability of these processes is still a challenge, particularly due to limited flake sizes [1]. Current LPE methods that are widely investigated by researchers include sonication [2], shear mixing [3], and high-pressure homogenization [4]. Sonication is a cavitation-dominated process, while shear-mixing and high-pressure homogenization are shear-dominated forces accompanied with cavitation and collision effects. The cavitation and collision effects involved in these methods can induce significant defects in the resulting material, as well as the long process time for sonication limit the scalability of these methods [5]. In this work, a new LPE method is introduced, in which exfoliation occurs due to high shear forces developed among successive stationary and high-speed rotating discs. CFD simulations are performed for the device to evaluate the resulting shear forces acting on the fluid. A structured hexahedral mesh is employed in the simulations with k-ω SST turbulence model for accurate near-wall resolution. Simulations are performed in the transient regime with a timestep of $1*10^{-5}$ s. Mesh sensitivity study is conducted employing mesh size range from 0.5 to 9.5 million to obtain mesh independent results. In this work, a broad range of rotational speeds from 1,000 to 10,000 RPM is examined, and the impact of each speed on flow behavior and shear rate will be presented. A snap of the results is shown in Figure 1 which depicts the velocity and strain-rate contours for the flow domain at 5000 rpm with the strain rate reaching a maximum value of $4.5*10^{6}$ s^{-1} and an average value of $5.4*10^{4}$ s^{-1}, which exceeds the minimum shear-rate required for graphene exfoliation (10^{4} s^{-1}) [3]. Overall, this method has the potential to produce larger flakes with minimum defects due to shear force dominance, which facilitates the efficient scalable production of graphene and 2D materials inks to be used in different applications.

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Figures

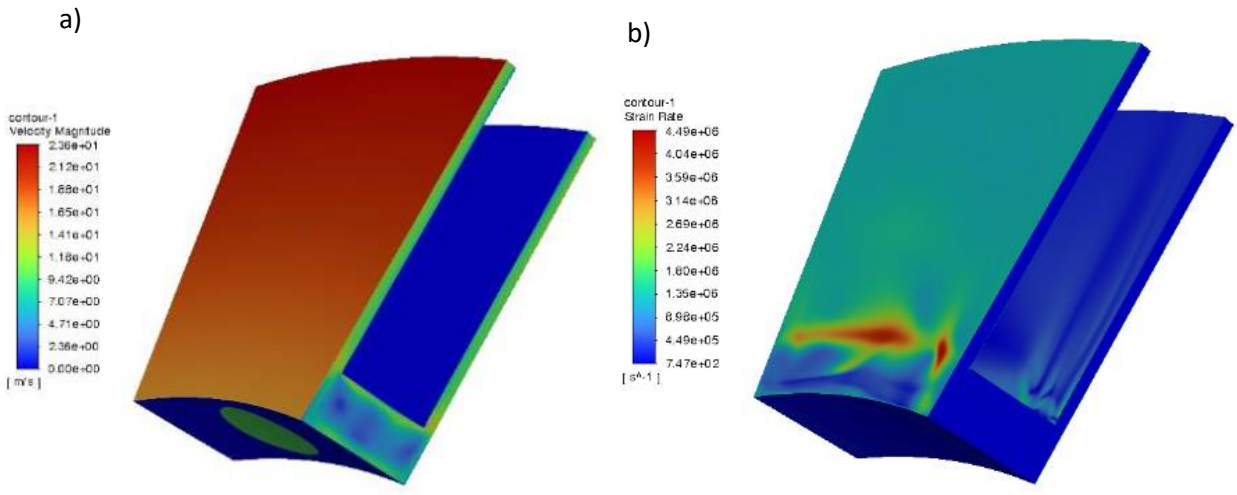

Figure 1: a) Velocity contour, and b) Strain rate contour.

Elucidating proton permeation and hydrogenation behaviour in graphene-based materials from DFT calculations

Daniel Bahamon[1,2], Yuting Li[1,2], Mohammad Y. Al Hamadi[1], Nirpendra Singh[1], Marcelo Lozada-Hidalgo[1,3,4], Lourdes F. Vega[1,2]

[1] *Research and Innovation Center for graphene and 2D-materials (RIC2D), Khalifa University of Science and Technology, PO Box 127788, Abu Dhabi, UAE.*
[2] *Research and Innovation Center on CO_2 and Hydrogen (RICH Center), Chemical and Petroleum Engineering Department, Khalifa University, PO Box 127788, Abu Dhabi, United Arab Emirates.*
[3] *Department of Physics and Astronomy, The University of Manchester, Manchester, UK.*
[4] *National Graphene Institute, The University of Manchester, Manchester, M13 9PL, UK.*

daniel.garcia@ku.ac.ae

Two-dimensional materials (*e.g.*, graphene and h-BN) offer a prospect of membranes that combine negligible permeability to gases with high proton conductivity, and could outperform the polymer-based existing proton exchange membranes used in various applications including fuel cells [1],[2]. Besides the well-investigated pristine graphene, there are hundreds of known two-dimensional materials that have not been explored from a permeability perspective. Hence, to guide the design and selection of promising 2D-structures, Density Functional Theory (DFT) calculations have been used as a high-throughput computational method for a first screening based on descriptors related to the permeability of the 2D-membranes [3]. Focus has been paid to functionalized graphene structures such as graphene oxide (GO) and fluorographene, to graphene-derivatives including non-metallic substitutions such as B, N, P, etc., and to other reported one-atom layer structures such as silicene, germanene and phosphorene. Simulations have been validated with experimental results (when available) and used as a guide for the rational selection of the best 2D materials for this application.
Results demonstrate that chemical functionalization can be used to enhance proton transparency without compromising gas impermeability. In particular, the enhancement is attributed to microscopic corrugations of the underlying graphene lattice, which are caused by functional groups bonded to the graphene surface [4]. In addition, surface hydrogenation has a similar enhancement effect in the studied materials. Furthermore, it was found a tendency to lower energy barriers for structures having larger pore sizes in their 6-atom rings (see Figure 1). For instance, boron substitution facilitates permeation, also attributed to a distortion induced by B atoms with larger atomic radii and an elongation of the B-C bond length; conversely, nitrogen atoms were identified as unfavourable for proton transport due to the distortion in carrier mobility. The revealed molecular-insights could expand the potential application of such 2D-materials in hydrogen-related technologies.
This work is financed by the Research and Innovation Center for graphene and 2D-Materials (RIC2D) under the RIC-2D-D001 project. Computational resources from the Almesbar HPC at KU are also gratefully acknowledged.

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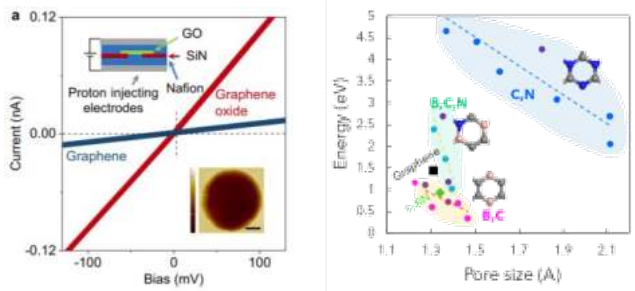

Figure 1: (**left**) Comparison of proton permeation (I-V characteristic) for graphene and GO monolayers. (**right**) Calculated DFT energy barriers of graphene-derivative structures, and correlation with the relaxed pore size of the permeated ring.

Phthalocyanine-Doped Nanofiber Membranes Utilizing Photosensitization for the Remediation of Persistent Pollutants in Wastewaters

Hooralain Bushnaq[1,2], Sisi Pu[1], Catherine Munro[1], Giovanni Palmisano[1,3], Srinivas Mettu[1,3], and Ludovic F. Dumée[1,2*]

[1] *Khalifa University, Department of Chemical and Petrochemical Engineering, Abu Dhabi, United Arab Emirates Organization*

[2] *Research and Innovation Center on 2D Nanomaterials, Khalifa University, Abu Dhabi, United Arab Emirates*

[3] *Research and Innovation Center on CO2 and Hydrogen (RICH), Khalifa University, Abu Dhabi, United Arab Emirates*

**Ludovic.dumee@ku.ac.ae; +971563842672*

h.bushnaq@hotmail.com

Recent studies highlight the increasing prevalence of microplastics in various environments, posing risks due to their composition and as carriers of microbial pathogens through biofilms [1]. Wastewater treatment plants play a pivotal role in mitigating microplastics' environmental release [2]. Therefore, integrating efficient microplastic removal technologies is essential for reducing biological and pollutant loads. Traditional treatments often result in harmful disinfection by-products, while photocatalytic methods, particularly those employing photosensitization, offer a less toxic and effective solution. Phthalocyanines (Pcs) have shown considerable promise due to their high absorption coefficient in both ultraviolet and visible spectral ranges, and their role in broadening the light absorption range [3]. This study investigates the incorporation of Pcs into polymeric membranes to generate visible-light active photo-responsive microfiltration membranes with enhanced photodynamic activity and filtration capabilities. Cellulose acetate-based electrospun nanofibrous membranes with pore sizes ranging from 1 to 2 µm were used. Several classes of Pcs, including Cobalt phthalocyanine (CoPc), Zinc phthalocyanine (ZnPc), Tetra-amino zinc phthalocyanine (TAZnPc), and Tetra-sulfonated aluminum phthalocyanine (TSAlPc), were incorporated into the membranes using two approaches to produce mixed matrix membranes (MMM) and grafted membranes (GM). The integration of these Pcs was shown to influence the membranes' structural and functional properties, enhancing catalytic, antibacterial, and antiviral performance, as well as the rejection of microplastics and bacterial inactivation in filtration systems. The homogenous fibrous structure of the membranes was confirmed by scanning electron microscopy (SEM), and the successful incorporation of Pcs was validated by Fourier transform infrared spectroscopy (FT-IR), X-ray photoelectron spectroscopy (XPS), and UV-visible diffuse reflectance spectroscopy (DRS). The photo-decontamination capabilities of the modified membranes were initially evaluated using methylene blue dye, with the degradation process following the Langmuir-Hinshelwood model and exhibiting pseudo-first-order kinetics. ZnPc MMM and TAZnPc GM showed the highest degradation rate constants of 0.026 min^{-1} and 0.0195 min^{-1}, respectively. The antimicrobial efficacy was further assessed through the photoinactivation of gram-negative E. coli, with each membrane variant demonstrating distinct growth inhibition percentages. Additionally, the membranes achieved complete microplastic rejection, a 2.5-log reduction in E. coli, and a 2-log reduction in Influenza A virus in filtration systems, highlighting their efficacy in bacterial and viral inactivation. The findings underscore the potential of Pcs-photosensitized cellulose acetate membranes for advanced water treatment applications, combining enhanced filtration capabilities with photodynamic activity for pollutant degradation and microbial inactivation.

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Wavelength-Dispersive Optical axes in Natural and Artificial Anisotropic Materials

Georgy Ermolaev
Dmitriy Grudinin, Ilia Fradkin, Andrey Vychnevyy Aleksey Arsenin, Valentyn Volkov
Emerging Technology Research Center, Dubai Internet City, Emmay Tower, Dubai, UAE
Luis Martin-Moreno
Instituto de Nanociencia y Materiales de Aragón (INMA), CSIC-Universidad de Zaragoza, Zaragoza, Spain
Kostya Novoselov
National Graphene Institute (NGI), University of Manchester, Manchester, M13 9PL, UK
Department of Materials Science and Engineering, National University of Singapore, Singapore 03-09, Singapore

ermolaev-georgy@xpanceo.com

Anisotropic materials play a pivotal role in contemporary nanophotonics applications, such as polaritonic physics [1], subdiffractional guiding [2], and strong light-matter coupling [3]. However, anisotropic materials have static optical axes, which prevent their complete manipulation of light in anisotropic devices. Here, we found that natural van der Waals crystals rhenium disulfide and diselenide demonstrate wavelength-dispersive optical axes owing to noncollinear excitons. It results in unusual far-field and near-field responses with the opportunity to control light propagation with even a slight wavelength shift. Moreover, we developed a technology for engineering systems with wavelength-dispersive optical axes via carbon and transition metal dichalcogenide nanotubes. It allows us to design almost any rotation of optical axes. Thus, the discovered phenomenon of wavelength-dispersive optical axes offers a novel route for light manipulation without nanostructuring.

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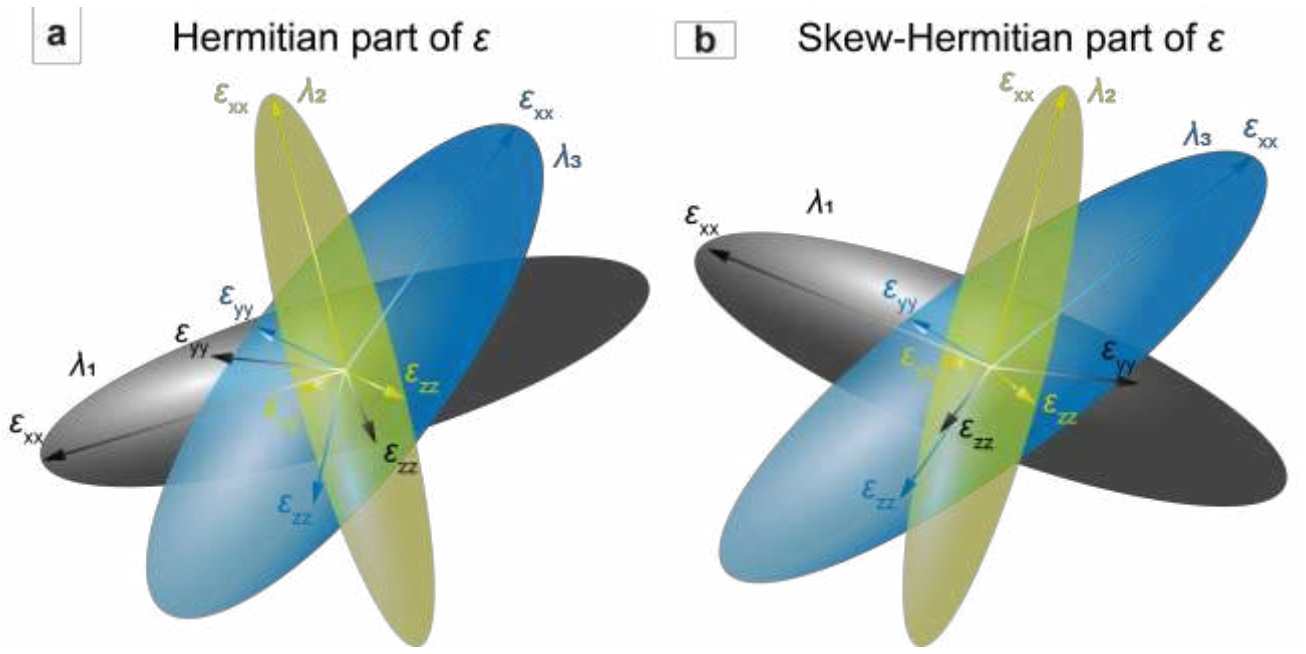

Figure 1: Schematic illustration of principal optical axes rotation.

Anisotropic optical response and emergent chirality in van der Waals arsenic trisulphide homostructures

D. A. Ghazaryan[1], K. V. Voronin[2], A. N. Toksumakov[3], G. A. Ermolaev[4], A. S. Slavich[3], M. I. Tatmyshevski[3], A. A. Vyshnevyy[4] , I. Kruglov[3], D. G. Baranov[3] , A. V. Arsenin[4], V. S. Volkov[4], K. S. Novoselov[5, 6, 7]
[1]*Laboratory of Advanced Functional Materials, Yerevan State University, Alek Manukyan 1, Yerevan, Armenia*
[2]*Donostia International Physics Center (DIPC), Donostia/San-Sebastián, 20018, Spain*
[3]*Moscow Center for Advanced Studies, Kulakova str. 20, Moscow, 123592, Russia*
[4]*Emerging Technologies Research Center, XPANCEO, Dubai, Internet City, Emmay Tower, Dubai, United Arab Emirates*
[5]*Institute for Functional Intelligent Materials, National University of Singapore, 117544, Singapore, Singapore*
[6]*National Graphene Institute (NGI), University of Manchester, Manchester, M13 9PL, UK*
[7]*Department of Materials Science and Engineering, National University of Singapore, Singapore, 03-09 EA, Singapore*
dav280892@gmail.com

The growing family of van der Waals crystals is recognized as a promising platform for the investigation of novel effects and creation of a variety of functional devices. The nature of their out-of-plane bonds that are stacking the comprising two-dimensional layers, *i. e.*, their explicit layered structure, instantly suggests the emergence of anisotropic properties. Furthermore, the subfamilies of van der Waals crystals that also naturally possess in-plane anisotropic electronic, optical and mechanical properties, appear more interesting as they significantly enrich the research scope [1]. Though the nature of in-plane bonds in constituent two-dimensional layers of van der Waals crystals is covalent, in view of anisotropic optical properties, their low-symmetry crystal structures establish one of the major factors behind its robustness [2]. Here, we will present our recent findings of strong biaxially anisotropic optical response of van der Waals arsenic trisulphide [2] along with a novel approach of an engineering of the chiraoptical response in trilayers of these crystals assembled into a helical homostructure [3]. Unlike the chiral response arising in twisted graphene or two-dimensional transition metal dichalcogenide based moiré homo- or hetero- structures [4, 5], our approach suggests an emergence of chirality entirely established on the effect of biaxial optical anisotropy of the van der Waals crystal. It demonstrates prospects of engineering the chiraoptical response at an intermediate level between the molecular and mesoscopic one due to the tailored arrangement of initially non-chiral layers.

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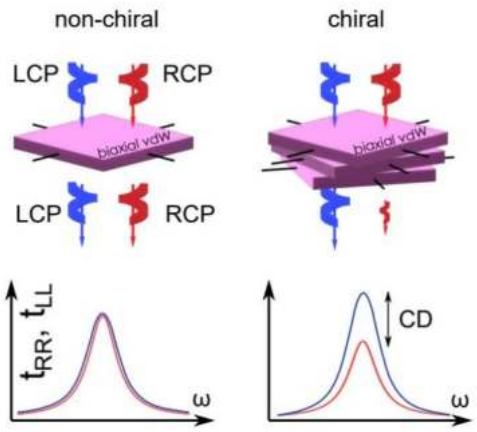

Figure 1: Engineering chirality in van der Waals homostructures comprising biaxially anisotropic arsenic trisulphide layers arranged in a helical fashion.

3D printing functional CNT-modulated nanoporous membranes for Energy Applications

Vinay Gupta, Kumar Shanmugam
Department of Physics, Khalifa University, Abu Dhabi, UAE
James Watt School of Engineering, University of Glasgow, Glasgow, G12 8LT, UK
vinay.gupta@ku.ac.ae

A self-standing 3D-printed PLA/sulfur/CNT cathode with high sulfur loading based on a biodegradable low-cost commercial polylectic acid (PLA) as the binding was fabricated via a facile robocasting 3D printing process (Figure 1a). The PLA/sulfur/CNT cathodes with different CNT loadings (3, 5, 7, and 10 wt%), interconnected porosities (10%, 30%, 50%, and 70%) and thicknesses (100, 200 and 300 µm) were 3D printed by utilizing in-house nanoengineered filaments Figure 1b). A nanoporous network of CNTs is developed (Figure 1c). Coin cells were fabricated (inset of Figure 1d) and their electrochemical performance is analyzed. The 3D-printed sulfur/CNT cathode shows excellent electrochemical performance in terms of capacity, cycling stability, and rate retention by facilitating Li+/e- transport at the macro-, micro-, and nano-scale in Li-S batteries. Meanwhile, the areal loading of the sulfur/carbon cathode can be easily controlled by the number of stacking layers during 3D printing process. The Li-S batteries assembled with the 3D-printed sulfur/CNT cathodes with a sulfur-loading of 6 mg cm^{-2} deliver an initial capacity of 1096 mA h g^{-1} (100 µm thick) and high capacity retentions of % within 100 cycles at 0.5 C (Figure 1d). Moreover, cathodes with sulfur-loadings of 11 mg cm−2 (200 µm thick) and 17 mg cm^{-2} (300 µm thick) show lower initial specific discharge capacities of 810 mA h g^{-1} and 542 mA h g^{-1} due to increased thickness. However, the areal capacity of 17 mg cm^{-2} (300 µm thick), 11 mg cm^{-2} (200 µm thick), and 11 mg cm^{-2} (200 µm thick) show areal capacity (at areal current density) of 9.2 (2.84 $mAcm^{-2}$), 8.91(1.84 $mAcm^{-2}$), and 6.5 mAh cm^{-2} (1.0 $mAcm^{-2}$), respectively.

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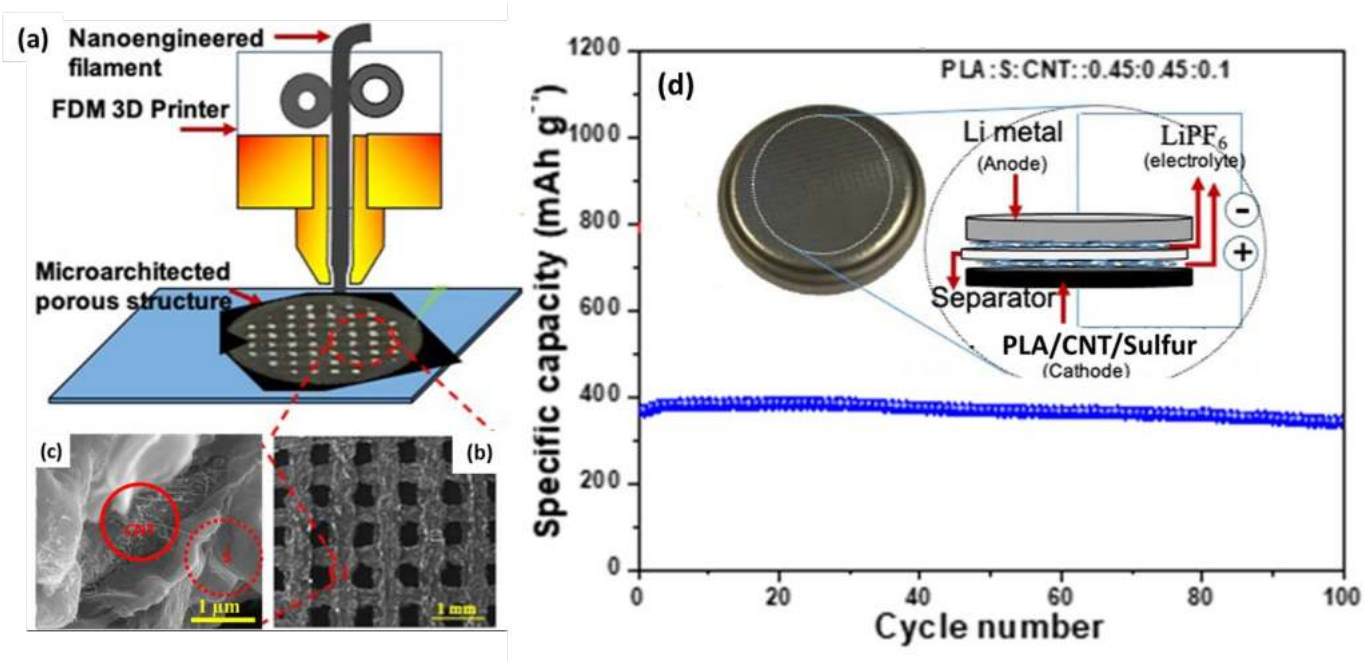

Figure 1: (a) Fabrication of PLA/S/CNT nanocomposite involving solvent casting, filament extrusion, and 3D printing. (b) A 3D printed PLA/S/CNT cellular nanocomposite with 10wt.% CNT loading (100 µm). (c) SEM images of a 3D printed PLA/S/CNT cellular nanocomposites with different 10% CNT loading. (d) Cyclic stability of a 3D printed PLA/S/CNT nanocomposite electrode at 0.5C rate (inset shows the schematics of the coin cell).

Ultrahigh Inter-Cation Selectivity from Chemically Nanoconfined Fluidic Channels

Seunghyun Hong[1], Marcos V. Surmani Martins[2], Faisal AlMarzooqi[1], Slaven Garaj[3]

1 Center for Membranes & Advanced Water Technology (CMAT), Khalifa University of Science and Technology, P.O. Box 127788, Abu Dhabi, United Arab Emirates
2 Department of Physics and Astronomy, School of Natural Sciences, The University of Manchester, Manchester, UK
3 Centre for Advanced 2D Materials, National University of Singapore, Singapore 117542

seunghyun.hong@ku.ac.ae

Overcoming the structural limitations at the nanoscale presents a significant challenge in the design of membranes for effective and scalable separation processes. In this context, nanostructured graphene-based membranes emerge as a promising solution, offering a versatile platform that can be tailored to meet specific requirements. However, the high yield and processability of graphene oxides (GOs) introduce complexities in controlling their features and properties during synthesis. This study aims to explore the material properties of various GOs to gain a deeper understanding of the key characteristics that influence their performance in ion-selective membranes. Notably, we employ a multidisciplinary approach for the first time to reveal how structural and chemical features impact ion transport at the nanoscale, ultimately enhancing the monovalent-selective capacity of GO laminates. Our findings show that in a low defect regime, the prevalent concentration of organosulfate groups—often resulting from conventional synthesis methods—plays a crucial role beyond mere steric effects. These groups significantly contribute to improved ionic selectivity between mono- and multivalent ions. We emphasize that these stronger interlayer interactions fostered by organosulfate groups provide an effective means to control membrane swelling with angstrom precision. As a result, we observe a remarkable four-fold increase in K^+/Mg^{2+} inter-cation selectivity, achieving 94 % Mg^{2+} rejection under osmotic transport conditions. Furthermore, even when interplanar distances are expanded to boost water fluxes, the inter-cation selectivity remains competitive with that of state-of-the-art membranes.

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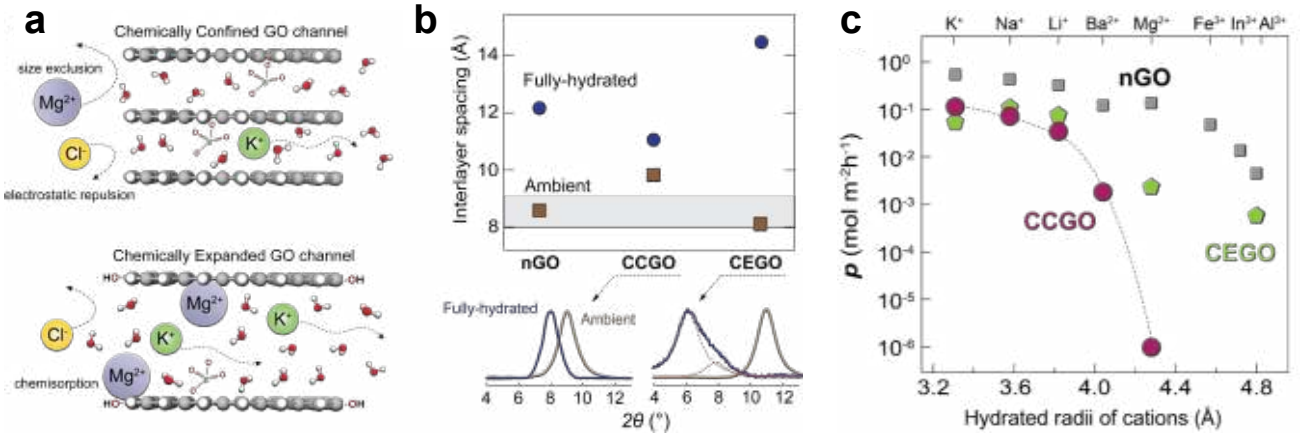

Figure 1: Ion-selective transport through chemically nanoconfined fluidic channels in graphene oxide-based membranes

Tunable Release of Ions from Graphene Oxide Laminates for Sustained Antibacterial Activity in a Biomimetic Environment

Kun Huang, Swathi Suran, Negin Kamyar, Farzad Foroutan, Premlal Balakrishna Pillai, Xuzhao Liu, John Vaughan, Darren Wilson, Philip J. Day, Rahul R. Nair
National Graphene Institute, Booth Street East, Manchester, United Kingdom
kun.huang-4@manchester.ac.uk

Abstract

Silver has long been recognized for its potent antimicrobial properties, but achieving a slow and longer-term delivery of silver ions presents significant challenges. Previous efforts to control silver ion dosages have struggled to sustain release for extended periods in biomimetic environments, especially in the presence of complex proteins. This challenge is underscored by the absence of technology for sustaining antimicrobial activity, especially in the context of orthopedic implants where long-term efficacy, extending beyond 7 days, is essential. In this study, the tunable, slow, and longer-term release of silver ions from the two-dimensional (2D) nanocapillaries of graphene oxide (GO) laminates incorporated with silver ions (Ag-GO) for antimicrobial applications are successfully demonstrated. To closely mimic a physiologically relevant serum-based environment, a novel in vitro study model using 100% fetal bovine serum (FBS) is introduced as the test medium for microbiology, biocompatibility, and bioactivity studies. To emulate fluid circulation in a physiological environment, the in vitro studies are challenged with serum exchange protocols on different days. The findings show that the Ag-GO coating can sustainably release silver ions at a minimum dosage of 10 µg cm−2 day−1, providing an effective and sustained antimicrobial barrier for over ten days.

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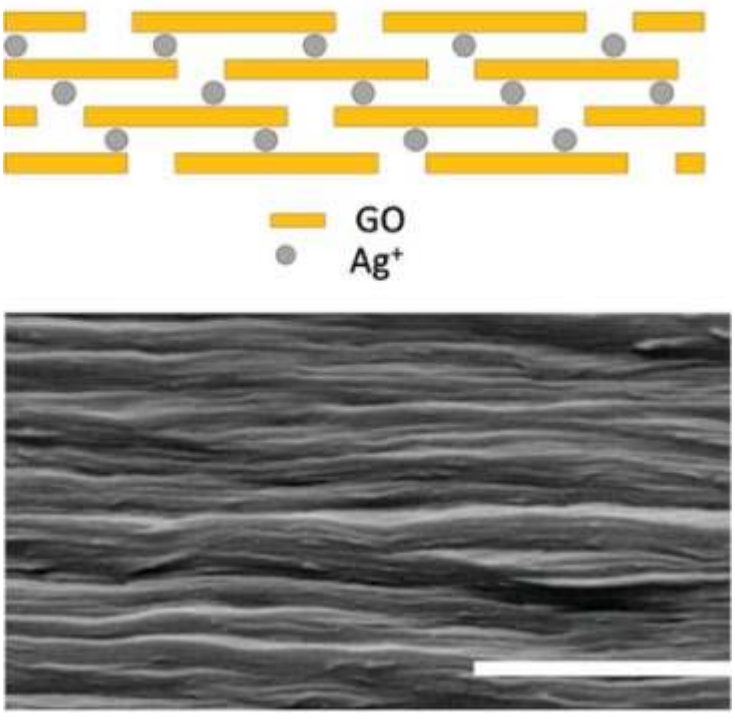

Figure 1: Schematic showing Ag^+ ions incorporated in the interlayer spacing of GO laminate

Can the Recent FAB Progress in 2D Transistors Serve 2D Photodetectors?

Yury Illarionov, Muhammad Zubair Nawaz
Southern University of Science and Technology, 1088 Xueyuan blvd, Shenzhen, China
illarionov@sustech.edu.cn

The tremendous amount of research on photodetectors with 2D channels has recently resulted in creation of a big zoo of prototypes with different layouts and operation principles [1]. This makes it complicated to select the most suitable 2D photodetector technology and move towards further integration, as finding the optimum trade-off between the technology-related aspects and performance characteristics remains complicated.

In this work we suggest to complement the recent advances of the optoelectronics community with what we have achieved working on 2D field-effect transistors (FETs) which are already being explored by the semiconductor industry [2,3]. First, back-gated FET-like 2D photodetectors, which in our opinion is the optimum way to go, would give an extra degree of freedom to modulate the device performance as compared to two-terminal devices (Fig.1a). However, currently available FET-like 2D photodetectors are impractical due to the use of thick oxides and resulting high operation voltages up to 70V [4]. Thus, scalable crystalline insulators such as CaF_2 [5] and Bi_2SeO_5 [6] previously used in 2D FETs should be very beneficial for 2D photodetectors as they would enable stable performance within CMOS-compatible few Volts operation range (Fig.1b), thereby also lowering power consumption. Next we will have to take into account that the use of a single 2D material as an active layer in photodetectors is typically not sufficient to achieve all desired performance parameters at once [7]. Thus, our recent results on CdS_xSe_{1-x}/PbI_2 heterostructures which enable photodetectors with simultaneously high photoresponsivity and fast time response (Fig.1c) will have to be considered. Finally, for CMOS circuits a buried back gate [4] is required for individual control of each particular device on the chip. Combining all these findings will bring us to the desired structure of a future 2D photodetector shown in Fig.1d.

In summary, we believe that future FET-like photodetectors employing scalable gate insulators, heterostructure channels and local back gates would be very attractive for future integrated circuits as they should simultaneously have superior performance and facile CMOS-friendly processing technology.

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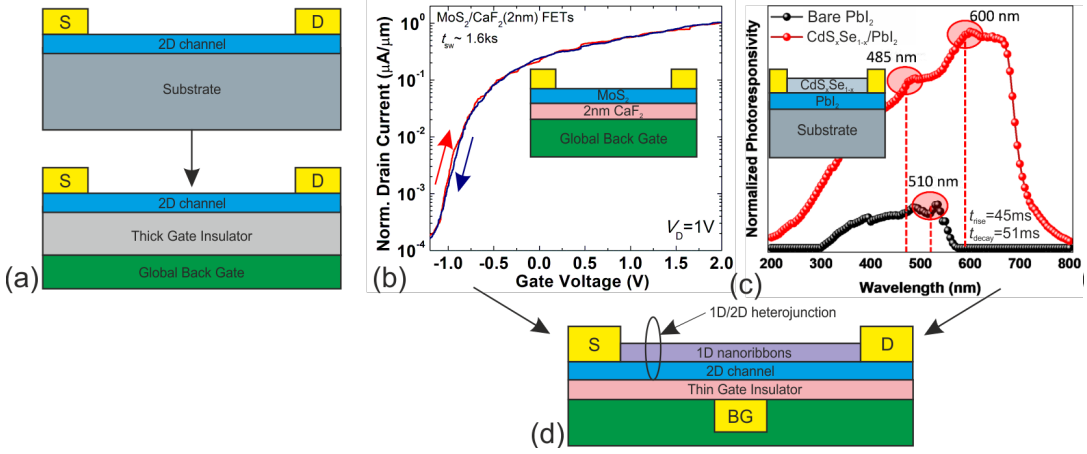

Figure 1: (a) Schematics of a two-terminal 2D photodetector (top) and a FET-like device with global back gate (bottom). (b) Back-gated MoS_2 FETs with 2nm CaF_2 insulators offer stable operation within few Volts bias range. (c) Photodetectors based on 1D CdS_xSe_{1-x}/2D PbI_2 heterojunctions exhibit fast photoresponse in a broad spectrum range. (d) Schematics of FET-like 1D/2D heterostructure photodetector with thin insulator and local back gate which could combine our advances made in scalable 2D FETs and heterojunction photodetectors.

Recent advances in personalized solution for bone regeneration

Mariana Ionita, Raluca Dobrisan, Alin Georgian Toader
Faculty of Medical Engineering, National University of Science and Technology Politehnica Bucharest, Gh. Polizu 1-7, 011061 Bucharest, ROMANIA
Advanced Polymer Materials Group, National University of Science and Technology Politehnica Bucharest, Gh. Polizu 1-7, 011061 Bucharest, ROMANIA
Contact@E-mail : mariana.ionita@upb.ro

Bone health is critically important to overall health and quality of life, representing a burgeoning problem for the demographics of an ageing society [1]. Conversely, multiple myeloma (MM) is characterized by bone marrow colonising neoplastic clonal plasma cells that produce organ damage including lytic bone lesions, fractures or spinal compression contributing to poor life quality causing bone lesion even more difficult to heal. On the other hand no bone substitute has proven to be fully clinically feasible, concerns regarding complex hierarchical constructs or lack of microvascular network still being important challenges [1]. In the current work we aim to improve implementation of existing cellular / acellular bone substitutes for the serious complication of non-union bone fractures, but also aim to devise new regenerative medicine products for prompt remediation for a donor-specific hBMSC osteogenic deficiency and alleviate MM complication. Functionalized nanostructured scaffolds fabricated by coupling 3D printing / bioprinting with novel biopolymer/ graphene-based inks modified / bioconjugated with ASOs are explored for local delivery of antisense oligonucleotides (ASOs) targeting favourable biodistribution and ncRNA inhibition. Our findings provide insights into the potential of GO-reinforced biopolymer composites as promising biomaterials for 3D printing sophisticated architectures for bone tissue engineering and emphasize the importance of GO concentration, material architecture, and biomimetic design in developing effective and clinically relevant regenerative therapies for bone regeneration and bone regeneration in MM conditions [2].

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Graphene/Polymer Nanocomposites: New Materials with Improved Functional Properties)

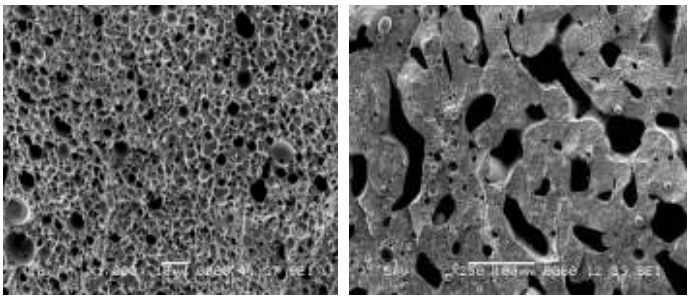
Muhammad Z. Iqbal
Chemical and Petroleum Engineering, United Arab Emirates University, United Arab Emirates
mziqbal@uaeu.ac.ae

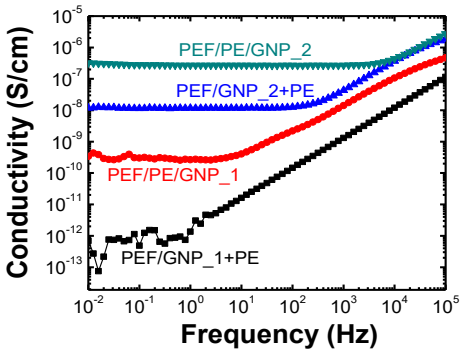
A new era of bio-based polymers replacing existing synthetic polymers has been growing at a tremendous speed. The interest in bio-renewable polymers further increased since some countries have banned single-use plastics for daily use, for example United Arab Emirates. Following the world patterns, companies such as Coca Cola are in line to change extensively consumed PET polymer with a bio-based alternative to share the global efforts in reducing synthetic polymer consumption. Bio-renewable poly (ethylene furandicarboxylate) (PEF) has been regarded as a possible substitute of PET for different applications. Being a new polymer in the market awaiting its commercial production line, PEF has to be studied towards various applications in the polymer market or at least within the application areas of PET.

This presentation is focused on our recent results on blending PEF with other potential polymers to improve its functional properties. Blends of PEF with synthetic polyolefins and bio-based poly (lactic acid) (PLA) and their nanocomposites were developed. The results are periodically benchmarked against standard PET to delineate a picture of practicality of the research results. Typically used commercial compatibilizers were incorporated to develop a thin interface between PEF and polyolefins whereas the concentration of the compatibilizers controlled the final morphology of the blends. The relations between on the one hand component properties and processing conditions and on the other hand blend morphology were rationalized based on classical theories for morphology development of polymer blends.

In the second part of this work, graphene nanosheets and single wall carbon nanotubes were locked at the interface of co-continuous PEF blends to produce electrically conductive composites. Owing to the development of an extremely thin polymer/polymer interface, a very small amount of nanofillers was able to electrically percolate the blend matrix. Moreover, conductive blends with changing blend ratio and graphene concentration are reported. In addition, membranes developed from PEF blends using electrospinning will be presented with unique switchable emulsification and demulsification applications in water-in-oil emulsions. More work is underway to predict filler packing at the polymer/polymer interface which will help in engineering conductive blends based on renewable polymers for mass applications.

Figures





2D material- enhanced superhydrophobic protective coating

Kishore Kumar Jena, Kin Liao
Department of Aerospace Engineering
Khalifa University of Science and Technology, PO Box- 127788, Abu Dhabi, United Arab Emirates
E-mail: Kishore.jena@ku.ac.ae

Abstract

The propose of this work is to develop superhydrophobic coatings by using 2D materials. The objective was achieved by developing hybrid coatings through sol-gel process and functionalization reaction. The role of hybrid molecules was particularly important for enhancing the hydrophobic properties of the hybrid coatings. The approach of current research is to develop a low temperature sol-gel coating process that gives better performance on metal surface. In this work two hybrid coatings were synthesized by two different mechanisms. 3-trimethoxy silyl propyl diethylene triamine and 3-trimethoxysilyl propyl methacrylate (TMSPM) precursors were mixed by stirring under nitrogen environment at 50 °C for 24 hours to formulate TSP-TM @HYBRID coating. The TSP-GLY @HYBRID coating was synthesized by ring opening polymerization process using 3-trimethoxy silyl propyl diethylene triamine and 3-glycidoxypropyltrimethoxysilane (GPTMS) silane precursors. In the second step 2D material (graphene) was synthesized from graphite flasks and thermal reduction process. The functionalization of 2D material was done by using amine (APTES) sol-gel precursors. In the final step TSP-TM @HYBRID coating and TSP-GLY @HYBRID coating were mixed with functionalized graphene to synthesize 2D material-based hybrid coating materials. The novelty of this work was the development of hybrid coatings by two different mechanisms and role of silane coupling agent. In this work, we explore the possibility of developing hybrid materials using 3-trimethoxy silyl propyl diethylene triamine, 3-glycidoxypropyltrimethoxysilane (GPTMS) ,3-trimethoxysilyl propyl methacrylate (TMSPM) silane coupling agent and functionalized graphene.

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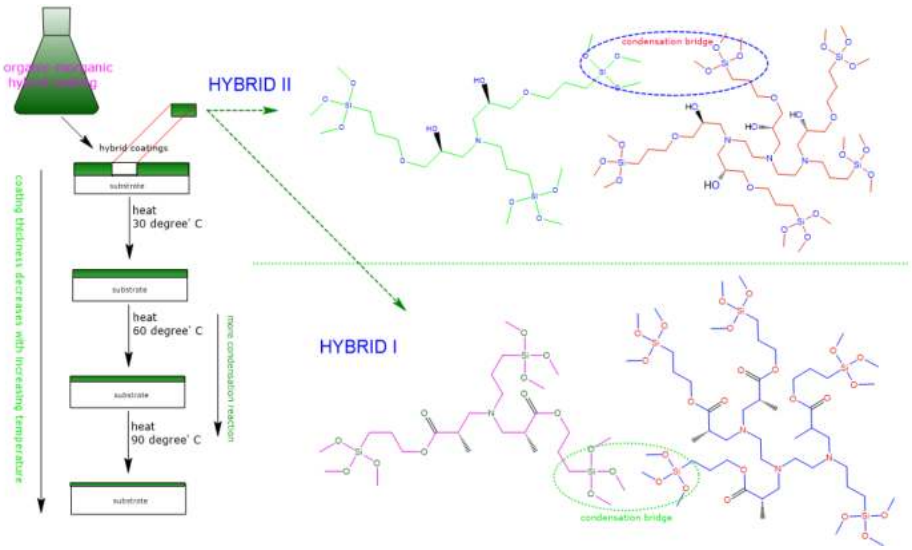

Figure 1: Synthesis procedure of HYBRID I and HYBRID II from siloxane precursors and 2D materials

3D Printing Nanoporous Nanocomposite Membranes

Hari Kalathil Balakrishnan, Laura Carvalho, Robel Tekle, Hassan Arafat, Ludovic F. Dumée
Khalifa University, Research & Innovation Center for Graphene and 2D Materials (RIC-2D), Abu Dhabi, United Arab Emirates
harikrishnan.balakrishnan@ku.ac.ae

The incorporation of nanoporosity into 3D-printed materials presents a promising opportunity to overcome the limitations of traditional fabrication methods in membrane technology [1]. However, current advancements in 3D printing face challenges in directly producing scalable macro materials with the necessary nanoporosity. To address this, we propose a novel strategy that combines ultraviolet (UV)-based 3D printing with polymer monolith chemistry [2] [3]. This enables the fabrication of membrane and separation materials with customizable geometries, controlled porosities, and integrated modular features. This approach not only streamlines the fabrication process but also allows for the integration of two-dimensional (2D) materials as well as nanosheets paving the way for the development of functional membranes with photocatalytic and electrocatalytic properties. Titanium dioxide (TiO_2) was chosen for its non-toxic properties in the development of membranes with superior photoactive/photocatalytic properties, increased permeability, and reduced fouling tendencies. [4] . Simultaneously, graphene nanosheets with higher mechanical properties, enhanced ionic and proton conductivity, and electrocatalytic properties, along with antifouling properties, were used to develop electrocatalytic membranes [5]. The current strategy facilitates the development of catalytic membranes with pore features ranging from ~ 10 nm to several hundred nm. Conventional phase inversion techniques are limited in terms of the maximum 2D material loading (~ 5-10 wt%) due to rheological, mechanical, and uniform distribution challenges caused by agglomeration [6]. In contrast, the proposed technique and the wide range resin chemistries enable much higher nanosheet and nanomaterials loading, up to 30 wt% and higher, with enhanced dispersion and uniform distribution through layer-by-layer control. Furthermore, the process allows for the creation of highly customized membranes with precise deposition of 2D materials in a highly automated and reproducible manner.

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Figure 1: 3D-printed graphene-based membranes with various sizes. SEM image confirms the porous nature of the 3D-printed membrane.

Resistive switching in memristors based on 2D materials

Zineb Kerrami[1], Gaelle Bigeard[1], François Triozon[2], Alessandro Cresti[1]
[1] *Univ. Grenoble Alpes, Univ. Savoie Mont Blanc, CNRS, Grenoble INP, CROMA, 38000 Grenoble, France*
[2] *CEA-Leti, 17 avenue des Martyrs, 38054 Grenoble, France*
zineb.kerrami@grenoble-inp.fr

The resistive switching mechanism in atomristors is driven by an external electric field that induces the migration of metallic ions from the contacts to the 2D material. The resulting conductive filament connects the electrodes, enabling different resistance states [1]. However, understanding the physics behind filament evolution and device performance remains a complex challenge. In this study, we employ density functional theory and non-equilibrium Green's function method to investigate the electronic and transport properties of monolayer and multilayer 2D materials sandwiched between two metallic electrodes. We consider structural defects and substitutional doping as key factors in the transition from low resistance state (LRS) to high resistance state (HRS). Our examination includes various 2D materials such as 1T-MoS_2 and 2H-MoS_2 (representing conductor and semiconductor phases of TMDs), graphene, and hBN. We illustrate how the electrical conductivity could be influenced by the thickness of the 2D material and the electronic behaviour at the interface with the electrodes. Furthermore, we investigate the effect of atomic vacancies and metal ion substitutions on the transport properties. These defects introduce localized states within the bandgap, which alter the electronic properties and then affect charge transport across the 2D material, thus enabling resistance switching between LRS and HRS.

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Figures

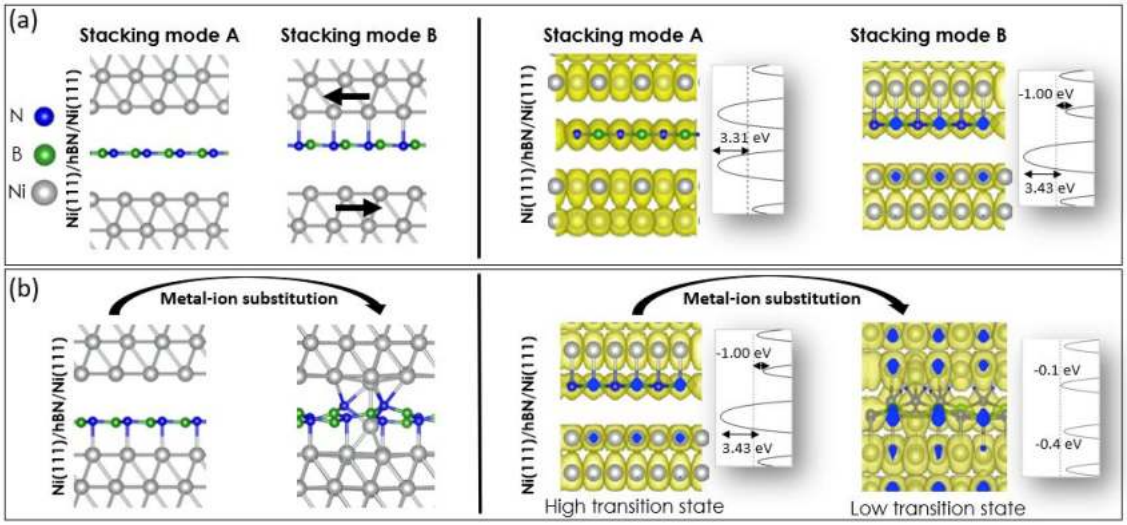

Figure 1: (a) Structural illustration (Left) and charge distribution (Right) of hBN in different stacking modes. Inset figure shows the averaged electrostatic potential. Reduced tunnelling barrier due to N-Ni bond formation at the interface in stacking mode B. (b) Structural illustration (Left) and charge density distribution (Right) of pristine and defected Ni/hBN/Ni systems. Charge distribution reveals enhanced charge density at the interface, attributed to the effect of metal-ion substitution. The averaged electrostatic potential shows no tunnelling barrier after metal-ion substitution, which indicates higher electronic transmission and then higher conductivity.

Acknowledgements

This work is supported by the LabEx Minos under the contract ANR-10-LABX-55-0, and by the ANR SWIT Grant (ANR-19-CE24-0004). It is implemented using HPC resources from GENCI–IDRIS (Grant 2023 A0140914157), GENCI–TGCC (Grant 2024 AD010914993), and the GRICAD infrastructure (https://gricad.univgrenoble-alpes.fr), which is supported by Grenoble research communities.

Improving the Gas Barrier Properties of Polymer Seals using Graphene

Tayyab Khan[1], and Ian Kinloch[1]
[1]National Graphene Institute, Henry Royce Institute and Department of Materials, School of Natural Sciences, The University of Manchester, Oxford Road, Manchester, M13 9PL, UK.
tayyab.khan@manchester.ac.uk

Abstract:

Preventing chemical and gas leakage is critical in the petrochemical, food, and automotive industries. High-performance seals generally made of fluoropolymers (e.g., PTFE, FKMs) are facing an uncertain future due to recent health-related legislation. In this study, ultrahigh molecular weight polyethylene (UHMWPE) and graphene nanoplatelets (GNP) nanocomposites were manufactured using hot pressing for sealant applications. The thermal properties were investigated through differential scanning calorimetry (DSC) and thermogravimetric analysis (TGA) techniques. The mechanical performance was evaluated through dynamic mechanical analysis (DMA) and tensile tests. Furthermore, the gas barrier performance in terms of CO2 permeability was assessed using a locally manufactured permeability rig (Figure 1).
The SEM micrographs confirmed a segregated core-shell structure where GNPs covered the outer surface of individual polymer particles. The DSC results showed a linear increase in the crystallinity of the nanocomposites up to 3 wt.% of GNP loading, followed by a notable drop due to agglomeration at higher concentrations. A significant improvement in the thermal stability of the nanocomposites was also observed with an increase in the GNP concentration. The DMA results also showed a linear increase in the storage moduli of the nanocomposites with an increase in the GNP concentration. Meanwhile, the tensile strength of the nanocomposites increased up to 1 wt.% GNP concentration, followed by a notable decrease at higher concentrations. The tensile moduli of the nanocomposites showed a similar linear increase with the GNP concentration as observed in the storage moduli. A significant improvement in CO_2 permeability was also observed with the addition of GNPs to the neat UHMWPE, showing great potential for sealant applications. The gas permeability results revealed a drop of around 50% in the average permeability of the specimens incorporating only 1 wt.% (around 0.47 vol.%) GNP compared to the neat UHMWPE specimens.

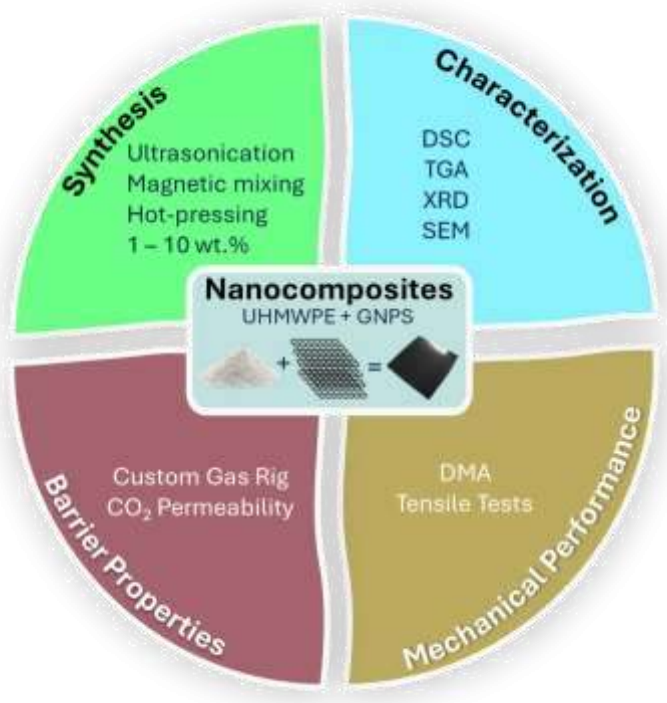

Figure 1: Graphical Abstract

Laser Propulsion of Three-Dimensional Graphene Structures For Space Applications

Omnia Khattab [1], Rami Elkaffas [1], Basel AlTawil [1], Carlo Lorio [2], Sean Swei [1], Yarjan Abdul Samad [1,3]
[1] Department of Aerospace Engineering, Khalifa University of Science and Technology, Abu Dhabi,127788, United Arab Emirates.
[2] Center for Research and Engineering in Space Technologies, Université libre de Bruxelles, Belgium.
[3]Cambridge Graphene Centre, University of Cambridge, Cambridge, CB3 0FA UK.
100062658@ku.ac.ae

Abstract

Advancements in space exploration enhance our understanding of the universe and drive cross-cutting technological innovation [1]. Photonic propulsion, using light's momentum to generate thrust, is a promising alternative to traditional systems [2]. It offers higher velocities, improved thrust-to-weight ratios, greater efficiency, reduced spacecraft mass by eliminating need for propellant, making it ideal for long-duration missions [3]. Recent studies highlight the potential of graphene & related materials (GRMs) for light propulsion due to their exceptional properties; graphene aerogels have low density (>0.16 mg/cm^3) [4], high electrical conductivity (>100 S/m) and a Young's modulus (>20 MPa) [5,6]. In this work we produce three-dimensional graphene structures using a novel intercalation, expansion, and liquid phase exfoliation technique. The study utilized directional freezing to optimize the microstructure and pore alignment of 3D graphene structures for laser propulsion applications, testing their application in simulated space environment in a state-of-the art setup. We tested a suspended graphene aerogel with a density of 0.16 g/cm³, at a vacuum level of 2x10^{-5} torr and with laser power input of 7 watts. Graphene 3D structure deflected by 2.7 mm in the x- and 0.009 mm in the y-direction, as analyzed using Tracker video analysis software. Experiments controlled for laser wavelength at 422 nm and less than 1-second strike time revealed variations in propulsion characteristics based on density and vacuum environment. This study is the first to develop an innovative setup for intensively investigating graphene 3D structures' propulsion, advancing beyond previous research on reduced graphene oxide.

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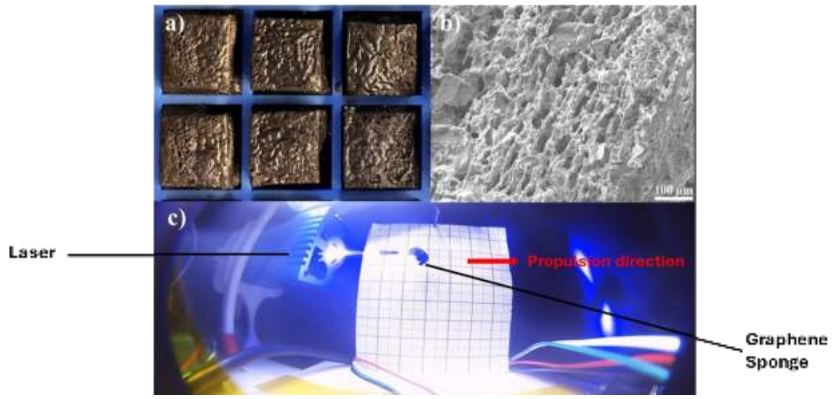

Figure 1: (a) Cubic Graphene Aerogels, (b) Aligned pores under SEM, (c) Laser Propulsion snapshot

Highly efficient titanium anodes with electrocatalytic coating of mixed oxides based on ruthenium, palladium and iridium for industrial disinfection of water with sodium hypochlorite

[1]D.V. Korolev, [1]S.N. Saltykov**,** [2,3]A.Y. Cherkesov, [2,3]I. V. Pchelnikov [2,3]L.N. Fesenko**,** [3]M.V. Liplyavka, [3]M.S. Lipkin

[1]MMC Nornicel, 1st Krasnogvrdeyskiy proezd, 15, Moscow, Russia, 123100
[2]Scientific and production enterprise ECOFES,
[3]Platov South-Russian State Polytechnic University (NPI), Prosveshcheniya str., 132, Novocherkassk, Rostov region, Russia, 346428

KorolyovDV@nornik.ru

Sodium hypochlorite is used as a safe alternative to chlorine in the disinfection of drinking water. Sodium hypochlorite is obtained by electrolysis of a solution of table salt or natural chloride-containing waters. The anode material has the greatest influence on the efficiency of electrolysis, electrical and electrochemical parameters, the economy of the process and its operating regulations, the design of devices and their durability. It is very important to choose the optimal coating with a long service life and high chlorine release ability. The most effective anode material is ruthenium titanium oxide anode, since it is this that allows one to achieve the highest concentration of hypochlorite (up to 9–10 g/l chlorine equivalent) with a high current yield of chlorine (60–70%). However, such anodes has a limited service life due to the irreversible loss of ruthenium oxide during anodic polarization. More effective are three-component anode coatings containing iridium (oxide-iridium ruthenium-titanium anodes), which increase corrosion resistance up to 8 times compared to ruthenium-type anodes. On the other hand, the cost of iridium is 7÷8 times higher than the cost of ruthenium, which significantly affects the economic aspects of using such anodes in the water disinfection industry with sodium hypochlorite. Palladium has a lower cost compared to iridium (3.5÷4 times) and at the same time is a highly active catalyst. The use of palladium as part of the electrocatalytic coating of anodes with partial replacement of iridium makes it possible to reduce the cost of such anodes and increase their efficiency in chlorine output over current without significantly reducing the corrosion resistance of such a multicomponent system. The addition of palladium oxides to mixed oxide electrodes causes an increase in catalytic activity due to a change in the ratio of oxygen and chlorine overpotentials. The possibility of the formation of oxides Pd_xO_y, at high current densities, having a high redox potential, leads to enhanced catalysis by the redox mechanism, as well as to an increase in the corrosion resistance of the electrode due to the protective effect of palladium in relation to titanium.

Figures

	Ru-Ir/Ti	RuPdIr/Ti
Specific consumption of electricity, kWh/kg of act.Cl.	3,6**	3,3
Service life, years	2,5	3*
The cost of the anode, USD/m^2	460	450

Table 1: Comparative features of developed Pd-based anode in comparison Ru-Ir - analogue

AI-guided screening of van der Waals materials with high optical anisotropy

Ivan Kruglov[1], Georgy Ermolaev[1], Lyudmila Bereznikova[1], Gleb Tselikov[1], Andrey Vyshnevyy[1], Alexey Arsenin[1], Valentyn Volkov[1]
Emerging Technologies Research Center, XPANCEO, Dubai Investment Park First, Dubai, United Arab Emirates
ikruglov@xpanceo.com

Large optical anisotropy observed in a broad spectral range is of paramount importance for efficient light manipulation in countless devices. As a result, natural materials with giant anisotropy ($\Delta n > 1$) are in growing demand both for scientific and industrial purposes. In this regard, transition-metal dichalcogenides (TMDCs) in a bulk configuration are promising candidates because of their strongly anisotropic vdW structure, which naturally leads to a large intrinsic birefringence [1-4].

ML methods can boost the search for materials with high optical anisotropy. In this work, we trained ALIGNN graph neural network to predict birefringence of materials based only on their crystal structure and composition (Figure 1) [5]. Average error on test and validations sets was 0.02. To train this model, we collected a unique database of known layered van der Waals materials, which consisted of their crystal structures and optical properties, calculated in density functional theory (DFT) and for some of them measured using scanning ellipsometry. In the database, theoretically calculated and experimentally measured optical constants are in perfect agreement.

Therefore, we developed a machine learning model, which can predict birefringence of materials with accuracy, close to DFT methods, but with a much higher speed. This allowed us to screen the existing databases of crystalline materials (MaterialsProject and GNOMe) and we found novel candidate materials with high optical anisotropy, which was then confirmed in DFT and GW calculations and experimental measurements.

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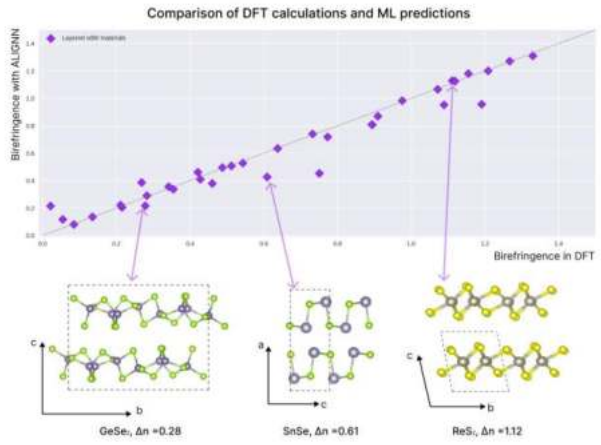

Figure 1: Machine learning model to predict birefringence of layered van der Waals materials

Graphene and its derivatives-based composites for industrial applications

Jitender Kumar
TACC Ltd., Mandideep, Bhopal, India
jitender.kumar@lnjbhilwara.com

Abstract

The exceptional mechanical, thermal, electrical, and optical properties of graphene have sparked widespread interest in its potential applications across various industries. The integration of graphene and its derivatives, such as graphene oxide and reduced graphene oxide, into composite materials has emerged as a promising approach to harness their unique properties. Graphene-based composites have shown significant potential in enhancing the performance of materials used in energy storage and conversion, aerospace, automotive, biomedical, and construction applications. By leveraging the unique properties of graphene, these composites offer opportunities for innovation and advancement in various industrial sectors.

Mechanical Composites

Graphene-based mechanical composites have been developed to enhance the mechanical properties of materials such as polymers, metals, and ceramics. The addition of graphene to polymer matrices has been shown to improve their tensile strength, stiffness, and toughness. For example, graphene-reinforced polypropylene composites have been demonstrated to exhibit improved mechanical properties, making them suitable for applications in the automotive and aerospace industries. Graphene-based composites have also been explored for use in advanced composite materials for aerospace applications, where they offer improved mechanical properties, reduced weight, and enhanced durability [1].

Energy Storage Composites

Graphene-based composites have been widely investigated for energy storage applications, including batteries, supercapacitors, and fuel cells. Graphene-based electrodes have been shown to improve the performance of lithium-ion batteries, with enhanced charge/discharge rates and cycle life. Graphene-based supercapacitors have also been developed, offering improved energy density and power density. Additionally, graphene-based composites have been explored for use in fuel cells, where they offer improved catalytic activity and durability [2].

Thermal Composites

Graphene-based thermal composites have been developed for applications in thermal management and energy harvesting. Graphene-based thermal interface materials have been shown to improve the thermal conductivity of materials, making them suitable for use in electronic devices and thermal management systems. Graphene-based composites have also been explored for use in thermoelectric devices, where they offer improved thermoelectric performance and efficiency [3].

Cement Composites

Graphene based cement composites could contribute towards major improvement in the properties of concrete, including significant changes in the microstructure. Various researchers are working all over the globe regarding application of graphene-based materials in Cementous application for sustainable concrete, mortar & paste. Cement alone contributes to 8% of global CO_2 production, incorporation of graphene in cement composites could reduce this CO_2 emission by 20% at least [4].

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Novel Heterostructured Holey Graphene-$CoTiO_3/TiO_2$ Nanocomposite Enabled Photocatalytic Mixed Matrix Membranes for Antibiotics Removal

Mahendra Kumar[1,2] Aya Fadl Aboukhater[1,2], Hassan A. Arafat[1] and Shadi W. Hasan[1,2]
1Research and Innovation Center in Graphene and 2D Materials (RIC-2D), Khalifa University, Abu Dhabi, UAE
[2]Center for Membrane and Advanced Water Technology, Khalifa University, Abu Dhabi, UAE
mahendra.kumar@ku.ac.ae

Discharging hospital wastewater without prior treatment is responsible for potentially transporting antibiotics-laden wastewater into water resources, which poses a significant threat to human health and the ecosystem [1,2]. To overcome this problem, photocatalysis and membrane filtration-enabled photocatalytic membrane reactors (PMRs) have emerged as a potential tool to remediate hospital wastewater and antibiotics contaminated water resources [3,4]. High photodegradation efficiency photocatalysts and advanced membranes are needed to develop photocatalytic membrane reactors. In this study, HGN-$CoTiO_3/TiO_2$ nanocomposites are first produced by integrating $CoTiO_3/TiO_2$ with 2D holey graphene (HGN), and sophisticated instrumental data validate the formation of HGN-$CoTiO_3/TiO_2$ nanocomposites. HGN-$CoTiO_3/TiO_2$ nanocomposites are proficient in the photocatalytic degradation of antibiotics aqueous solution over a short period of exposure to light radiation. The mixed matrix membranes (MMMs) with different loading of HGN-$CoTiO_3/TiO_2$ are also fabricated from HGN-$CoTiO_3/TiO_2$, PVP, and PVDF via the nonsolvent-induced phase separation method. All the membranes demonstrated typical asymmetric porous structures with a compact skin layer and porous sublayer with finger-like pores. The pure water flux, antifouling, and photocatalytic degradation efficiency are tunable upon varying the loading content of HGN-CoTiO3/TiO2 within the matrix of MMMs. The maximum pure water flux is observed for 5 wt.% HGN-$CoTiO_3$ incorporated membrane while the best antifouling and antibiotics photodegradation abilities are attained for 15 wt.% HGN-$CoTiO_3/TiO_2$ loaded membrane used in dead-end and vacuum filtration under direct exposure to light radiation. The integrated adsorption and photocatalytic membrane reactor can be manufactured using HGN-$CoTiO_3/TiO_2$ and MMMs for hospital wastewater treatment.

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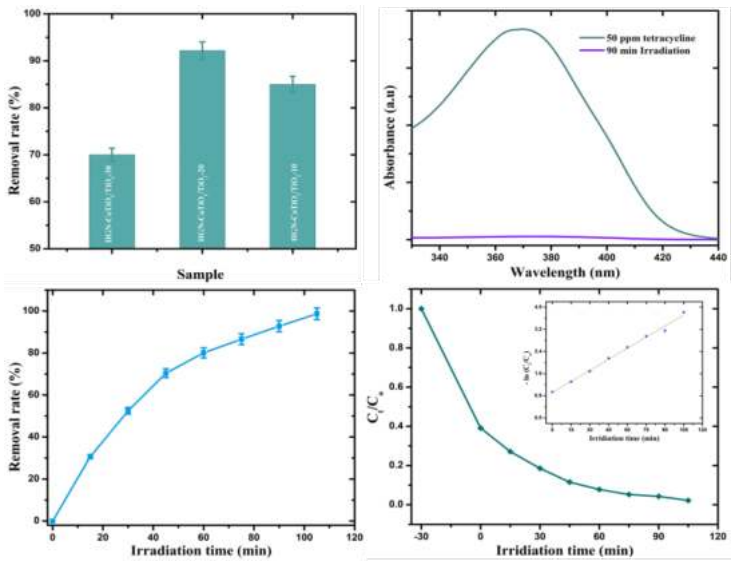

Figure 1: Photocatalytic performance of HGN-$CoTiO_3/TiO_2$ nanocomposite in degradation of antibiotic solution.

Computational modeling of modified 2D materials with deep eutectic solvents for water contaminant removal

Tarek Lemaoui, Ahmad S. Darwish, Anjali Goyal, Hassan A Arafat, Enas Nashef
Khalifa University, Research and Innovation Center on 2D Nanomaterials (RIC2D), Abu Dhabi, United Arab Emirates
tarek.lemaoui@ku.ac.ae

Abstract

The widespread presence of contaminants such as heavy metals, dyes, PFAS, pharmaceuticals, and pesticides in the aquatic environment poses a significant threat to public health and ecological balance. This work introduces a novel approach to water treatment technology, focusing on the computational modeling of two-dimensional (2D) materials, including graphene (Gr), graphene oxide (GO), and reduced graphene oxide (rGO) modified with natural deep eutectic solvents (NADESs) for effective contaminant removal. The study used Density Functional Theory (DFT) calculations and COSMO-RS analysis to evaluate the affinity and selectivity of these 2D materials and NADESs for various contaminants. The results showed that GO exhibited a significantly higher affinity for a broad range of pollutants compared to Gr and rGO, suggesting its superior potential in water purification. Additionally, among the tested NADESs, thymol-based DES demonstrated the best performance in enhancing the removal of contaminants. The findings underscore the promise of 2D materials and NADESs in developing sustainable, efficient water treatment technologies. These results provide a strong foundation for future experimental work and the development of novel materials that can be applied in various applications, such as membrane fabrication, adsorption, catalysis, and sensor development, all designed to improve the removal efficiency of a wide range of contaminants from water.

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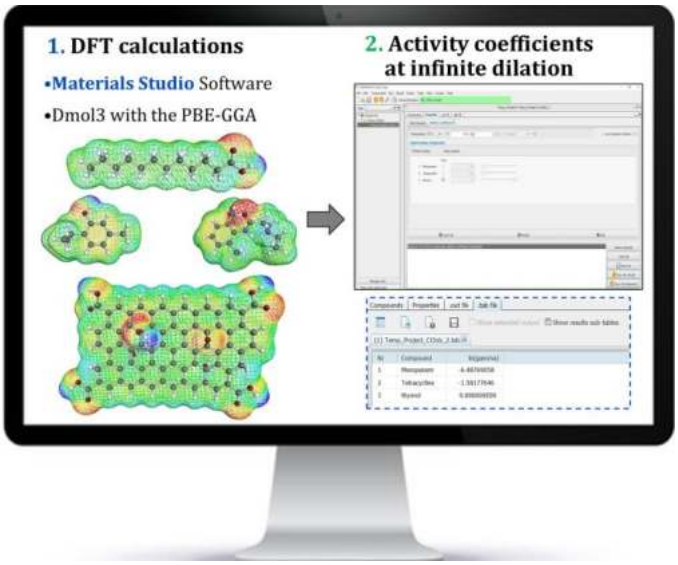

Figure 1: Quantum chemical calculations for 2D materials modified deep eutectic solvents.

Palladium-composite membrane application for the separation of high-purity hydrogen from gas mixtures

Leontyev A.[1], Saltykov S.[1], Podkolodnaya Yu.[1], Khimich A.[1], Shirin N.[2], Vitkovskii V.[2], Roslyakov I.[2], Napolskii K.[2], Prikhno I.[2], Poyarkov A.[2], Eliseev A.[2], Lukashin A.[2]

1 – Palladium Technology Center, MMC Norilsk Nickel, 15, 1st Krasnogvardeysky Drive, Moscow, Russia

2 – Lomonosov Moscow State University, 1, Leninskie Gory, Moscow, Russia

LeontevAVi@nornik.ru

Hydrogen is a clean and efficient energy carrier, and the hydrogen economy is currently seen as a potential solution for energy security. Therefore, the extraction and purification of hydrogen from gas mixtures is an extremely relevant issue. Membrane technology serves as the most effective and economically viable alternative for the extraction of high-purity hydrogen.

Various hydrogen-selective membranes can be represented by carbon molecular sieves, dense metallic, silicon oxide, polymer, and composite membranes. The main drawbacks of commercial membrane samples include high cost and low performance, which makes composite membranes consisting of a permeable substrate and a coated selective palladium layer of great scientific and practical interest. A properly chosen support and an optimal Pd active layer will achieve high selectivity and significant permeability for effective gas separation.

The active palladium layer applied to the support gives selectivity to the material. This layer should be as thin as possible, while also being gas-tight with minimal defects. Various methods are used for deposition, including magnetron sputtering, chemical vapor deposition, electroplating, and others.

Porous Vycor glass, metal substrates, polymers, and ceramics are used as supports for composite membranes. The permeability of the support and the thickness of the selective layer influence the membrane's performance.

In the present work, laboratory methods have been developed for synthesizing composite membranes based on a porous ceramic substrate with varying pore diameters in the range of 50-150 nm from anodized aluminum oxide with a palladium layer. The use of anodized aluminum oxide as a support determined the mechanical and thermal stability of the material, as well as the ability to control geometric parameters (pore diameter and spacing between their centers) during anodization. The authors established that by varying the voltage, electrolyte composition, concentration, and temperature, the porous structure of the ceramic substrate can be regulated. The application of the palladium active layer through vacuum and magnetron sputtering ensured the selectivity of the composite membrane. The authors highlight the exceptional importance of nanofibers in the pores of the ceramic substrate, as they promote adhesion and retention of the deposited selective layer on the surface of the anodized aluminum oxide.

The obtained composite membranes have successfully passed laboratory tests for determining the gas permeability of composite membranes using model mixtures of H2/N2, and tests are currently being conducted on real gas mixtures containing CO and CO2. Positive research results showed that the developed prototypes of composite membranes based on a porous ceramic substrate hold promise for future use in technologies for the extraction of pure hydrogen.

The research group continues to optimize the technology for producing composite membranes and is testing new methods for creating the selective layer, with the aim of developing a prototype that will occupy its niche in the hydrogen technologies of the future.

Ag-assisted construction of multiple interfaces in $Ti_3C_2T_x$/g-C_3N_4@Ag composite films for enhanced electromagnetic interference shielding

Baosong Li, Kin Liao
Department of Aerospace Engineering and Research & Innovation Center for Graphene and 2D Materials (RIC2D), Khalifa University of Science and Technology, Abu Dhabi, UAE
baosong.li@ku.ac.ae

The proliferation of electronic devices leads to the generation of significant amounts of electromagnetic radiation, resulting in various detrimental effects, such as temporary device disturbances, environmental pollution, and even potential risks to human health [1]. MXene-based heterogeneous structures with multiple interfaces have inspired significant interest due to their remarkable performance when applied in smart electronic and energy storage devices [2]. Herein, two-dimensional (2D) $Ti_3C_2T_x$/g-C_3N_4@Ag composite films were assembled in a layered structure with multiple interfaces and simultaneously displayed outstanding electromagnetic interference (EMI) shielding effectiveness and distinguished pseudocapacitive performance. Beneficial from the heterogeneous structure, Ag-assisted construction of multiple interfaces, and controllable composition, the composite film containing 10 wt.% of g-C_3N_4@Ag nanosheets exhibited exceptional EMI shielding effectiveness of 51.4 dB and high absolute shielding effectiveness of 25855 dB cm^2 g^{-1}. The high EMI shielding effectiveness largely depends on the enhanced absorption of electromagnetic waves, stemming from local dipolar polarization, the porous architecture, and multiple interface interactions in the composite film.

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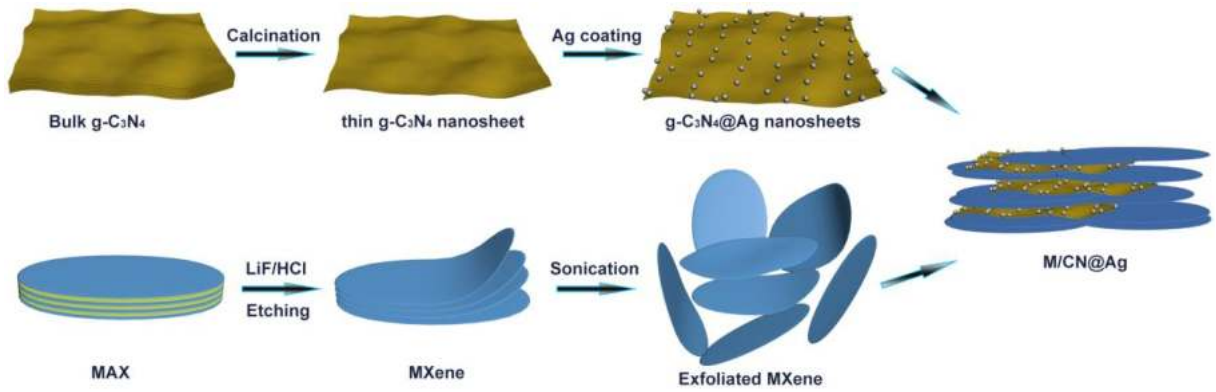

Figure 1: Schematic diagram of the synthesis of $Ti_3C_2T_x$/g-C_3N_4@Ag composite film.

Enhanced removal of short-chain PFAS from water using modified Graphene Oxide membrane

Eubert Mahofa[a,b], Sally El Meragawi[a,b], Akshat Tanksale[c], and Mainak Majumder[a,b]

[a]*Nanoscale Science and Engineering Laboratory (NSEL), Department of Mechanical and Aerospace Engineering, 20 Research Way, Monash University, Clayton, VIC 3800, Australia*
[b]*ARC Research Hub for Advanced Manufacturing of 2D Materials, 20 Research Way, Monash University, Clayton, VIC 3800, Australia*
[c]*Department of Chemical and Biological Engineering, Monash University, Clayton, VIC 3800, Australia*
eubertmahofa@monash.edu

Abstract

Per- and polyfluoroalkyl substances (PFAS) are highly persistent in the environment and can accumulate in human bodies, leading to significant health risks [1]. Traditional methods struggle to effectively remove short-chain PFAS (those with fewer than eight carbon atoms) from water [2]. In this study, we developed a beta-cyclodextrin modified graphene oxide (GO-βCD) membrane featuring asymmetrically sized nanochannels that interact favourably with these persistent pollutants. We enhanced water flux by incorporating an intercalant that enlarges the nanochannels and modifies the chemistry to improve PFAS transport through complexation and coordination sites. Our innovative GO-βCD membrane successfully eliminates over 90% of PFBA, PFPeA, PFHxA, and PFOA from water mixtures, achieving a high permeance of 21.7 ± 2 $Lm^{-2}h^{-1}bar^{-1}$, which surpasses that of standard NF270 membranes, while concentrating these contaminants in the retentate. By combining permeation experiments with molecular dynamics simulations and transition state theory [3], we showed that the energy barrier for PFAS transport is higher in the GO-βCD structure compared to both GO-αCD and pristine GO. This modified membrane features strategically placed sites that effectively impede PFAS transport under realistic conditions, ensuring long-term performance (up to 24 hours) at concentrations typical of drinking and recreational waters.

Keywords: beta-cyclodextrin, short chain PFAS, graphene oxide membrane, nanofiltration, energy barriers.

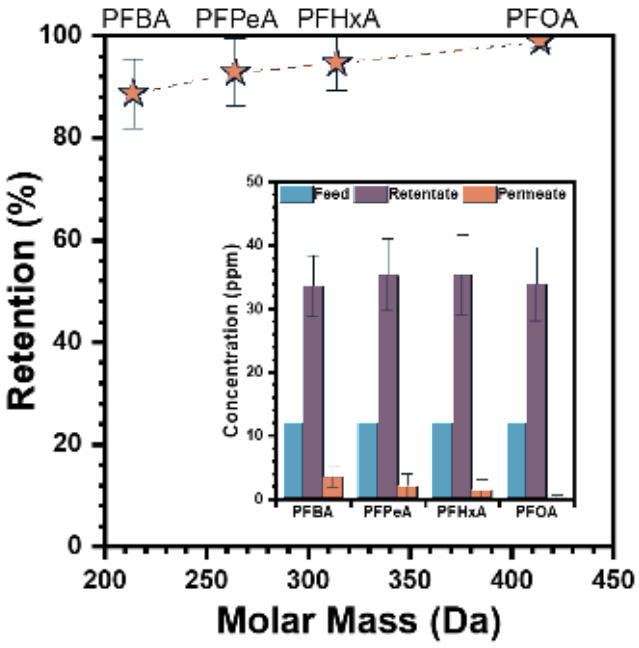

Figure 1: Retention of mixtures of PFAS with an inset displaying mass balance detail

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15.5 MeV Proton Irradiation Treatment of Liquid Phase Exfoliated Graphene

Narek Margaryan[a], Hovhannes Badalyan[a], Tigran Ohanyan[a], Eduard Aleksanyan[a], Astgik Hovhannisyan[b]
[a] *A. Alikhanyan National Science Laboratory (Yerevan Physics Institute), Yerevan 0036, Armenia*
[b] *Scientific Technological Center of Organic and Pharmaceutical Chemistry, 26, Azatutian ave., Yerevan, 0014, Armenia*
n.margaryan@yerphi.am

Exceptional Physical properties, including lightweight nature of graphene make it a highly promising material for space applications [1,2]. However, the impact of proton irradiation, a common phenomenon in space environments, on the structural integrity and functional properties of graphene remains a critical area of research. This study aims to fill this gap by investigating the effects of proton irradiation on liquid-phase exfoliated graphene. We focus specifically on the alterations in infrared spectra and structural characteristics of graphene induced by irradiation with 15.5 MeV protons [3]. Our analysis reveals that organic molecules and functional groups adsorbed on graphene during exfoliation elevate the Fermi level, suppressing graphene's infrared absorption through the Pauli blocking effect. We demonstrate that proton irradiation, at fluences up to 1×10^{15} proton/cm^2, effectively removes adsorbed molecules and functional groups, thereby eliminating Pauli blocking effect. These findings contribute to a better understanding of the behaviour of graphene under proton irradiation, essential for its utilization in space-centric applications such as thermal coatings, electronics, and optical devices.

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Investigating integration of perylene derivative molecules with monolayer MoS_2: Insights into hybrid interface properties

Mohammed EL Amine Miloudi, Oliver Kühn
Institute of Physics, University of Rostock, Albert-Einstein-str. 23-24, 18059 Rostock, Germany

Oliver.kuehn@uni-rostock.de

Integrating organic molecules with two-dimensional (2D) materials represents a transformative advancement, expanding processes within two dimensions and facilitating van der Waals (vdW) heterostructures. This synergistic alliance harnesses the unique properties of finite 2D materials found in nature, seamlessly merging with a diverse array of purposefully designed organic molecules. Despite their immense potential, the ability to tailor and synthesize molecules with predictable properties remains virtually boundless [1]. Organic compounds, renowned for their high absorption capacities yet limited mobility and charge stability, starkly contrast with inorganic compounds known for relatively low absorption but exceptional charge transport properties [2]. The deliberate assembly of van der Waals heterostructures, combining inorganic compounds with organic molecules, holds promise for synergistically exploiting the advantageous characteristics of both material classes. Molybdenum disulfide (MoS_2), a prominent member of transition-metal dichalcogenides (TMDs), is a highly promising 2D semiconductor for transistors, optoelectronics, and catalysis applications. In contrast, widely utilized as dyes, perylenes offer tunable optical properties through modifications to their core structure. This study systematically investigates the structural, electronic, and optical features of MoS_2/perylene hybrid systems employing density functional theory (DFT), incorporating diverse perylenes such as perylene diimide (PD), perylene orange (PO), and perylene red (PR). The research emphasizes the precise modulation of properties within the hybrid system, providing insights into the intricate interplay between MoS_2 and perylenes, including strain effects. This elucidation sheds light on synergistic effects, paving the way for advanced applications across diverse disciplines and contributing to a deeper comprehension of 2D material integration and the tailored design of materials for specific functionalities.

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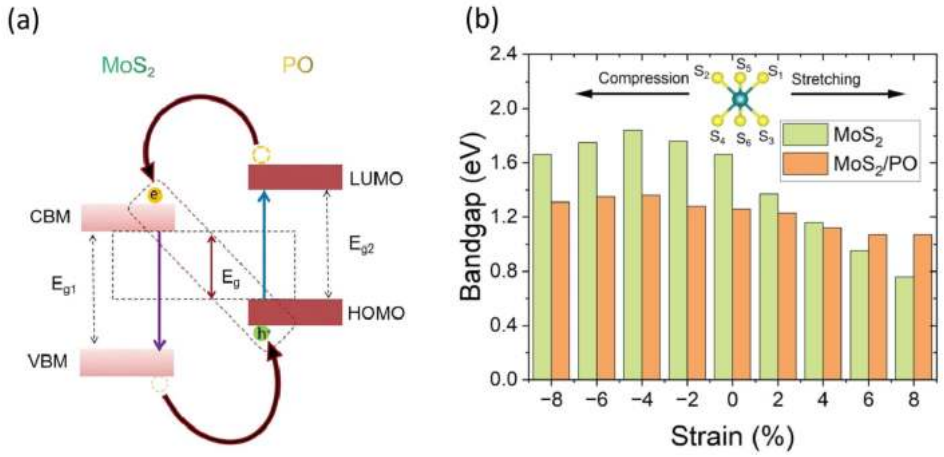

Figure 1: (a) Schematic of interface band alignment relative to Fermi energy (E_F), and (b) evolution of band gap (E_g) in strained MoS_2 and MoS_2/PO systems.

Ionogel-based electrodes for non-flammable high-temperature operating electrochemical double layer capacitors

Alberto Morenghi[1]
Agnese Gamberini[1], Tobias Burton[2], Alix Ladam[2], Ahmad Bagheri[1], Matteo Abruzzese[1], Hossein Beydaghi[1], Valentina Mastronardi[1], Elena Calcagno[1], Samaneh Vaez[1,3], Alberto Morenghi[1], Teresa Gatti[3], Anais Falgayrat[2], Sebastiano Bellani[1], Sebastien Fantini[1], and Francesco Bonaccorso[1,4]

1 Bedimensional S.p.A., Lungotorrente secca 30R, 16163 Genova, Italy.
2 Solvionic, 11 Chemin des Silos, Toulouse, 31100 France.
3 Department of Applied Science and Technology, Politecnico di Torino, Corso Duca degli Abruzzi 24, 10129 Torino, Italy.
4 Istituto Italiano di Tecnologia, Graphene Labs, Via Morego 30, 16163 Genova, Italy.

a.morenghi@bedimensional.it

Electrochemical double-layer capacitors (EDLCs) are a type of supercapacitors (SCs), which have garnered significant attention as suitable energy storage solution for several applications ranging from automotive, to smart grids, wind turbines, and power electronics [1]. However, their limited energy density (E_s) and narrow operating temperature range pose challenges for wider adoption, especially in harsh environments [2, 3]. This study introduces a novel approach for the fabrication of the SC electrodes using ionogels, improving the overall performances and overcoming the temperature limitations of conventional SCs. This study presents a novel strategy utilizing ionogel-based electrodes to improve the energy density of EDLCs, while expanding their operational temperature range. The ionogel electrodes were fabricated by formulating electrode slurries with an ionic liquid (1-ethil-3-methylimidazolium bis(fluorosulfonyl)imide (EMIMFSI)) and water as the liquid medium, avoiding the need for organic solvents and eliminating expensive drying procedures. The ionogel-electrode approach facilitates efficient contact between the porous electrode surface and the electrolyte, preventing gas entrapment in the pores, ensuring uniform wetting, and eliminating the need for time-consuming pre-conditioning steps. This simplifies industrial assembly processes significantly [4]. Ionogel-electrodes exhibited remarkable rate capability and capacity retention (~92 % over 100 h of floating time) due to the extended electrolyte penetration into the electrode pores, hardly achievable with conventional electrodes. At a power density of 12.96 kW kg^{-1}, the ionogel-based EDLC retains 33 Wh kg^{-1} which is ~83 % of the energy density measured at a low power of 0.14 kW kg^{-1} (40 Wh kg^{-1}). In contrast, conventional EDLCs retain 65 % of its energy density in the same specific power range. Moreover, the operating temperature window is enlarged thanks to the thermal stability of EMIMFSI-based electrolyte which enables to retain ~24 Wh kg^{-1} still at 100 °C while conventional SC are limited under 65 °C. Overall, this research presents a promising pathway for advancing EDLC technology through innovative electrode fabrication methods and IL-based electrolytes.

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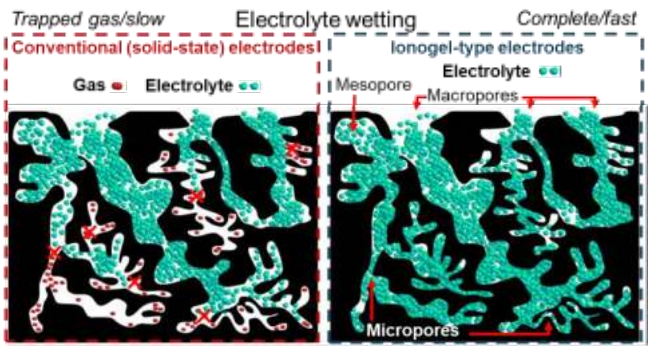

Figure 1. Sketch of the electrolyte wetting processes for conventional (solid-state) and ionogel-type electrodes.

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Exploring the anti-inflammatory effect of $Mo_2Ti_2C_3$, Ta_4C_3 and Nb_4C_3 in murine monocytes and macrophages.

Giorgia Longo[1,2], Linda Giro[2,3], Laura Fusco[3,4], Natalya Resto-Trujillo[2], Mohammad Oliaeimotlagh[2], Amir Khan[2], Benjamin Chacon[4], Christopher Shuck[4], Martina Pigazzi[2], Yuri Gogotsi[4], Lucia Delogu[3,5], Klaus Ley[2], **Marco Orecchioni[2]**

1. Women and Child Health Department, Haematology-Oncology Clinic and Lab, University of Padova, Padova, Italy;
2. Immunology Center of Georgia, Augusta University, GA, USA
3. Department of Biomedical Science, University of Padua, Padua, Italy;
4. A. J. Drexel Nanomaterials Institute and Department of Materials Science and Engineering, Drexel University, Philadelphia, PA, USA;
5. Department of Biological Sciences, Khalifa University of Science and Technology, Abu Dhabi, UAE.

morecchioni@augusta.edu

Abstract

Macrophages are innate immune cells with varying phenotypes and functions that are influenced by their microenvironment. The distinction between the classical M1 and M2 phenotypes, even if with limitations, has been crucial in understanding their involvement in inflammation[1]. Recently, single-cell technologies have revealed a complex range of macrophage activation states, each contributing differently to maintaining physiological balance and affecting the development and progression of diseases. Identifying the origins and function of these macrophage subsets and effectively modulating their phenotype remains a complex challenge. MXenes, a new category of two-dimensional transition metal carbides and nitrides, show promise in the biomedical field owing to their notable features, such as biocompatibility [2]. MXenes' unique chemical properties allow for their detection at the single-cell and tissue level using mass cytometry (CyTOF), which shows great promise for biomedical applications[3]. We found that MXenes can be internalized by myeloid cell precursors, monocytes, and macrophages without affecting their survival or differentiation. Early evaluations of MXenes uptake by monocytes have shown their detectability even after 30 minutes of incubation, which is partially driven by Clathrin-mediated endocytosis. RNA sequencing and CyTOF analysis also found that MXenes can modulate both monocytes and macrophage phenotype, driving an anti-inflammatory M2-like response by reducing proinflammatory markers expression (**Figure 1**) and driving anti-inflammatory markers like CD28[4]. In vivo, peritoneal macrophages exhibit similar phenotype shifts upon MXenes uptake. These findings position MXenes as exciting new tools for detecting and regulating macrophage function, with promising implications for future biomedical applications.

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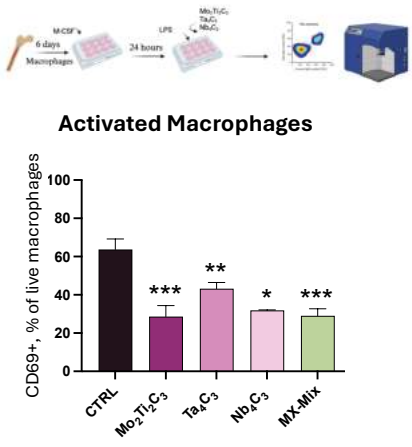

Figure 1: MXenes inhibit the activation of bone marrow-derived macrophages treated with LPS

Advancing Nanoplastic Separation with Niobium Dicarbide Composite Electro-Membranes

Mariam Ouda, Shadi W. Hasan
Khalifa University, Abu Dhabi, UAE
mariam.ouda@ku.ac.ae

Abstract

Water scarcity and pollution by micro- and nanoplastics (MNPs) are pressing global challenges that threaten water security and ecosystem health. These pollutants, prevalent in aquatic systems, compromise the efficiency and longevity of water purification technologies due to their resistance to traditional filtration methods. This study introduces a pioneering approach to water treatment through an electro-membrane filtration system featuring niobium-based MXene (Nb_2CT_x) integrated into sulfonated polyether sulfone (SPES) membranes, aimed at effectively separating nanoplastics and improving the sustainability of water purification systems. The integration of Nb_2CT_x into the SPES membranes results in marked improvements in their physiochemical properties, particularly in enhancing hydrophilicity, porosity and conductivity. The optimized membrane with 5 wt% Nb_2CT_x demonstrates superior water flux, attributable to the synergistic effects of increased hydrophilicity and porosity. The application of an electric field during the filtration process significantly enhances the removal efficiency of PMMA nanoplastics. This electrocoagulation mechanism, promoted by the electric field, facilitates nanoplastic aggregation and floc formation, reducing fouling. Figure 1 shows the effect of applied electric field on the flux and rejection, and outlines the mechanism that leads to this result. This study establishes a new benchmark for the efficiency and sustainability of water treatment technologies by utilizing the properties of 2D materials.

Figures

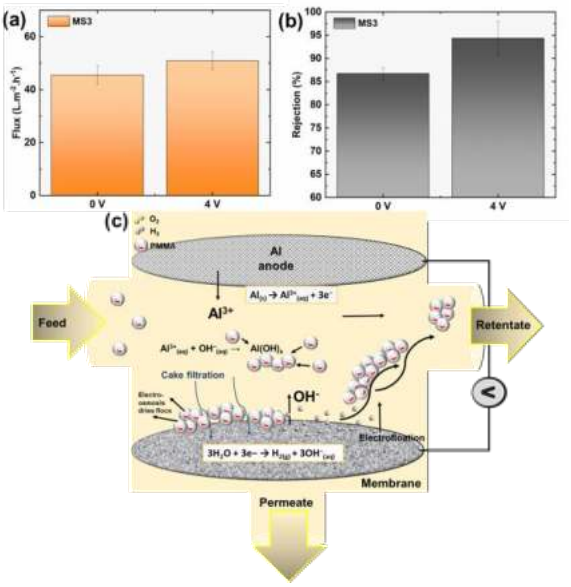

Figure 1: (a) Flux and (b) rejection with and without electric field; (c) Schematic representing the removal mechanism due to electric field.

Reactive retention of heavy metals using self-indicator polymeric membranes

Andreea Madalina Pandele
Advanced Polymer Materials Group,Gheorghe Polizu 1-7, Bucharest, Romania
Pandele.m.a@gmail.com

Abstract

Heavy metals are some of the most hazardous environmental contaminants as they can be found widely in the Earth's crust and affect all ecosystem components such as water, soil and even air. They can enter easily into the human body and represent a health hazard even at very low concentrations. Considering this, various technologies were developed for the removal or immobilization of heavy metals commonly found in water and wastewater. These remediation procedures include precipitation and coagulation, ion exchange, membrane filtration, bioremediation, heterogeneous photocatalysis and adsorption. Membrane separation processes occupy a central place in the development of green technologies since they are more efficient and economical in time and energy. The main advantages of membrane processes consist in their increased selectivity and high separation capacity. Membrane selectivity as well as the retention capacity are evaluated through specific techniques which ultimately appraise the membrane efficiency (percentage of species dissolved or dispersed in the feed solution which are retained by the membrane).
The aim of the current project is to synthesize novel polymeric membranes with self-indicating properties that simultaneously exhibit two roles: the efficient removal of heavy metals from real water samples and also provides a visual indication of the separation capacity without subsequent analysis, through a color change of the membrane's surface. These modified membranes will thus be able to retain heavy metal cations.

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Polymelamine-Modified Graphene Electrodes for Enhanced Claudin18.2 Detection

Kanagavalli Pandiaraj and Shimaa Eissa*

Department of Chemistry, Khalifa University of Science and Technology, Abu Dhabi, P.O. Box 127788, United Arab Emirates
Contact: kanagavalli.pandiaraj@ku.ac.ae

Abstract

Recent advancements in nanotechnology have led to the development of carbon-based nanomaterials, including graphene (Gr), graphene oxide (GO), and carbon nanotubes (CNT), which significantly enhance the performance of electrochemical biosensors[1]. Their high surface area, mechanical strength, and excellent electrical conductivity make them ideal candidates for diagnostic and environmental applications[2]. This study investigates polymelamine (PM) electrodeposition on screen-printed electrodes (SPEs) modified with various carbon-based materials, such as carbon (C), Gr, GO, CNT, and carbon nanofibers (CNF). While PM has been previously explored on substrates like graphene-doped carbon paste, there is a lack of comprehensive comparisons among these commercial carbon nanomaterials. Cyclic voltammetry (CV) was utilized to assess the electron transfer properties. Defect density, and chemical composition of the modified electrodes were characterized with the support from Raman spectroscopy and X-ray photoelectron spectroscopy (XPS). Figure 1 presents scanning electron microscopy images of the bare Gr and PM-Gr modified electrodes, showing the polymer layer coating the electrode surface. PM-modified Gr and CNT/SPEs exhibited pronounced and stable redox behaviour in phosphate-buffered saline (PBS). The presence of terminal amine functionalities on the PM-modified electrodes enabled the effective immobilization of anti-CLDN18.2 antibodies via EDC-NHS chemistry. This facilitated the sensitive detection of Claudin18.2 (CLDN18.2), a critical biomarker frequently overexpressed in gastrointestinal and oesophageal cancers[3,4]. The detection limits achieved were 7.9 pg/mL for PM-modified Gr/SPE and 0.104 ng/mL for PM-CNT/SPE, indicating the superior sensitivity of these electrodes. The PM-modified electrodes also exhibited reagentless signalling capabilities, demonstrating exceptional performance in CLDN18.2 detection. Overall, this research offers a promising approach for the early diagnosis of gastric cancer, effectively addressing a pressing clinical need in cancer detection and management.

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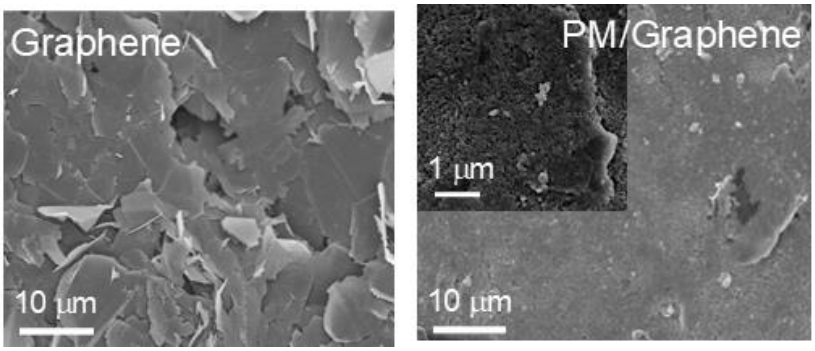

Figure. 1 SEM images of graphene and polymelamine modified graphene electrodes

Plasma-Treated LDPE/GNP Liners to Enhance Bonding with CFRP for Hydrogen Storage Applications

Jabir Ubaid, J Jefferson Andrew, Wesley J Cantwell, Kamran A Khan, Rehan Umer
Khalifa University, Abu Dhabi, United Arab Emirates
rehan.umer@ku.ac.ae

Abstract

Hydrogen storage is critical for the widespread adoption of hydrogen as a clean energy source, especially in high-pressure applications like fuel cell vehicles [1,2]. Type IV hydrogen storage tanks, featuring a polymer liner paired with a carbon fiber-reinforced polymer (CFRP) outer layer, are a promising option due to their lightweight structure and capacity to store hydrogen at pressures up to 700 bar, with polyethylene being one of the most suitable liner materials for these tanks [2,3]. However, a key challenge with these systems is the potential for delamination between the liner and CFRP during rapid depressurization, which can occur due to differences in material properties and hydrogen permeation [3]. Improving the bonding between the liner and CFRP is essential to enhance the overall reliability and safety of these hydrogen storage tanks. Plasma treatment has shown promise in improving the adhesion between polymers and composites by modifying surface energy, roughness, and chemistry [4]. Additionally, graphene nanoplatelets (GNP) have emerged as a potential additive for enhancing the properties of polymers, including bonding performance [2]. This study investigates the effects of varying GNP concentrations on the bonding performance of plasma-treated low-density polyethylene (LDPE)/GNP composites with CFRP. The experimental results from the wedge peel tests, shown in Figure 1, indicate that plasma treatment significantly improved the bonding performance of LDPE/GNP with CFRP across all GNP concentrations. While GNP incorporation initially reduced wedge peel strength and fracture energy in untreated samples due to increased surface roughness, plasma treatment mitigated these effects, enhancing both surface wettability and interfacial interactions. The combination of GNPs and plasma treatment produced a synergistic effect, with higher GNP content yielding improved bonding performance after treatment. These findings suggest that plasma-treated LDPE/GNP composites offer a promising route for improving the performance of hydrogen storage systems, optimizing the interface between the LDPE liner and CFRP for safer, more reliable operation.

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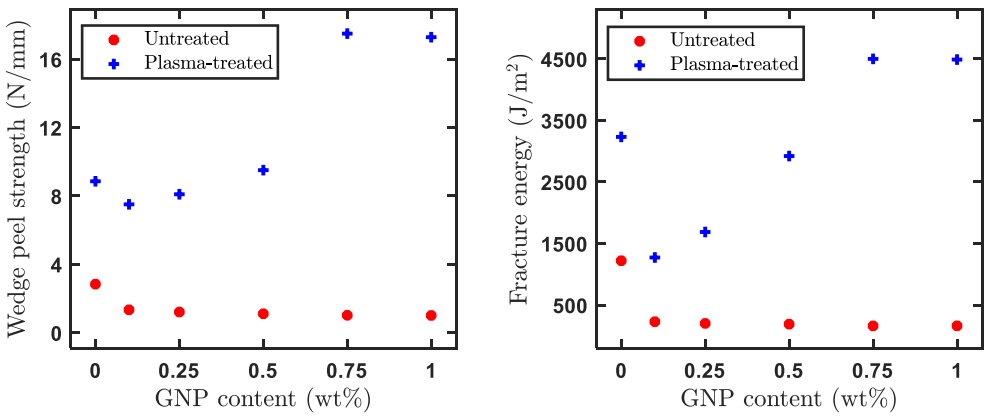

Figure 1: Wedge peel test results of LDPE/GNP bonded with CFRP.

Influence of swelling and penetrants' adsorption on the performance of graphene oxide membranes

Petukhov Dmitrii[1], Andrei Chumakov[2], Johnson Daniel[1]
[1] - *Water Research Center, New York University Abu Dhabi, PO 129188, Abu Dhabi, UAE*
[2] - *Deutsches Elektronen-Synchrotron DESY, Notkestraße 85, 22607 Hamburg, Germany*
dp3916@nyu.edu

Graphene oxide (GO) membranes exhibit unique properties in nanofiltration and reverse osmosis processes. Their performance and rejection characteristics are influenced by the interlayer distance, which is governed by two competing factors: GO swelling in liquid phases [1] and penetrant adsorption [2]. The latter can reduce flux by decreasing the interlayer distance or reducing the available interlayer volume for permeate transport. GO membranes show high rejection rates for both anionic and cationic dyes [3], with permeance values ranging from 5 to 15 l/(m²·bar·h) for water or alcohol solutions. The near-complete rejection of dyes is attributed to size exclusion, as methylene blue (MB) ions are considered larger than the interlayer spaces in GO. In this study, we investigate the filtration characteristics of GO membranes for separating cationic (Methylene blue, MB) and anionic (Methyl orange, MO) dyes. During filtration, we observed that the permeate flux remained constant or slightly increased for MO solutions, while MO rejection decreased from 100% to 85%. In contrast, for the cationic MB dye, a significant and irreversible decrease in permeate flux occurred, with rejection remaining around 100% (Figure 1). To understand this effect, we conducted an adsorption study of the dyes on graphene oxide. Negatively charged MO molecules adsorb weakly onto graphene oxide, with an adsorption capacity of around 50-70 mg/g(GO). However, for the positively charged MB, the adsorption capacity is much higher, reaching 600 mg/g (GO). To study real filtration conditions, these experiments were carried out in aqueous dye solutions during the *in situ* experiment using the Grazing-Incident Wide-Angle X-Ray Scattering (GIWAXS) technique (P03 beamline, synchrotron PETRA III, DESY). The interlayer distance *d* of GO membranes after filtering a certain volume of dye solution was analyzed (Figure 2). Parameter *d* in a 10 mM NaCl solution was measured to be 12.9 Å. After filtering a small volume of dye solution, the *d*-spacing decreased to 11.7 Å, with further filtration causing significant shrinkage to 10.4 Å. For negatively charged MO molecules, which do not adsorb between GO nanoflakes, the interlayer space decreased slightly from 12.9 Å to 12.4 Å, likely due to the compaction of the GO structure under external pressure. The reduction in permeate flux during MB filtration can be explained by two effects: (i) the adsorption of MB molecules in the interlayer space and (ii) the resulting shrinkage of the interlayer distance, both of which significantly reduce the available volume for water transport. Therefore, MB and other anionic dyes are not suitable for testing size exclusion effects in GO membrane permeation, as sorption effects can lead to high rejection rates of anionic dyes.

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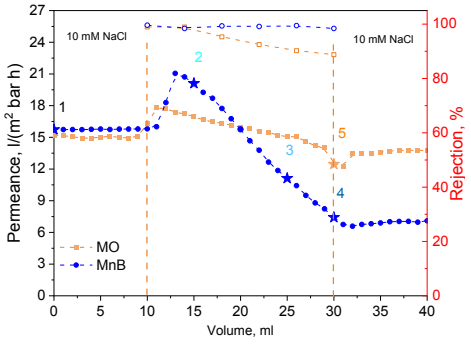

Figure 1. Dependence of GO permeance and rejection during dye solutions filtration

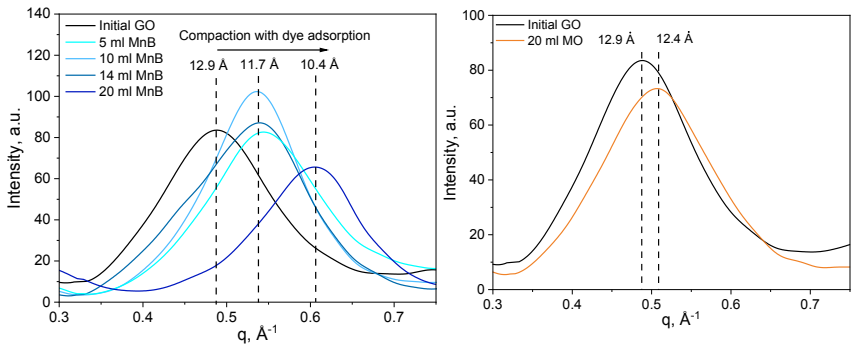

Figure 2. GIWAXS patterns for membranes after dyes filtration. Numbers correspond to the volume indicated on figure 1

Strain-Engineered MoS2/WS2 and XS2/VS2 (X=Mo, W) Heterostructures for Hydrogen Generation and Spintronics Applications

R.Thangavel and Saurav Lahiri, *Department of Physics, Indian Institute of Technology (Indian School of Mines), Dhanbad, Jharkhand 826004, India*

rthangavel@iitism.ac.in

Abstract

Innovative semiconductor heterostructures, MoS2/WS2 and XS2/VS2 (X=Mo, W), offer promising solutions for solar energy-driven hydrogen generation and advanced opto-spintronics applications. This study comprehensively examines their structural, electronic, photocatalytic, and magnetic properties under biaxial strain using density functional theory (DFT) and Monte Carlo (MC) simulations. The MoS2/WS2 heterobilayer, with its most stable stacking configuration (conf-1), shows a low interlayer binding energy of −18.07 meV/Å² and type II band alignments, which enhance charge carrier mobility and reduce recombination rates. This heterostructure also exhibits superior visible light absorption (8.3 × 10^5 cm^{-1}) compared to its monolayers. Its band positions under tensile and compressive strains are suitable for hydrogen evolution (HER) and oxygen evolution reactions (OER), highlighting its potential for water-splitting applications. The strain-induced red shifts in absorption edges further indicate its capability for efficient solar energy harvesting. Concurrently, the XS2/VS2 heterostructures reveal notable ferromagnetic properties, with indirect band gaps and type II heterojunctions ideal for opto-spintronics devices. They maintain high Curie temperatures (TC) of 299.08 K (MoS2/VS2) and 301 K (WS2/VS2) as determined by MC simulations. While the WS2/VS2 heterostructure transitions to a half-metal under tensile strain beyond 1%, both heterostructures retain their semiconducting nature under other strains. This strain-induced tunability of electronic and magnetic properties underscores their versatility for customized device applications. These findings pave the way for further exploration of 2D van der Waals heterostructures in hydrogen generation and opto-spintronics. Strain engineering emerges as a critical tool for optimizing their performance, suggesting a wide range of potential applications in energy and technology sectors.

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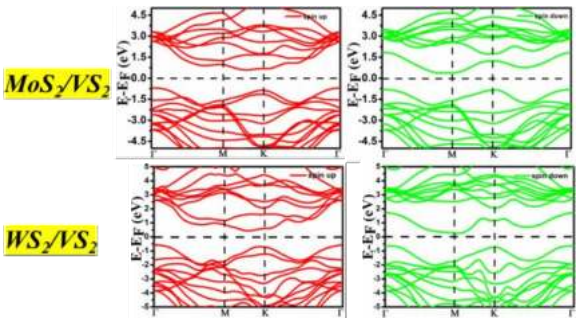

Figure 1: HSE Spin polarized band structure for (a) spin up (b) spin down channel of MoS2/VS2 while (c) spin up and (d) spin down of WS2/VS2 heterostructure

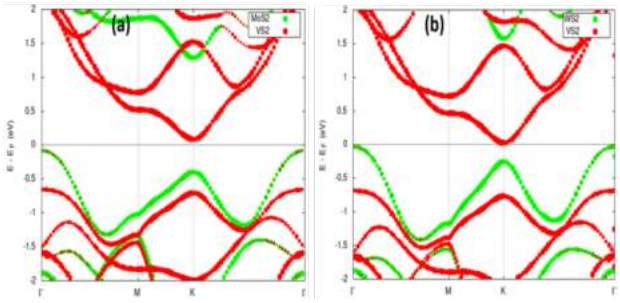

Figure 2: PBE+U computed projected band structure of (a) MoS2/VS2 and (b) WS2/VS2 heterostructure

Excitation-Tunable Gap-Mode TERS from 2D Semiconductors

João Lucas Rangel[a], Marc Chaigneau[a], Andrey Krayev[b]*

[(a)] HORIBA France SAS, Palaiseau, France
[(b)] Horiba Instrument Incorporated, Novato, United States of America

*e-mail of corresponding author: andrey.krayev@horiba.com

Resonant excitation is well-known to enhance SERS/TERS scattering from analytes ranging from molecules to 3D materials. Here, we investigate the dependance of TERS scattering from mono- and bi-layers of WS_2 and MoS_2 in intimate contact with silver on the excitation laser wavelength (within 473nm-830nm spectral range). This is achieved by collecting the TERS maps of the same area featuring both the mono-and the bi-layers with the same probe at six different excitation wavelengths. We found that the response from the mono- and bilayers is very different: the ratio of the A'/A_{1g} peaks that represent similar out-of-plane Raman mode for the mono- and the bi-layer correspondingly, features a sharp dip at A exciton for both MoS_2 and especially for WS_2 (existing laser set matched the excitonic bands in WS_2 particularly well). For the latter material the 632.8nm excitation is very close to A exciton (~620nm) and consequently, TERS response from the monolayers obtained with this most popular laser wavelength for TERS measurements, was dramatically decreased compared to excitation at 671nm and 594nm, making the resonant excitation counterproductive. We propose that this phenomenon arises from intermediate (Fano resonance) or strong coupling (Rabi splitting) between the A exciton in WS_2(MoS_2) and the junction plasmon. This is akin to the so-called Fano(Rabi) transparency experimentally observed in far field (coherent) scattering from transition metal dichalcogenides between two plasmonic metals. Naturally, TERS provides direct control of the gap plasmon, and in turn exciton-plasmon coupling, compared to the rigid geometries that were previously employed in diffraction limited measurements. In effect, our observed phenomenon opens new frontiers for the varied excitation gap-mode TERS as the platform to study fascinating quantum phenomena in systems with intermediate-to-strong coupling between excitons and plasmons in ambient conditions.

Using Graphene and Topological Insulators to Advance U.S. Measurement Science

Albert F. Rigosi, Ngoc Thanh Mai Tran, Jason M. Underwood, Yanfei Yang, Alireza R. Panna, Dean G. Jarrett, and David B. Newell
National Institute of Standards and Technology (NIST), Gaithersburg, MD 20899, United States
afr1@nist.gov

Since 2017, epitaxial graphene (EG) has been the base material for the U.S. national standard for resistance. Nanoscale devices based on EG have been expanded to include specially designed arrays to rapidly expand access to quantized resistance at values other than $h/2e^2$ via mathematical star-mesh transformations. In addition to these developments, an alternative research avenue in electrical metrology has also formed around the use of magnetically doped topological insulators (MTIs), which seek to replace graphene as a standard due to its exhibition of the quantum anomalous Hall effect (or zero-field quantized resistance) [1-3]. Results will be presented on both material systems to show the benefits gained by the measurement science community, along with benefits applicable to many research endeavours focused on the fabrication of small-scale devices.

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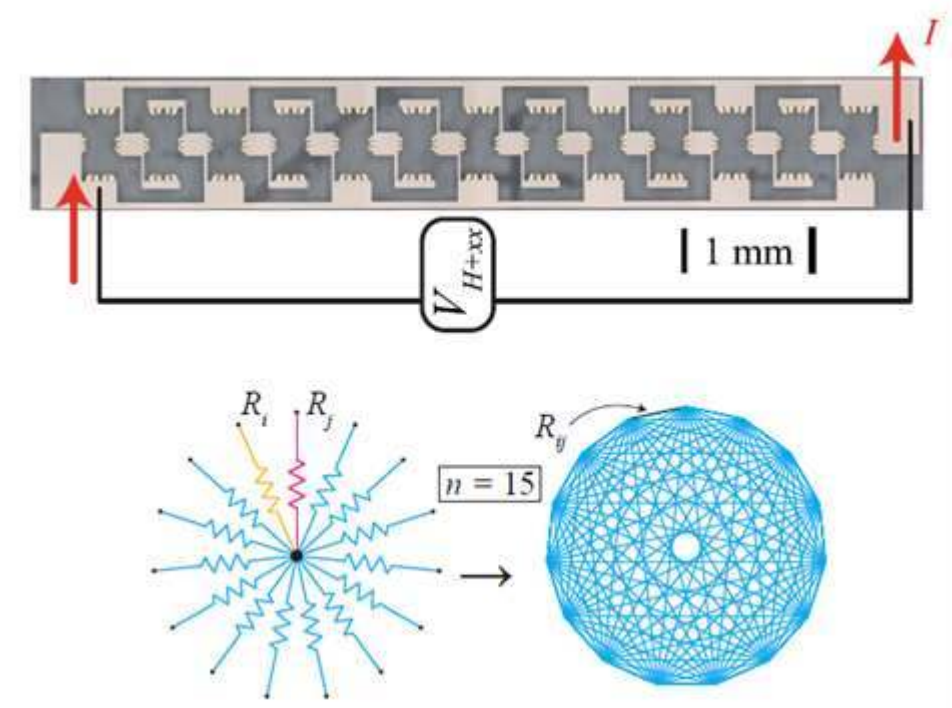

Figure 1: (Top) An example 13-element graphene-based array for obtaining quantized resistances other than h/2e2. (Bottom) A mathematical star-mesh transformation for a 10 GΩ quantum electrical standard is illustrated, representing a possible configuration that is within fabrication capacities.

Library of Rubbable and Rubbing Materials for obtaining Nanostriped Two-Dimensional Sheets, Nanostructures and Nanocomposites by the Surface Rubbing Method

Gagik Shmavonyan[1], Levon Misakyan[1], Areg Shmavonyan[1, 2], and Theresia Knobloch[3]
[1]National Polytechnic University of Armenia, 105 Teryan street, 0009, Yerevan, Armenia, [2]Yerevan State University, 1 Alex Manoogyan street, Yerevan, 0025, Armenia, [3]TU Wien, Institute for Microelectronics, Gusshausstr. 27-29, 1040, Vienna, Austria
gshmavon@yahoo.com

Here, we report pioneering research on creating comprehensive library of rubbable and rubbing materials (bulk and low-dimensional) consisting of a few tens of inorganic (with different crystal systems) and organic materials. Inorganic materials include carbonaceous and non-carbonaceous crystalline and amorphous materials, while organic materials comprise non-living and living materials.

In the library the materials are classified by taking into account their chemical composition and physical properties focusing on their crystal structures, as well as mechanical and surface properties.

The library was created by mechanically rubbing layered and non-layered bulk and nanosized materials (inorganic, inorganic-organic and organic powders) with two substrates with ultra-flat to rough (non-porous, porous) surfaces by Surface Rubbing method [1-5].

Unique nanomaterials with complex architectures and tailored functionalities and nanostructures are obtained, such as:
- Self-assembled 2D nanostripes with tunable sizes, shape, distribution density and surface morphology,
- Pure and composite nanostriped 2D sheets,
- Mixed-dimensional nanostriped nanocomposites,
- Nanoengineered nanostructures with different architecture and surface morphology.

Moreover, the Surface Rubbing method allows fabricating nanostriped heterostructures and 2D devices based on nanostriped nanomaterials. These novel nanostriped nanomaterials and nanostructures offer novel characteristics and lead to a wide range of potential applications.

Besides, a nanoscale phenomenon enabling materials exhibit extraordinary and unprecedented properties and behaviour at the nanoscale, driving advances across multiple fields has been discovered by us.

The research was carried out within the framework of 22el-048 "Establishment of Remote Laboratories" program of the contractual (thematic) funding of scientific and scientific-technical activities provided by the Higher Education and Science Committee of the Ministry of Education, Science, Culture and Sports of the Republic of Armenia.

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Waste Heat to Energy: From 2D Materials Perspective

Nirpendra Singh
Department of Physics, Khalifa University of Science and Technology, Abu Dhabi-127788 UAE
*The Research & Innovation Center for Graphene and 2D Materials (*RIC-2D*), Khalifa University of Science and Technology, Abu Dhabi-127788 UAE*
Nirpendra.Singh@ku.ac.ae

Abstract (Arial 10)
Waste heat is everywhere, and every bit of waste heat recycled into green energy can reduce greenhouse emissions, promote sustainable development, and impact the economy. Thermoelectric generators can generate electricity from waste heat and can also be used to convert even tiny heat into electricity for sensors. The development of efficient devices, however, requires materials with a robust thermoelectric response. Two-dimensional (2D) materials have unique electronic properties due to the quantum confinement and prevent heat transfer between two layers, making them excellent thermoelectric materials. We design 2D materials and their heterostructure using innovative approaches to optimize thermal transport properties by optimizing the electronic properties and simultaneously reducing the thermal conductivity of 2D materials. In this talk, I will discuss a wide perspective and various design principles of 2D materials and their possible applications in thermoelectric generators.

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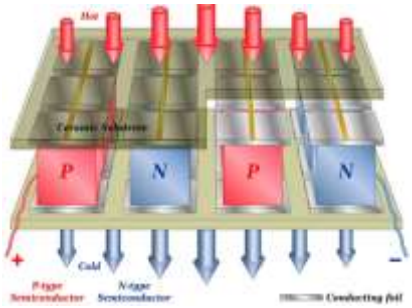

Figure 1: Schematic of a thermoelectric module

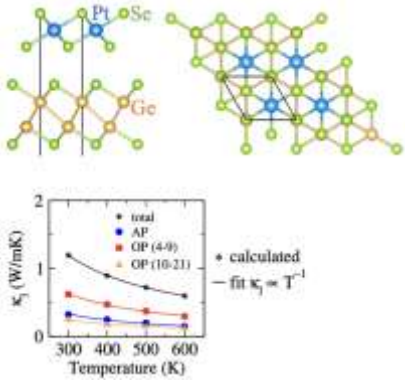

Figure 2: Thermoelectric properties of van der Waals Heterostructure $PtSe_2$/γ-GeSe

Advancing Graphene for Commercial Applications: Enhancing HVAC Filters for Sustainable Indoor Air Quality in Abu Dhabi Office Buildings

Deepak Sridhar, Ryan Shacklock, Colin van der Kuur
Zentek Ltd., 24 Corporate Court, Guelph, Canada
dsridhar@zentek.com

Graphene, despite its promising properties, has faced significant challenges in commercialization over the past two decades. Issues such as scaling production, developing disruptive products, market demand, regulatory hurdles, and economic feasibility have limited its widespread adoption. This study explores the application of a proprietary silver-graphene oxide (AgGO) formulation which is produced on a large scale for treating HVAC in-duct air filters, and theoretically enumerates its performance in Abu Dhabi office buildings.

The AgGO-treated MERV-A 9-A (M9AZG) filters (Figure 1) provide an average pathogen removal efficiency of 67% over six months [1], outperforming untreated filters with similar ratings. This improved performance is attributed to enhanced mechanical filtration mechanisms such as interception and diffusion, driven by the surface properties of the AgGO. The AgGO on the filter fibres increases the surface area and also creates a rugged topography that aids in capturing smaller particles like infectious aerosols. The results suggest that AgGO enhances filtration without increasing pressure drop, providing a more energy-efficient solution, along with enhanced protection from pathogens for maintaining indoor air quality (IAQ).

In the context of the UAE's goal of achieving net-zero emissions by 2050, the building sector is critical, which contributes about 28% of greenhouse gas emissions [2]. Abu Dhabi, with approximately 46 million square feet of office space [3], could save $9.8 million annually by replacing MERV 13 filters with M9AZG filters. This stems from fewer filter replacements, reduced waste, and lower energy costs. Additionally, this would result in 45% energy savings and reduce CO2eq emissions by approximately 5,050 tonnes per year. This aligns with the UAE's 40% CO2eq reduction target by 2030, demonstrating that graphene-based air filtration technologies can help decarbonize buildings without additional equipment installations or modifications, offering both sustainability and health benefits for a wide range of sectors, including commercial buildings, retail spaces, and institutions of all sizes.

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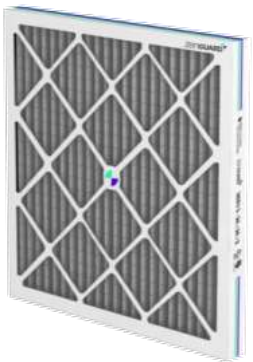

Figure 1: M9AZG (ZenGUARD™) filters used in the experimental evaluation.

Deeper insights into 2D-Materials by Imaging spectroscopic Ellipsometry (ISE) and Imaging Mueller Matrix Ellipsometry (IMME)

Peter H. Thiesen
Park System GmbH, Stresemannstr. 30, 37079 Göttingen
Peter-Thiesen@Parksystems.com

Imaging Spectroscopic Ellipsometers (ISE) combine the benefits of ellipsometry and optical microscopy in a single device. The unification of the two technologies creates a unique metrology tool that redefines the limits of both ellipsometric measurements and polarization-contrast microscopy. The enhanced spatial resolution of imaging ellipsometers (about 1 µm) expands ellipsometry into new areas of microanalysis, microelectronics, and bio analytics. Imaging Ellipsometry is an all-optical, non-contact metrology technique that excels at the layer-thickness and material characterization of micro-structured thin-film samples and substrates.

In the field of 2D materials characterization, Imaging Spectroscopic Ellipsometry enable the determination of optical properties of micro crystals [1],[2],[3]. The data are required for a better understanding of 2D material based devices [4],[5].

From the macroscopic point of view, ellipsometric contrast micrographs or microscopic maps of Delta and Psi can be stitched and offer a fast, non-contact, wafer-scale, atomic layer resolved imaging of 2D materials [6] on a variety of substrates. Including maps recorded at different wavelengths, a specific search for microcrystals with a dedicated number of layers or a predefined thickness was reported. Recent studies also show the possibility of imaging buried layers [7].

The focus of the talk will be on applications of Imaging Müller matrix ellipsometry for anisotropic microcrystals characterization. Micrographs of 11 elements of the Müller Matrix, normalized to element 1 were recorded at different wavelength and orientations for different microcrystals like Black Phosphorous or Bi_2SeO_5 (Fig, 1),

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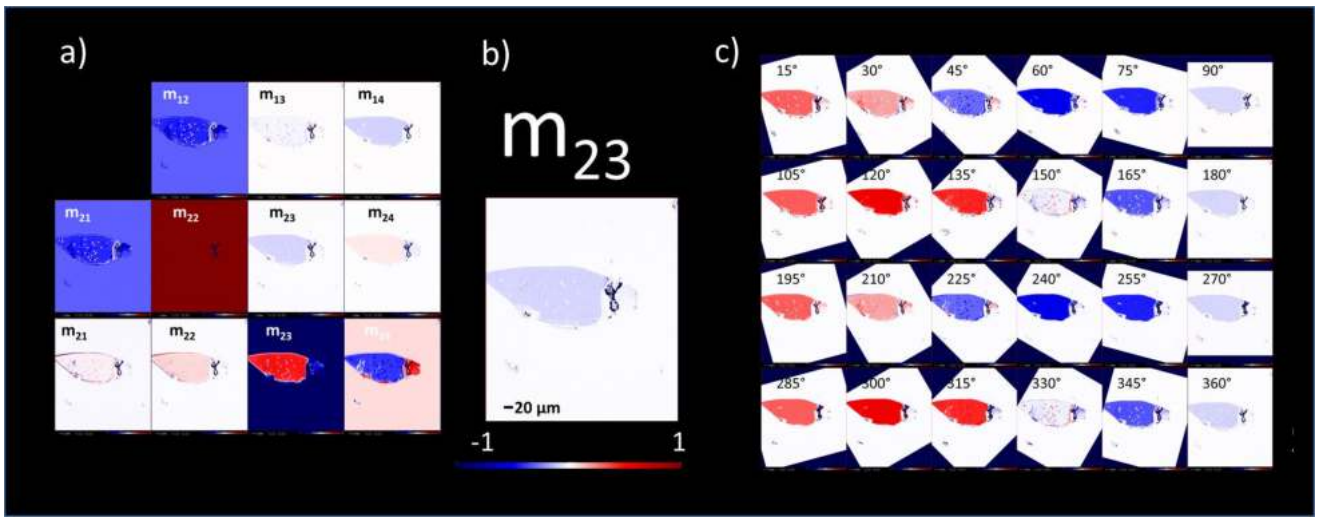


Figure 1: Microscopic Maps of 11 elements of the Müller Matrix (a), the element m_{23} in detail (b) and rotated (c) of a Bi_2SeO_5 microcrystals on SiO2 | Si substrate.

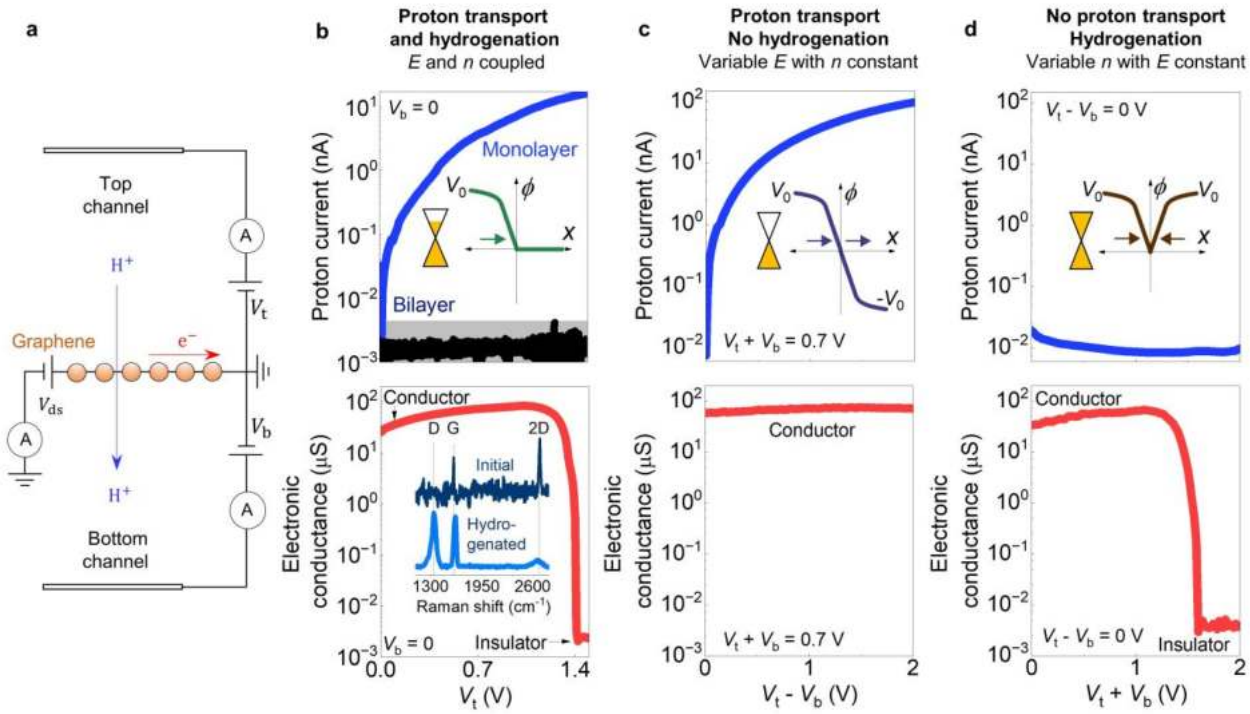
Control of proton transport and hydrogenation in double-gated graphene

Jincheng Tong[1,2]
Y. Fu[1,2], D. Domaretskiy[1], F. Della Pia[3], P. Dagar[1,2], L. Powell[1], D. Bahamon[4,5], S. Huang[1,2], B. Xin[1,2], R. N. Costa Filho[6], L. F. Vega[4,5], I. V. Grigorieva[1], F. M. Peeters[6,7], A. Michaelides[3], M. Lozada-Hidalgo[1,2]

[1] *Department of Physics and Astronomy, The University of Manchester, Manchester M13 9PL, UK*
[2] *National Graphene Institute, The University of Manchester, Manchester M13 9PL, UK*
[3] *Yusuf Hamied Department of Chemistry, University of Cambridge, Cambridge, CB2 1EW, U.K.*
[4] *Research and Innovation Center on CO2 and Hydrogen (RICH Center) and Chemical Engineering Department, Khalifa University, PO Box 127788, Abu Dhabi, United Arab Emirates*
[5] *Research and Innovation Center for graphene and 2D materials (RIC2D), Khalifa University, PO Box 127788, Abu Dhabi, United Arab Emirates*
[6] *Departamento de Física, Universidade Federal do Ceará, 60455-900 Fortaleza, Ceará, Brazil*
[7] *Departement Fysica, Universiteit Antwerpen, Groenenborgerlaan 171, B-2020 Antwerp, Belgium*
Jincheng.tong@manchester.ac.uk

Abstract
Graphene's basal plane can function as a perfectly selective barrier permeable to protons but impermeable to all ions and gases, stimulating its use in applications such as membranes, catalysis and isotope separation. Protons can also chemically adsorb on graphene and hydrogenate it, inducing a conductor-insulator transition intensely explored in graphene electronic devices. However, both processes face energy barriers that in the case of proton transport motivate strategies to accelerate it, such as introducing vacancies, incorporating catalytic metals or chemically functionalising the lattice, but these can compromise other properties like ion selectivity or mechanical stability. Here we show that independent control of the electric field E~ V nm^{-1} and charge carrier density n~10^{14} cm^{-2} in double gated graphene allows decoupling proton transport from lattice hydrogenation and can accelerate proton transport such that it approaches the limiting electrolyte current in our devices. Proton transport and hydrogenation can be driven selectively with precision and robustness that enables proton-based logic-and-memory graphene devices with orders-of-magnitude on-off ratios. Our results show that field effects can accelerate and decouple electrochemical processes in double-gated 2D crystals and demonstrate the possibility of mapping such processes as a function of E and n – a fundamentally different technique to study 2D electrode-electrolyte interfaces[Nature, 2024, 630(8017): 619-624.].

Figures



Nanoparticles of van der Waals materials with tunable size, shape and crystallinity for nanophotonic applications

Tselikov G.I., Ermolaev G.A., Tikhonowski G.V., Minnekhanov A.A., Arsenin A.V., Volkov V.S.
Emerging Technologies Research Center, XPANCEO, Dubai, 00000, United Arab Emirates
celikov@xpanceo.com

Two-dimensional (2D) van der Waals (vdW) materials have captured significant attention in scientific research due to their distinctive properties, which hold promise for next-generation electronic and optoelectronic devices [1]. However, the practical application of 2D materials in photonics faces limitations related to their form-factor – whether they are exfoliated flakes or grown through chemical vapor deposition (CVD) and epitaxial processes. At the same time, most effective way to manipulate light at the nanoscale involves interaction with nanostructured materials. Therefore, nanostructuring vdW materials offers a compelling avenue to advance nanophotonics by expanding its material database [2]. In recent years, diverse approaches have been explored to nanostructure anisotropic vdW crystals, resulting in the creation of nanophotonic devices such as waveguides, nanoantennas, and metasurfaces [3-5]. However, these approaches inherently lack the capability to form spherical substrate-free nanoparticles (NPs) from layered vdW crystals. Recently, this challenge was overcome by employing femtosecond (PLAL) technique to produce resonant NPs from MoS2 and WS2 both representing the class of transition metal dichalcogenides [6-7]. Our work demonstrates the feasibility of transforming a wide range of vdW crystals into colloidal nanoparticles with precise control over composition, shape, size, and crystalline structure.

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Figures

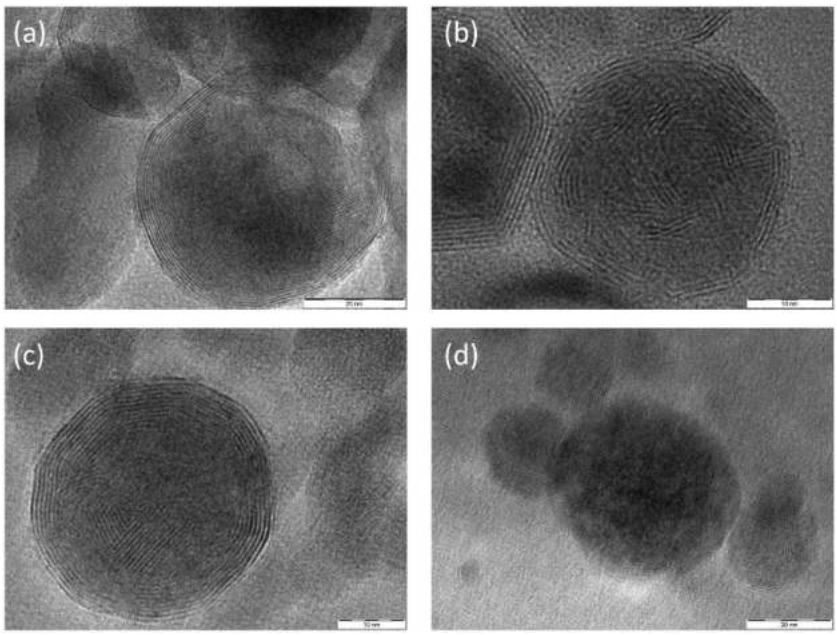

Figure 1: TEM images of colloidal (a) MoS_2, (b) WS_2, (c) $MoSe_2$ and (d) WSe_2 NPs produced by fs PLAL technique in deionized water.

MgH_2 confined in a graphene-organosilica heterostructure for hydrogen storage

Feng Yan
Petra E de Jongh, Petra Rudolf, Rahul Nair

Debye Institute for Nanomaterials Science, Utrecht University, Utrecht, 3584 CG, the Netherlands.
Zernike Institute for Advanced Materials, University of Groningen, Groningen, 9747 AG, the Netherlands.
National Graphene Institute, University of Manchester, Manchester, M13 9PL, UK.
feng.yan@manchester.ac.uk

Hydrogen is a promising alternative fuel that can push forward the energy transition because of its high energy density (142 MJ kg^{-1}), variety of potential sources, low weight and low environmental impact, but its storage for automotive applications remains a formidable challenge.[1] MgH_2, with its high gravimetric and volumetric density, presents a compelling platform for hydrogen storage; however, its utilization is hindered by the sluggish kinetics of hydrogen uptake/release and high temperature operation. Confinement of MgH_2 in nanoporous supports has been demonstrated to be an effective way to improve hydrogen desorption properties, since the particle size can be easily controlled by modifying the pore size of the scaffolds, and the direct inter-particle contact is avoided, which can further prevent particle agglomeration.

In this presentation, I shall discuss about our recent work, where we developed a novel layered heterostructure of reduced graphene oxide and organosilica with high specific surface area and narrow pore size distribution, which serve as a scaffold to host MgH_2 nanoparticles with a narrow diameter distribution around ~2.5 nm and superior hydrogen storage properties. Reversibility tests demonstrated that the dehydrogenation kinetics and re-hydrogenation capacity of the system remains stable over four cycles. Our results prove that MgH_2 confinement in a nanoporous scaffold is an efficient way to constrain the size of the hydride particles, avoid aggregation and improve kinetics for hydrogen release and recharging.[2]

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Use of graphene as chemical additive for anticorrosive and architectural paints

Xavier Raby, Valdirene Peressinotto
Gerdau Graphene, AV DRA RUTH CARDOSO 3518 ANDAR 4 CONJ 1, Sao Paulo, Brazil
xavier.raby@gerdaugraphene.com

It has already been demonstrated graphene exhibits unique electrical, mechanical, and thermal properties that can bring significant improvements for many technical applications [1]. Paint & coating industry is one of the sectors that should be deeply transformed by this new technology. The use of graphene as corrosive inhibitor in industrial coatings has been widely reported in the past [2] but the literature often presents fluctuating performance data under the broad term 'graphene'[3-4], which can be confusing, particularly for paint industry professionals unfamiliar with nanotechnology. Moreover, due to the extensive focus of global R&D efforts on anticorrosive properties [5], the benefits of graphene in architectonic and decorative coatings remain largely underutilized especially in regards with the waterborne latex resin coatings. The objective of this study is to provide clarity regarding real-life applications of graphene in corrosion-resistant coatings and to show the reasons why use of graphene can boost the performance of architectural coatings. Finally, as an illustration, examples of graphene-based chemical additives (figure 1) developed by Gerdau Graphene for different product lines will be presented:

- anticorrosive paints with enhanced corrosion resistance (possibility of substitution of conventional corrosion inhibitors);
- floor paint with enhanced durability;
- wall paint with increased wash resistance.

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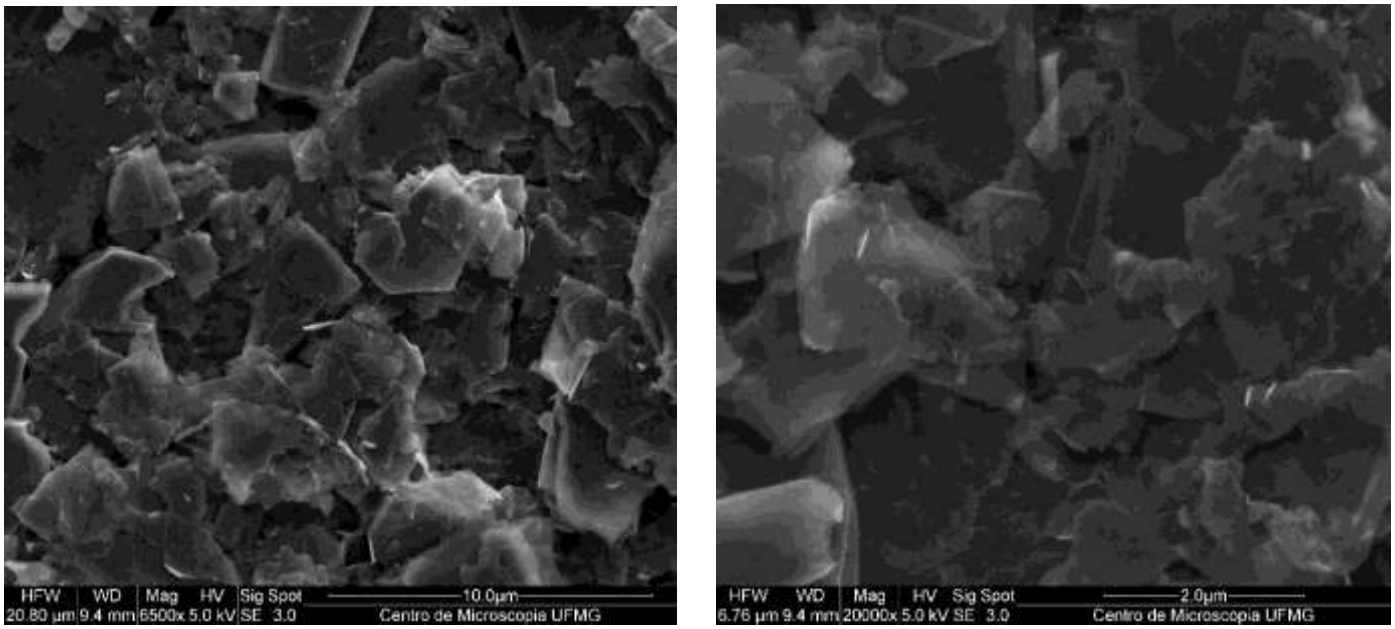

Figure 1: SEM images of an example of graphene dispersion in xylene previously dried used as a chemical additive for anticorrosive coatings

The origin and mitigation of defects induced by metal evaporation in 2D materials

Wenwen Zheng, Bin Yuan, Marco A. Villena, Kaichen Zhu, Sebastian Pazos, Yaqing Shen, Yue Yuan, Yue Ping, Chen Liu, Xiaowen Zhan, Xixiang Zhang, Mario Lanza*
King Abdullah University of Science and Technology, Thuwal 23955-6900, Jeddah, Saudi Arabia
wenwen.zheng@kaust.edu.sa

Evaporating metals on 2D materials is crucial for building electronic devices but often damages the material by breaking bonds and causing metal penetration, which degrades device performance. While ultra-high vacuum (10^{-9} Torr) evaporation reduces such damage, it is costly and inefficient. This study explores a simpler alternative by evaporating Au in moderate vacuum (5×10^{-6} Torr) on defect-free, mechanically exfoliated 2D materials. Cross-sectional TEM analysis reveals that this approach preserves the van der Waals interface with minimal defects. Density functional theory simulations suggest that surface water molecules slightly distort the crystal lattice, lowering the energy required for defect formation. Devices fabricated with Au/h-BN/Au structures at 5×10^{-6} Torr show reduced leakage current compared to those made at 3×10^{-5} Torr, offering a practical solution to integrate 2D materials into electronics.

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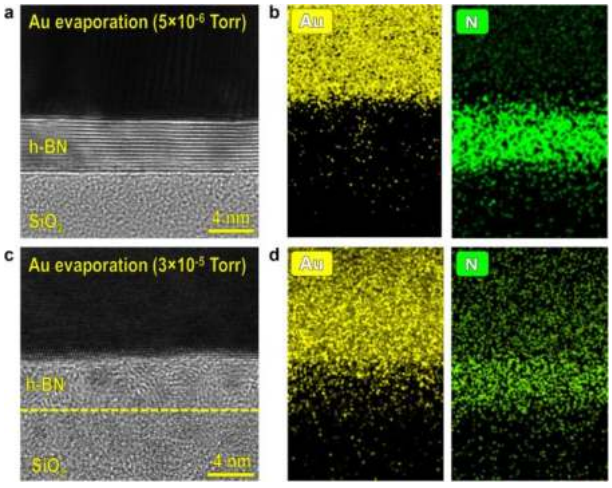

Figure 1: Morphological and chemical analysis of mechanically exfoliated h-BN flakes.

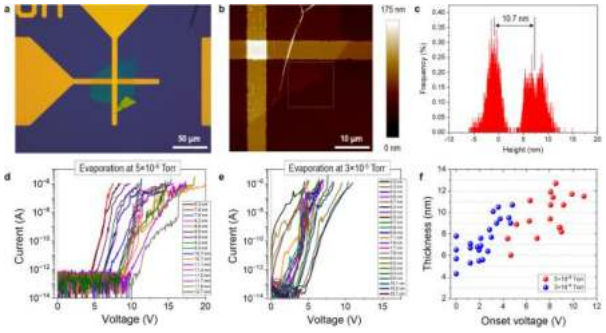

Figure 2: Leakage current across h-BN with Au electrodes evaporated at 3×10^{-5} and 5×10^{-6} Torr.

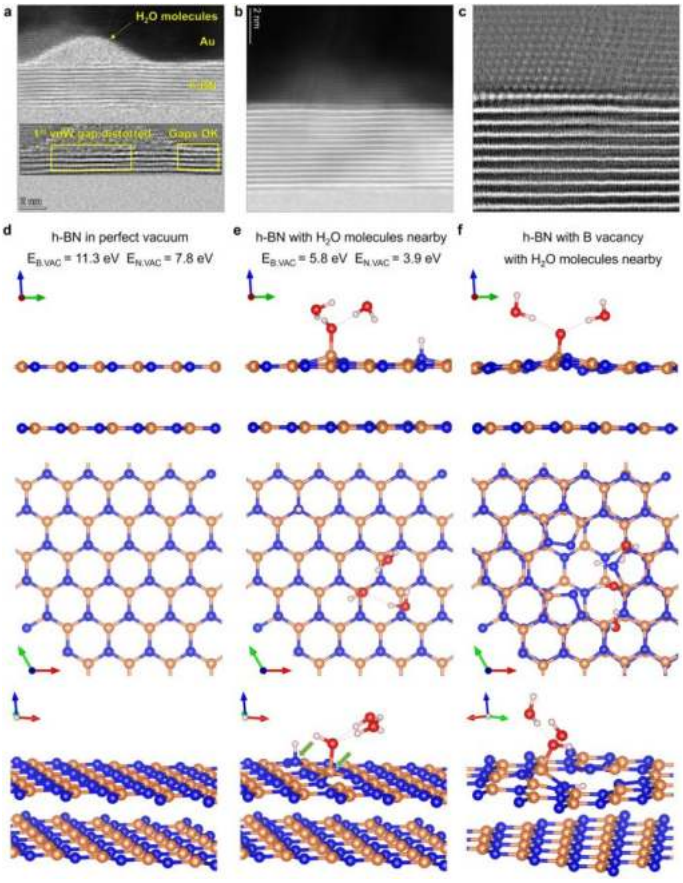

Figure 3: Origin of the evaporation-induced effects.

2D Nanocomposite Aerogels for Efficient Lithium Recovery from Aqueous Sources

Nour S. Abdelrahman, Seunghyun Hong, Hassan A. Arafat, Daniel Choi, Faisal Al Marzooqi*
Khalifa University, Department of Chemical, UAE
(e-mail: Nourabdelrahman13@gmail.com)

Abstract

With the increasing demand for lithium in industries such as electric vehicles and renewable energy, concerns have arisen regarding the depletion of global lithium reserves and the environmental impact of mining. This research focuses on the recovery of lithium from diverse water resources, including brine water, wastewater, and seawater, to address the need for sustainable lithium production. Our goal is to fabricate a high-performance adsorbent and incorporate it into effective lithium recovery technologies, thereby paving the way for a circular economy in the lithium-ion battery domain. One promising approach to be explored is the utilization of 2D material-based nanocomposite aerogels, leveraging modified cellulose—the most abundant polymer in the world—as the primary structural component. The use of these modified cellulose-based aerogels offers significant advantages, particularly in the ease of recovery and handling of the adsorbent material, which is more practical compared to dealing with nanomaterials separately. In this study, various modified cellulose-based aerogels were developed and tested as lithium ion-selective adsorbents, including those incorporating MXene, sulfonated graphene oxide, and ionic liquid. The performance of these aerogels in lithium-ion adsorption was evaluated successfully, providing insights into their potential application in lithium recovery technologies. The findings from this research could offer valuable pathways to reduce the environmental footprint of lithium extraction and enhance the cost-effectiveness of lithium recovery processes, contributing to the long-term sustainability of the lithium-ion battery industry.

From Brine to Battery: Exploring High-Efficiency Lithium Recovery with a Novel LDH Material

Mohammed Abujayyab, Shadi Hassan, Hassan Arafat, Fawzi Banat
Khalifa University of Science and Technology, PO Box 127788, Abu Dhabi, United Arab Emirates

m.a.a92@hotmail.com

Abstract
The rising demand for lithium, driven by the rapid expansion of the electric vehicle and renewable energy sectors, has underscored the need to identify effective extraction methods. Adsorption is emerging as a cost-effective technique for extracting lithium with high selectivity. This study explores the potential of a novel layered double hydroxide (LDH) and its derivatives for efficient lithium recovery from synthetic brine. The use of Li-Mn-Al LDH exhibited a high lithium adsorption capacity of 79.7 mg/g. To enhance adsorption performance, the influence of surface functionalization on LDH's adsorption capacity was investigated. Introduction of hydroxyl and carboxylic groups onto the LDH surface led to adsorption capacities of 87.72 mg/g and 126.985 mg/g, respectively. Additionally, a composite of LDH with waste-derived keratin was fabricated, resulting in a substantial increase in lithium uptake to 149.8 mg/g. This improvement is attributed to the synergistic effects of the LDH's layered structure and the keratin's high affinity for lithium ions. These findings highlight the potential of LDH-based materials, particularly when being functionalized or combined with keratin, as promising adsorbents for sustainable lithium recovery from brine solutions. Further optimization of synthesis conditions and adsorption parameters is warranted to translate these laboratory-scale results into practical applications.

Computational Approaches for Selecting Novel 2D materials for Proton Exchange Membrane Fuel Cells

M.Y Al Hamadi[1,2], D. Bahamon[1,2,3], N. Singh[1,3], Marcelo Lozada-Hidalgo[1,5], L.F Vega[1,2,3,*]
[1]Research and Innovation Center on Graphene and 2D materials (RIC2D Center), Khalifa University of Science and Technology, Abu Dhabi, United Arab Emirates
[2]Chemical and Petroleum Engineering Department, Khalifa University of Science and Technology, Abu Dhabi, United Arab Emirates
[3]Research and Innovation Center on CO2 and Hydrogen (RICH Center), Khalifa University of Science and Technology, Abu Dhabi, United Arab Emirates
[4]Physics Department, Khalifa University of Science and Technology, Abu Dhabi, United Arab Emirates
[5]Department of Physics and Astronomy. National Graphene Institute. The University of Manchester, M13 9PL, UK

100053592@ku.ac.ae

Abstract

In the quest for sustainable energy solutions, hydrogen production and utilization play a crucial role. Proton Exchange Membrane Fuel Cells (PEMFCs), known for their high efficiency, low emissions, and adaptability, represent a promising technology in this domain. However, traditional PEMs like Nafion underperform at high temperatures and low humidity, necessitating the exploration of alternative materials [1, 2].
Geim's team has shown that graphene, though impermeable to gases, demonstrates high proton conductivity [3]. This work is focused on investigating proton permeability across a range of two-dimensional (2D) materials by a computational modeling approach, with an initial focus on dichalcogenides. The study involves systematically examining the structures of these materials, engineering specific defects, and evaluating their proton conductivity and selectivity under various conditions [3, 4]. Quantum mechanical simulations and molecular dynamics are employed to model the structural integrity and stability of promising materials, with the goal of advancing the design of high-performance PEMs for hydrogen-based energy solutions.

Financial support from the RIC2D centre through project 2DMat4H2 (D0001) is gratefully acknowledged.

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Figures

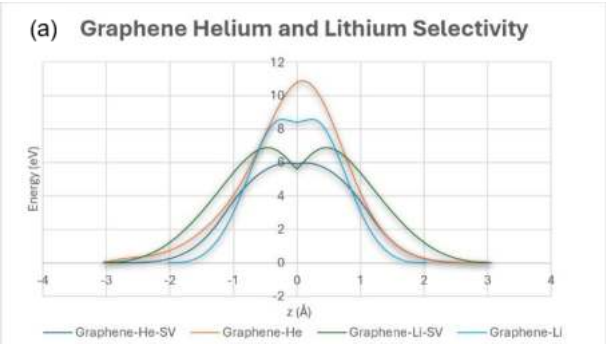

Figure (a): Permeation Energy of He and Li^+ through (1) Pristine Graphene ML, and (2) Graphene ML with single Carbon Vacancy

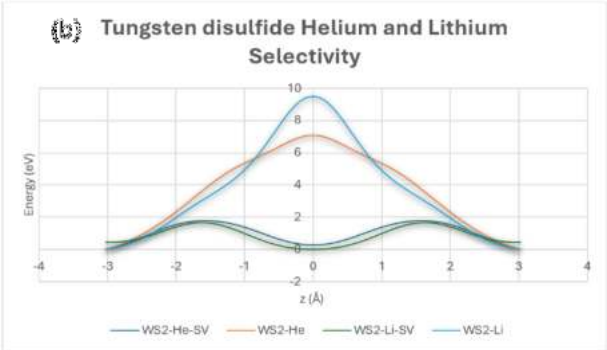

Figure (b): Permeation Energy of He and Li^+ through (1) Pristine WS_2 ML, and (2) WS_2 ML with single Tungsten Vacancy

Single atom-alloy Ni-based catalysts design for bio-oil upgrading

Seba Alareeqi[1], Daniel Bahamon[1], Kyriaki Polychronopoulou[2], Paulette Clancy[3], and Lourdes F. Vega[1,*]
[1] Research and Innovation Center on CO_2 and Hydrogen (RICH), Chemical and Petroleum Engineering Department. Khalifa University, Abu Dhabi, UAE.
[2] Center for Catalysis and Separations (CeCaS), Mechanical and Nuclear Engineering Department. Khalifa University, Abu Dhabi, UAE.
[3] Department of Chemical and Biomolecular Engineering, Johns Hopkins University, 3400 North Charles Street, Baltimore, Maryland, USA.
*seba.alareeqi2@ku.ac.ae, *lourdes.vega@ku.ac.ae

Biofuels production from biomass has been a worldwide interest in the hunt for sustainable fuels. A substantial hurdle in commercializing the conversion of biomass-derived feedstocks to *drop-in* hydrocarbons, or hydrogen, is designing a catalyst with high dehydrogenation activity, economic viability, long-term stability, and coke resistance. Attempting to refine the active-sites properties, single-atom alloy (SAA) catalysts have emerged as a pioneer class of heterogeneous catalysts with tuned surface properties. Herein, we employ descriptor-based density functional theory (DFT) calculations, combined with Microkinetic (MK) modelling and *ab initio* molecular dynamics (AIMD) simulations, to elucidate their role in upgrading modelled bio-oil compounds. The deoxygenation upgrading of phenolic O-moieties has been systematically explored on a wide range of SAA M-Ni-based catalysts (i.e., M=Pd, Pt, Cu, Co, Fe, Ru, Re, Rh, V, W, and Mo). Results reveal that the OH*-induced surface improve the SAA catalysts stability, designating their applicability under experimental deoxyeganton conditions. Moreover, the V-Ni catalyst showed the strongest adsorption energy (E_{Ads}) for all modelled O-moieties (**Figure1(a)**). This high E_{Ads} was elucidated to originate from the induced-electronic effect, evaluated by the lessened *d*-band shift (-0.84eV) in the partial density of states (PDOS) of V-Ni, relative to monometallic Ni at -1.3 eV (**Figure1(b)**). Linking the DFT Gibbs-free energy to MK analysis, the Mo-Ni site was shown to be the most active, both at low and high reaction temperatures. We then processed our investigation to conduct a DFT-screening of 26-doped SAA *bimetallic* and *trimetallic* Ni-based catalysts, combined with AIMD simulations, to access the dehydrogenation of acetic acid bio-oil towards green hydrogen (**Figure1(c)**). Results identified 3 *bimetallic* SAA M-Ni combinations, i.e., Cu-Ni, Zn-Ni, and Ag-Ni, with promising costing, stability, and dehydrogenation activity. Moreover, *trimetallic* dopants outperformed the *bimetallic* candidates, signifying 6 stable SAA catalysts with balanced adsorption and reduced coking susceptibility. The findings of this work enable the design of affordable, stable, and active SAA catalysts for multifunctional bio-oils upgrading reactions.

This work has been financed by Khalifa University of Science and Technology under the Research and Innovation Center on CO_2 and Hydrogen (RICH) and the Catalysis and Separation Center (CeCaS) (projects RC2-2019-007 and RC2-2018-024) and by the Abu Dhabi Award for Research Excellence (AARE19-223).

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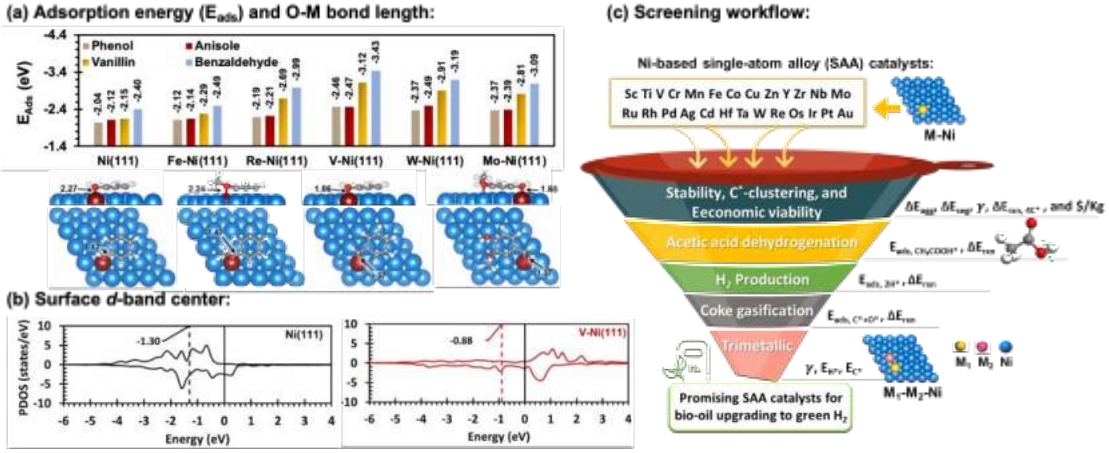

Figure 1: Adsorption energy (E_{ads}) of bio-oils on the M-Ni(111)-based surfaces and their configurations on V–Ni(111). Distances in Angstroms (Å). (b) Projected density of states (PDOS) of *d*-states for the Ni-M-Ni site. Solid black line: Fermi level. Dashed line: *d*-band center. (c) Hierarchical DFT descriptor-based assessment criteria for the discovery of promising SAA Ni-based catalysts for bio-oil upgrading to hydrogen.

Unravelling the Interaction of MXenes with Extracellular Vesicles

Maha Alhosani[1*], Olla Elkhatib[1*], Nabila Yasmeen[2*], Benjamin Chacon [5], Jawaher Alhammadi[2], Laura Fusco [3,5], Linda Giro [3], Marco Orecchioni[4], Yury Gogotsi [5], Anna-Maria Pappa[2], and Lucia Gemma Delogu[1,3]

**Those authors contributed equally to this work*
[1]Department of Biological Sciences, Khalifa University of Science and Technology, Abu Dhabi, UAE.
[2]Department of Biomedical Engineering, Khalifa University of Science and Technology, Abu Dhabi, UAE
[3] Department of Biomedical Science, University of Padua, Padua, Italy
[4] Immunology Center of Georgia, Augusta University, Augusta, Georgia
[5] A. J. Drexel Nanomaterials Institute and Department of Materials Science and Engineering, Drexel University, Philadelphia, PA, United States.

lucia.delogu@ku.ac.ae

Transition metal carbides, nitrides, and carbonitrides (MXenes) are emerging 2D materials with versatile chemistry, garnering significant interest in diagnostic and biomedicine[1]. Recent studies have revealed safe interactions of MXenes at tissue and cellular level[2], highlighting their potential for biomedical applications, such as encapsulation within extracellular vesicles (EVs) for future therapeutics. EVs are nanosized, membrane-bound particles that transfer biomolecules such as proteins, lipids, RNAs, DNA and nanomaterials into target cells [3]. Accumulating evidence shows that EVs have a role in intracellular communication, influencing processes like immune response and cancer progression[3,4]. Understanding whether MXenes are integrated into EVs, their chemistry and the intracellular communication between MXene, EVs and target cells may open new avenues to revolutionize targeted drug delivery. In this study, MXene-encapsulated EVs are extracted from immune cells of THP-1 cells by mechanical extrusion and chemical blebbing protocols. The obtained changes in hydrodynamic diameter and surface charges shed light on the dynamics of the interaction of MXene with EVs at different incubation time points. Scanning electron microscopy showed morphological changes induced by MXene encapsulated EVs on the cell membrane surface. Additionally, flow cytometric analysis is performed to gain deeper insight for the presence of specific extracellular and intracellular EVs surface markers. Future studies aim to delve into the potential use of MXene encapsulated EVs, extracted from THP-1 immune cells, for transfection of biomolecules and therapeutic tagging for biomedical purposes.

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A Graphene Oxide-Based Aptasensor for the Multiplexed Detection of Neonicotinoids in Food Samples

Asma Zaid Almenhali, Pandiyaraj Kanagavalli, and Shimaa Eissa
Department of Chemistry, Khalifa University of Science and Technology, Abu Dhabi, United Arab Emirates
100059171@ku.ac.ae

Neonicotinoids are a group of neurotoxic insecticides that are chemical analogues of nicotine [1]. They possess significant threats not only to the environment, but also to human health [2]. This underlines the importance of developing cost-effective detection tools for these insecticides. Graphene oxide is a popular choice of material in the development of such sensors due to the unique properties it presents like the presence of oxygenated functional groups, its high conductivity, and the simple preparation [3]. Nonetheless, no aptasensor was reported for the multiplexed detection of neonicotinoids. Recent years have seen a surge of interest in integrating aptamers with graphene in electrochemical biosensors, thanks to the remarkable properties of both materials. Herein, an electrochemical biosensor was fabricated by integrating three aptamers on a reduced graphene oxide screen printed electrodes for the detection of imidacloprid, thiamethoxam, and clothianidin. While the latter two were directly retrieved from the literature, the imidacloprid-specific aptamer underwent a truncation, which showed strong affinity with K_d = 20 nM when studied with cyclic voltammetry (CV) and differential pulse voltammetry (DPV). The biosensor displayed good sensitivity and a linear range from 0.01ng/mL to 100 ng/mL for imidacloprid, thiamethoxam, and clothianidin. It also demonstrated good selectivity to the three analytes against dinotefuran and one another. Spiked extracts of tomatoes and rice samples were tested for all three neonicotinoids and the recovery was in the range of 99.0% - 100.8%. This study highlights the potential for using reduced graphene oxide in developing electrochemical biosensors, which could be further extended to detect emerging organic contaminants.

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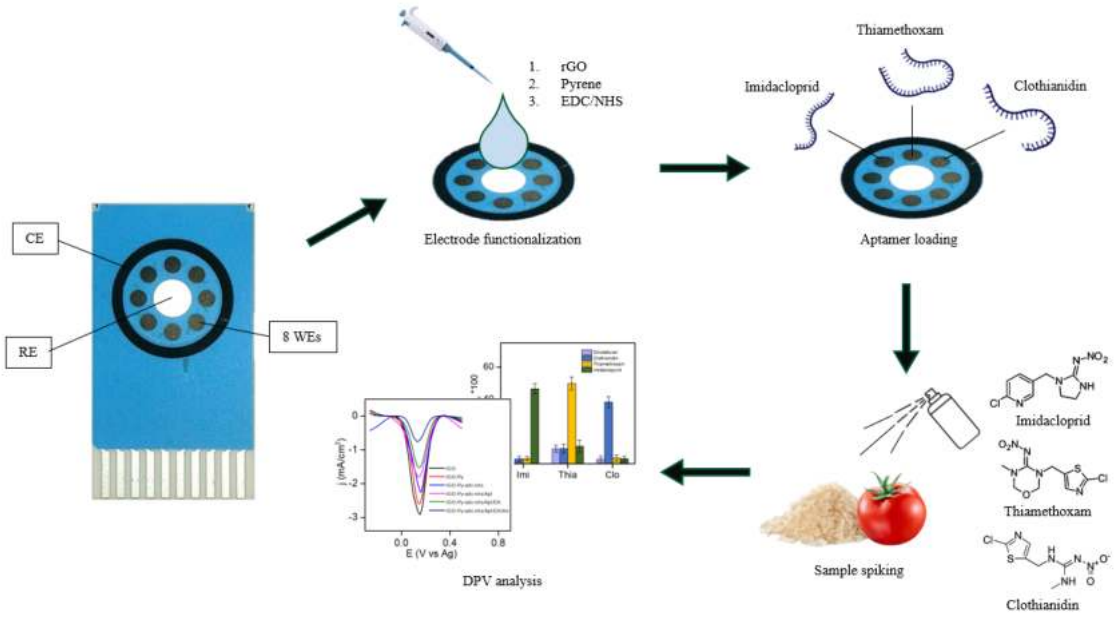

Figure 1: Schematic overview of the developed aptasensor

Carbon-Based 2D Electrocatalysts for Efficient Water Splitting

Presenting Author Mariam Alqubati[1,2], Co-Authors Yuting Li[1,2], Lourdes F. Vega[1,2,3]
[1]*Research and Innovation Center for Graphene and 2D Materials (RIC-2D), Khalifa University of Science and Technology, PO Box 127788, Abu Dhabi, United Arab Emirates*
[2]*Department of Chemical and Petroleum Engineering, Khalifa University of Science and Technology, PO Box 127788, Abu Dhabi, United Arab Emirates*
[3]*Research and Innovation Center on CO2 and Hydrogen (RICH Center), Khalifa University of Science and Technology, PO Box 127788, Abu Dhabi, United Arab Emirates*
100051892@ku.ac.ae

Abstract

One of the technological routes for achieving net-zero emissions is the use of low carbon hydrogen, for which more efficient and cheaper production technologies are needed. Two-dimensional (2D) carbon-based materials, including graphene and its doped variants, have gained significant attention as viable alternatives to noble metals for electrochemical water splitting due to their abundance, stability, and tunable electronic properties. Studies indicate that heteroatom-doped graphene and 2D porous carbon nanosheets demonstrate promising performance for water splitting; hydrogen evolution reaction (HER) and oxygen evolution reaction (OER) [1], [2]. Specifically, nitrogen and sulfur doping in graphene improves electron density distribution, creating active sites favorable for catalytic activity, especially under alkaline conditions [3]. Doped carbon structures additionally exhibit enhanced durability and efficient mass transport due to minimized catalyst aggregation [4]. Dual-doped graphene, for instance, has shown competitive catalytic performance with reduced overpotentials and enhanced kinetics in both HER and OER processes [5]. The objective of this work is to explore the potential of noble metal-free carbon-based electrocatalysts as cost-effective options for sustainable hydrogen production by a combined computational modeling – experimental approach. Density Functional Theory (DFT) calculations are used to study and optimize selected novel 2D materials, aiming to identify electrocatalysts with improved performance for scalable green hydrogen production.
This work is financed by the RIC2D center through project 2DMat4H2 (D0001). Computational resources from the RICH Center at Khalifa University are also acknowledged.

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An Alternative Cell Labeling System Based on the New Two-Dimensional Nanomaterials MXenes

Roberta Cagliani[1], Laura Fusco[1], Linda Giro[1,2], Maha Khaled Hasan Ahmed Alhosani[4], Olla Hazem Elkhatib[4], Chacon Benjamin[3], Klaus Ley[2], Marco Orecchioni[2], Yury Gogotsi[3], Lucia Gemma Delogu[1,4]

1. Department of Biomedical Science, University of Padua, Padua, Italy.
2. Augusta University, Immunology Center of Georgia, Georgia, United States.
3. A. J. Drexel Nanomaterials Institute and Department of Materials Science and Engineering, Drexel University, Philadelphia, PA, United States.
4. Department of Biological Sciences, Khalifa University of Science & Technology, Abu Dhabi, United Arab Emirates

roberta.cagliani@unipd.it

Abstract

Gaining deeper insights into immune cell functions is crucial for developing safe and effective therapeutic applications, especially due to the increasing use of immune cells to treat conditions like autoimmune diseases and cancer. Transition metal carbides and nitrides (MXenes),[1] a novel family of 2D nanomaterials, rapidly growing as multimodal nanoplatforms in biomedicine,[2–4] hold immense potential for tracking immune cells, a crucial aspect in precise diagnosis and treatment. Traditional cell labeling strategies have remained the same over two decades due to a lack of chemical versatility, limiting advancements in translational medicine. Furthermore, current cell labeling tools are incompatible with single-cell mass cytometry by time-of-flight (CyTOF), a globally adopted technology replacing flow cytometry. We propose a groundbreaking approach using MXenes as a model to address these limitations. Our strategy, Label-free sINgle-cell tracKing of 2D matErials by mass cytometry (LINKED) introduces a versatile, multiplexed label-free single-cell detection method based on CyTOF and ion beam imaging by time-of-flight (MIBI-TOF).[3] This technique overcomes chemical limitations and integrates seamlessly with CyTOF, allowing for nanomaterial detection and simultaneous measurement of diverse immune cell and tissue features.[3] This work holds immense potential to propel immunological research, enabling precise cell labeling and tracking for applications in translational medicine.

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Development of highly flexible nanoporous membranes – Potential of 3D printing technology

Laura F. P. Carvalho, Hari K. Balakrishnan, Hassan A. Arafat, Ludovic F. Dumée
Khalifa University, Department of Chemical Engineering, Abu Dhabi, United Arab Emirates
Research and Innovation Center on Graphene and Nanomaterials (RIC2D)

lauracarvalhoeq@gmail.com

Nanoporous membranes are a pivotal technology in supporting the future growth of water purification, desalination, and wastewater treatment industries owing to their ability to selectively remove contaminants at the molecular level. However, they struggle with limited mechanical and chemical resistance under compression, fouling and achieving high permeance [1]. Meanwhile, standard fabrication methods struggle with scalability, waste production, and narrowing the pore size distribution at low costs which is essential to water applications [2]. In contrast, Digital Light Projection (DLP) printing is promising as it allows precise control over membrane structure with high customization and minimal waste [3]. This poster will present the ongoing work of exploring the tools provided by DLP 3D printing to manufacture compression-resistant nanoporous membranes for wastewater treatment applications. We have implemented polymerization-induced phase separation (PIPS) techniques associating different monomers in additive manufacturing to impart flexibility, compressive strength, and overall stability to the material. By benefiting from DLP printing's versatility in fine-tuning membrane properties through specialized chemistries, our research investigates 2D nanomaterials. By incorporating graphene into the polymeric matrix, we not only may improve mechanical strength but also introduce additional functionalities such as anti-fouling systems that enhance performance and broaden the application scope of such composite materials. Therefore, as a proof of concept, this poster will present how DLP technology enables the production of 2D material membranes. Following, we will showcase a new compression test methodology in development to translate the characteristics bestowed on the membranes through 3D printing into measurable KPIs that represent their behavior under operation to further benchmark our membranes against commercial ones. Despite the wide variety of characterization techniques in the literature, a lack of standardization leads to the employment of procedures, like tensile testing, that provide parameters of limited relevance to real operational conditions. Finally, we expect to show that this newly developed methodology greatly contributes to the understanding of the compressibility of membranes and compaction over time effects that cause loss in flux performance, allowing the better engineering of materials that are mechanically sturdy without becoming brittle.

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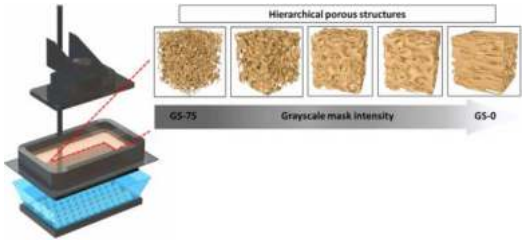

Figure 1: Scheme of DLP printing of porous structures (Adapted from [3])

Figure 2: DLP 3D printed membrane (RIC2D group proprietary picture)

Graphene Enhanced Concrete for Wastewater Treatment

Krishnan Chandrasekharapuram Ramakrishnan and Murugan Muthu
RIC-2D Research Center, Khalifa University, PO 127788, Abu Dhabi, UAE
krishnan.ramakrishnan@ku.ac.ae

Abstract

Heavy metal ions from wastewater strongly adsorb to graphene and its derivatives. They can even be immobilized on hydrated cement surfaces in pervious concrete mixes. In this study, the removal of copper, lead, cadmium and zinc in a fixed bed based on pervious concrete and graphene coated aggregates was examined by performing column experiments for 10 h. Lead removal was exceptional throughout the experiment, regardless of the water head that operated on such fixed beds. Copper removal reached 92% when this operating water head was kept empty. This fixed bed permeability was marginally reduced as suspended clay particles in the wastewater clogged the pore channels. Calcium ions from such concrete matrices leached into percolated water, but this leaching was reduced by the graphene coat, which strengthened the interface between the aggregate and the cement paste. These experimental findings show that graphene-engineered pervious concrete has great potential in industrial wastewater treatment.

Graphene-based Wavy Textile Integrated with Ecoflex™ for Tactile Sensor Applications

Rui Chang [1], Abdullah Solayman [1], Rohan B. Ambade [1,2], Yahya Zweiri [1], Yarjan Abdul Samad [1,2,3]

[1]*Advanced Research & Innovation Center, Khalifa University of Science & Technology, Abu Dhabi, UAE*
[2]*Department of Aerospace Engineering, Khalifa University of Science & Technology, Abu Dhabi, UAE*
[3]*Cambridge Graphene Center, University of Cambridge, CB3 0FA, UK*

100063086@ku.ac.ae

Graphene's outstanding electromechanical properties have garnered great interest for tactile sensors, enhancing robotic capabilities [1]. Higher sensitivity is crucial for tactile sensors, requiring deformable materials like rubber [2]. However, rubber-like materials exhibit the Mullins effect, causing undesirable resistance shifts [3]. This study aims to enhance sensitivity through new structural design modifications and mitigate resistance shifts. Wavy structures show significant deformation under applied forces [4, 5]. This work compares coated textile tactile sensors with flat and wavy shapes integrated into Ecoflex™ (Fig. 1a, b). Nonetheless, during cyclic loading tests, both sensors demonstrated resistance shifts over time (Fig. 1c, d), likely attributable to several factors reported in the literature [3, 6, 7]. To address this shift, the difference between initial and minimum resistance for each cycle (ΔR^*) was calculated (Fig. 1e, f). Under the same applied stress over 1000 cycles, the difference between the maximum and minimum resistances for a single cycle vary 20.78% for the wavy sensor and 60.07% for the flat sensor (Fig. 1c–f) on average, demonstrating long-term reliability. The wavy sensor exhibits higher sensitivity as it results in considerably higher normalized resistance than the flat sensor (Fig. 1g). Furthermore, under an applied stress of 95 kPa corresponding to a 13% strain, the sensitivity of the wavy textile sensor was 2.25 times higher than that of the flat fabricated textile sensor. This study demonstrates that graphene-coated textile tactile sensors with the wavy structure integrated into Ecoflex™ exhibit higher sensitivity and greater stability under dynamic loading than the flat structure.

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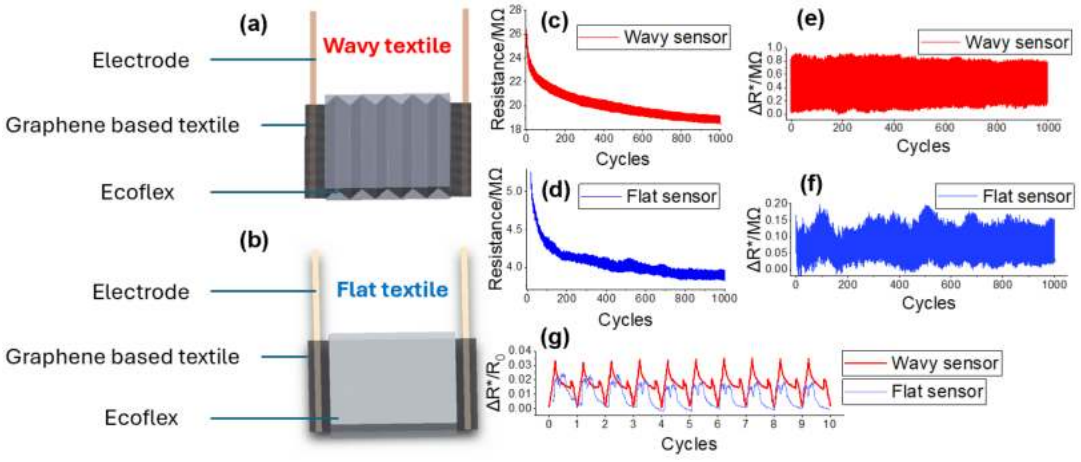

Figure 1: (a, b) Schematic illustration of wavy and flat graphene-coated textile tactile sensors integrated into Ecoflex™, (c, d) Resistance change across 1000 cycles loading test of wavy and flat textile sensors, (e, f) The difference between current resistance and fitted minimum resistance for each cycle (ΔR^*) across 1000 cycles loading test of wavy and flat textile sensors, (g) Normalized resistance change ($\Delta R^*/R_0$) across 10 cycles loading test of wavy and flat textile sensor.

Enabling fast-charging via layered ternary transition metal oxide design as anode materials for lithium-ion batteries

Yannis De Luna, Khaled Youssef, Nasr Bensalah
Qatar University, Doha 2713, Qatar
yannis.deluna@gmail.com

Abstract
Lithium-ion batteries remain at the forefront of battery technology – however, a new generation of electrode materials are required to satisfy new demands in large-scale and more advanced energy storage systems [1]. The application of transition metal niobates as battery anode material has attracted research interests due to their higher operating voltage, capacities, and rate capabilities compared to niobium oxides and conventional graphitic anodes [2]. Current battery technology utilizes cobalt as part of the electrode material, which is one of the most expensive transition metals with strained supplies from the growing demand for electric vehicles [3]. To distribute the use of transition metals, ternary transition metal oxides may have great potential for more cost-effective and high-rate anode materials. Furthermore, a trimetallic mixture of transition metal oxides as an anode material may provide multiple redox pathways for a speedier diffusion of Li^+ ions and higher theoretical capacity, enabling synergistic effects [4]. In this work, a ternary transition metal oxide based on Ni-Mn-Nb has been synthesized for the first time through a thermo-mechanochemical synthesis method. The as-prepared Ni-Mn-Nb anode was characterized and electrochemically evaluated as an anode material against Li/Li^+ (half-cell) and against NMC and LFP cathodes (full cells). For comparison, niobium pentoxide and binary transition metal oxides (Ni-Nb and Mn-Nb) were also prepared and tested as anode materials. The first discharge and charge capacities delivered by Ni-Mn-Nb anode at 0.1 A g^{-1} were 550 and 400 mAh g^{-1}, respectively. The ternary metal oxide design greatly enhanced its cycling performance after 7000 cycles with a reversible capacity of 93.8 mAh g^{-1} at a high current density of 2 A g^{-1} (10C) - the highest among the other anode materials in this work at a very high rate, synonymous to fast-charging. Post-mortem analysis revealed a stable SEI layer on the anode after cycling, which enabled the extremely stable cycling in 7000 cycles.

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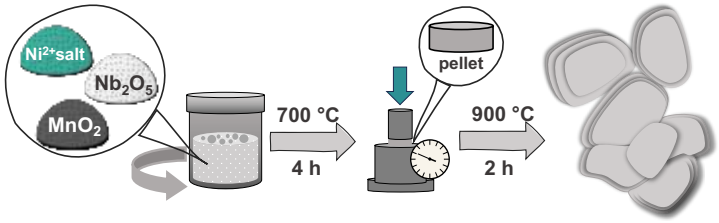

Figure 1: Schematic diagram of the thermo-mechanochemical synthesis used to prepare the layered ternary transition metal oxide (Ni-Mn-Nb).

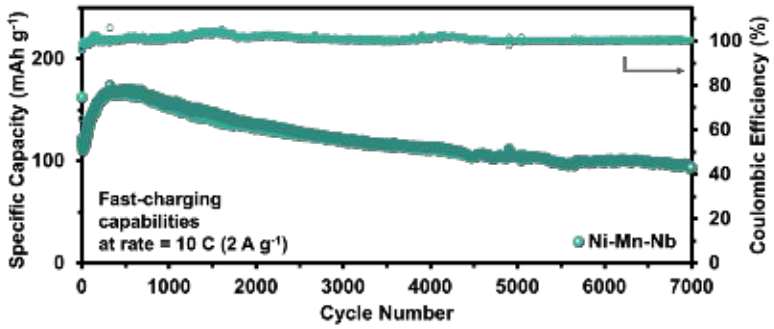

Figure 2: Long-term cycling performance of Ni-Mn-Nb oxide as anode material at a fast-charging rate of 10C.

Ferroionic 2D Material Integration for Enhanced Electro-Optic Functionality in Silicon Photonic Circuits

Ghada Dushaq [1]*, Solomon Serunjogi[1], Srinivasa R. Tamalampudi[1], and Mahmoud Rasras[1,2]
[1] *Department of Electrical and Computer Engineering, New York University Abu Dhabi, P.O. Box 129188, Abu Dhabi, United Arab Emirates.*
[2] *NYU Tandon School of Engineering, New York University, New York, USA*
ghd1@nyu.edu

Tunable optical materials are crucial in integrated photonic circuits, where precise refractive index control is essential for diverse applications [1,2]. Two-dimensional (2D) materials like transition metal dichalcogenides (TMDs) have shown promise [3,4], but efficient phase modulation in the short-wave infrared (SWIR) with low loss remains challenging.
In this work, we demonstrate the strong electro-refractive response of multilayer ferroionic $CuCrP_2S_6$ (CCPS) integrated into silicon photonics (SiPh) microring resonators (MRRs) in the near-infrared. The migration of Cu ions under an applied electric field enables refractive index tuning of approximately 2.8×10^{-3} RIU, while preserving extinction ratios and resonance linewidths. The devices exhibit low optical losses, with a modulation efficiency of 0.25 V·cm and a consistent blue shift in resonance wavelengths across both voltage polarities, outperforming previous TMD-based phase shifters.
Additionally, we observe polarization-dependent electro-optic tuning, with distinct responses for transverse electric (TE) and transverse magnetic (TM) modes. The dual optoelectronic and ionotronic capabilities of CCPS-based devices offer potential applications in phased arrays, optical switching, environmental sensing, optical imaging, and neuromorphic computing.

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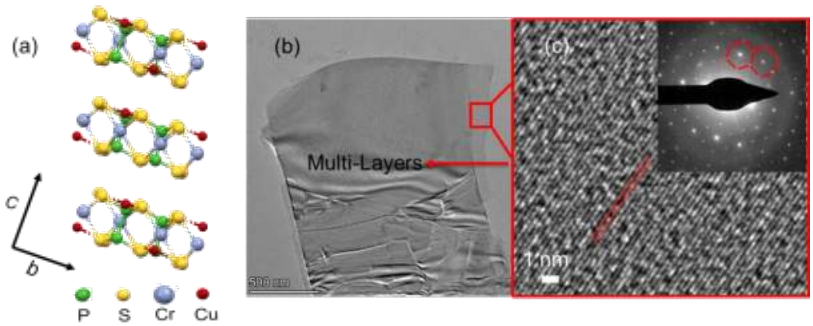

Figure 1: Structural characteristics of CCPS (a) 3D visualization of bc plane (ball-stick model) (b) high-resolution transmission electron microscopy (HRTEM) of multilayer CCPS captured at the red squared area.

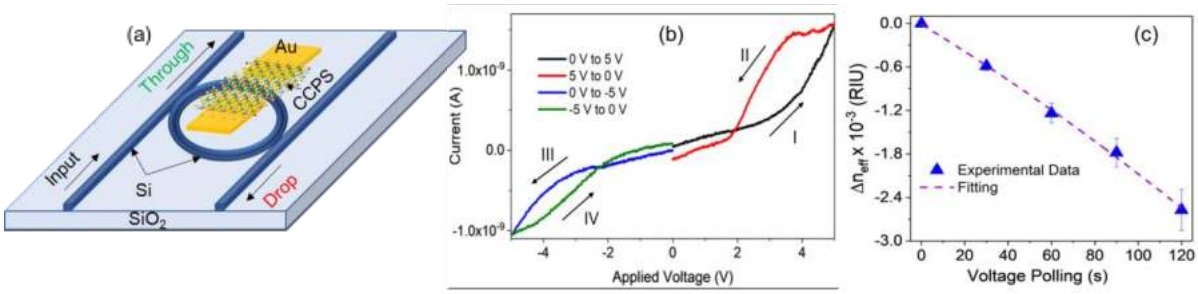

Figure 2: (a) Schematic configuration of the photonic design and CCPS integration (b) full I−V curves swept in the order 0 V→ 5 V → 0 V → -5 V → 0 V labeled as I, II, III, IV (c) the change in real part of effective index of refraction as a function of the polling time at E= $1x10^4$ V/cm.

Reduced Graphene Oxide/MOF-based Electrochemical Biosensor for Environmental and Diagnostic applications

Ragi Adham Elkaffas, Kanagavalli Pandiyaraj, M. Infas H. Mohideen and Shimaa Eissa*
Department of Chemistry, Khalifa University of Science and Technology, Abu Dhabi, P.O. Box
Ragi.elkaffas@ku.ac.ae

Abstract
This study presents the development of novel electrochemical biosensor platforms based on reduced graphene oxide (rGO) and metal-organic frameworks (MOFs) composites for the detection of water-borne pathogens and cancer-related biomarkers. By integrating GO with copper-based and chromium-based MOFs, enhanced electrocatalytic performance was observer for the composites. The combination of GO and MOFs was validated using characterization methods such as FT-IR, XRD, SEM, and XPS, confirming the successful formation of the composite. The large surface area and functional versatility of both materials enabled the covalent attachment of antibodies to develop the biosensor. These platforms offer rapid, sensitive, cost-effective, and portable detection, driven by the synergistic effects between rGO and MOFs. The resulting immunosensors exhibited high specificity and practical potential, making them promising for detecting other water-borne pathogens and cancer-related biomarkers. The combination of rGO with MOF composites offers a flexible approach to biosensing, underscoring their potential in diagnostics, environmental monitoring.

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Figures

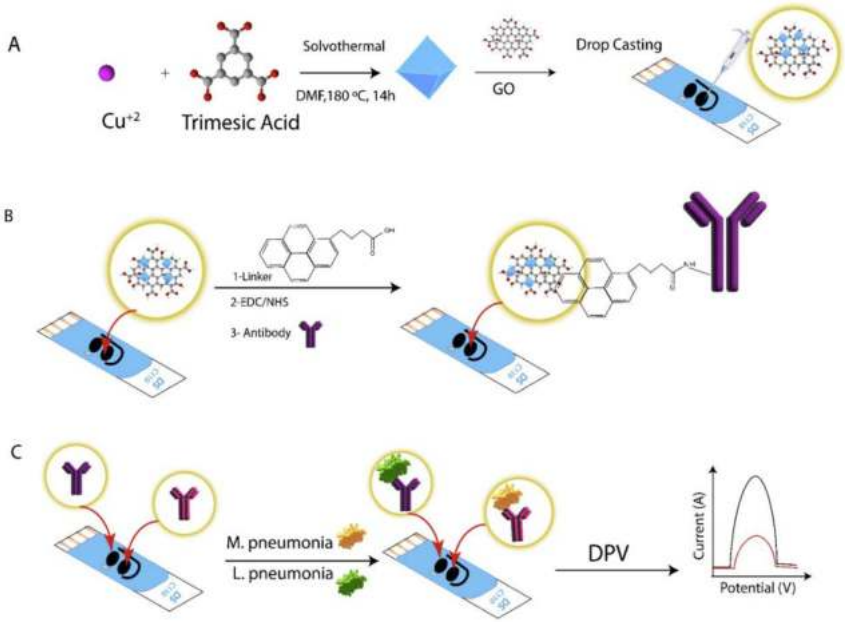

Figure 1: Illustration of (**A**) the synthesis method used for the preparation of the GO/Cu–MOF composite. (**B**) The steps for the fabrication of the immunosensor and (**C**) the dual detection of *M. pneumoniae* and *L. pneumophila* antigens using differential pulse voltammetry.

In-Situ Expansion of Intercalated Graphite in Scanning Electron Microscopy

Rami Elkaffas [a*]
Mohamed I helal [a*]
Yarjan Abdul Samad [a,b*]
[a] Department of Aerospace Engineering, Khalifa University of Science and Technology,
Abu Dhabi,127788, United Arab Emirates.
[b] Cambridge Graphene Centre, University of Cambridge, Cambridge, CB3 0FA UK.
Rami.Elkaffas@ku.ac.ae

Abstract

Graphene has been a focal point of research interest since its isolation by Novoselov and his team [1], who used micromechanical cleavage of graphite with scotch tape, marking a seminal moment in the field. Graphene's 2D hexagonal carbon lattice structure gives its distinct properties, including a remarkable tensile strength of 130 GPa and Young's modulus of 1.0 TPa [2], exceptional thermal conductivity at 5×10^3 W/mK [3], and electrical conductivity up to 80 MS/m [4]. a high surface area of 2630 m^2/g [5], outstanding electron charge transport properties (~200000 $cm^2V^{-1}s^{-1}$) [6]. Scanning Electron Microscopy (SEM) is known for characterizing surfaces from the millimeter range to the highest resolution. SEM has been reported to be capable of imaging many types of graphene, such as a few layers [8], a bilayer [9], and monolayer graphene on SiO_2 substrate [10]. This study presents a ground-breaking observation of the expansion between graphite layers, visualized for the first time through SEM. This process was carefully controlled and monitored, allowing an unprecedented view of graphite's structural evolution and manipulation at the nanoscale. A parametric study was done, and it was found that by adjusting the electron beam's voltage to 30kV and exposure duration to 30 seconds, we achieved controlled expansion of the graphite layers up to 20 times its original interplanar distance. Raman spectroscopy, XRD, and EDS analyses were conducted to confirm the success of the process. This work enhances our understanding of graphite's structural properties and opens new pathways for developing graphite intercalation-expansion into graphene technique.

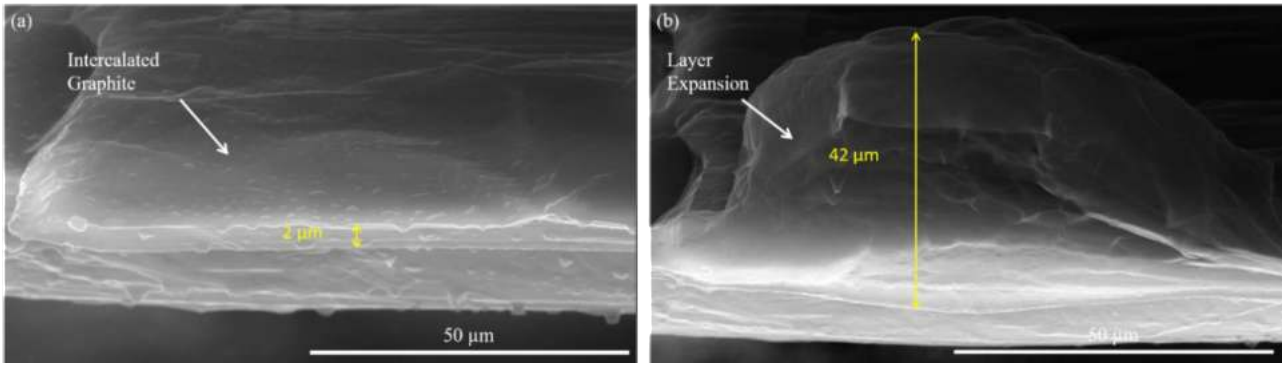

Figure 1: (a) SEM of Intercalated Graphite, (b) Expansion of Intercalated Graphite under SEM

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Low-Power Light Propulsion of Graphene-Wood Composites for Space Applications

Afnan Elmubasher, Rami Elkaffas, Basel Altawil, Carlo Iorio, Sean Swei, Yarjan Abdul Samad
Khalifa University of Science and Technology, Muroor Road, Abu Dhabi, UAE
Afnan.Elmubasher@ku.ac.ae

The past 60 years of space operations have filled Earth's orbits with defunct spacecraft that are composed of metallic materials like Aluminium (Al) which generates polluting particles such as alumina (Al_2O_3) during re-entry [1]. There is a need for sustainable materials like wood which decompose into safe organic vapors [2]. Additionally, graphene exhibits high electric conductivity (80 MS/m) [3], Young's modulus of 1 TPa [4], and strong EMI shielding efficiency (SE) of 90 dB which may be maintained under space conditions [2]. This study explores graphene-enhanced wood, combining the strengths of both materials. The method, shown in Figure 1, involves treating wood with $NaOH/Na_2SO_3$ to partially remove lignin and hemicellulose, creating micropores and enhancing flexibility [5]. Graphene, synthesized via microwave-assisted exfoliation of graphite flakes, is applied to coat the cell walls and pores. The wood is then heat-dried in a shaped die to achieve the desired form.

FTIR analysis of the delignified wood reveals partial removal of hemicellulose and lignin and shows that delignification increased bondage between fibers and graphene sheets. SEM images show that delignified wood has denser fibers compared to natural wood, with uniform graphene sheet distribution throughout fibers. Delignification increases tensile strength from 50 MPa to 170 MPa (a 240% increase), achieving a specific tensile strength of 191.2 MPa·cm³/g, 1.82 times greater than Al6061. The graphene-enhanced wood has a density of 0.89 g/cm³, making it 67% lighter than Al6061 [6]. It also exhibits 35 S/m electrical conductivity and an EMI SE of around 37 dB, exceeding the commercialization requirement of 20 dB.

Laser ablation propulsion tests were performed inside a Thermal Vacuum Chamber (TVAC), with a pressure of 2.5 x 10^{-4} Torr to simulate the high vacuum in space. High-speed videos of pendulum movement were analyzed through deep learning algorithms with MATLAB. Results showed a maximum thrust force of 0.658 mN, and hence a momentum coupling coefficient of approximately 42.85 μN/W, using a 450 nm laser diode at 0.86 W. This value is only achievable with Al at about 1000 times this power. Moreover, Graphene-wood composites showed an average mass consumption of 3.99x10^{-5} g/s, 97.07% lower than metals in vacuum with continuous-wave lasers (3x10^{-3} g/s) [7].

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Figures

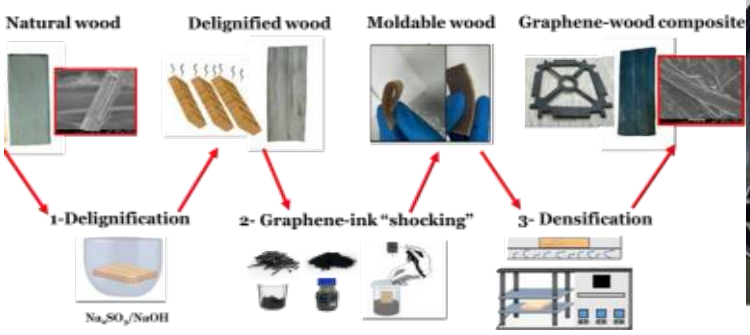

Figure 1: Graphene-wood production process.

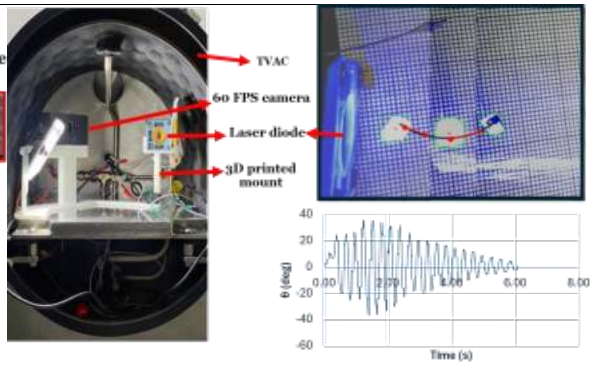

Figure 2: Experimental set-up and tracked sample movement with MATLAB.

Azobenzene Functionalized Light-Responsive Membranes for Solute Speciation during Water Purification

Mohammad Faraz, Fatima Mumtaz, Hari Balakrishnan, and Ludovic F Dumée
Khalifa University, Research and Innovation Center on 2D Nanomaterials (RIC2D), Abu Dhabi, United Arab Emirates
mohammad.faraz@ku.ac.ae

Abstract

Light-responsive membranes represent an innovative solution to address the critical challenges of water purification and desalination in the 21st century, particularly in the context of an escalating global water crisis. As freshwater resources become increasingly scarce, the need for innovative technologies that enhance the efficiency of water treatment processes is paramount. This study explores the integration of photo-responsive molecules, such as azobenzene compounds, into membrane surfaces to create materials that can dynamically regulate separation processes in response to light stimuli. Molecular design and chemical functionalization advances enable precise control over membrane properties under varying light conditions, including permeability, pore size, and surface characteristics. Our research focuses on the functionalization of alumina membranes with light-responsive molecules to produce light-tunable membranes for solute speciation in water purification. The functionalization of membranes with azobenzene moieties is validated through analytical tools, including XPS, FTIR, and laser profilometer. The wettability and pore size of the functional membranes can be tuned upon exposure to UV/Vis light for specific time intervals. These membranes demonstrate efficacy in the selective fractionation of pharmaceuticals (Sulfamethoxazole and tetracycline) from their aqueous solution or contaminated water during continuous exposure with light. This work not only demonstrates the potential of light-responsive membranes for tunable filtration systems but also highlights their role in enhancing the efficiency of water purification. By harnessing molecular engineering and photo-switchable chemistry, we aim to develop sustainable and effective water treatment technologies that contribute to addressing water scarcity worldwide.

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Assessment of Nb_4C_3 MXene Single-Cell Skin Interactions and Irritation Evaluation Using a Non-Animal Model: A Safe Material for Cutaneous Applications

Laura Fusco,[1,2] Benjamin Chacon[2], Erfan Rezvani Ghomi[2], Divij Matthew,[3] Beatriz Estrada-Hernaez,[4] Linda Giro[1], Roberta Cagliani,[1] Kara Spiller[4], Flavia Vitale[5], Yury Gogotsi[2], Lucia Gemma Delogu[1,6,*]

[1]Department of Biomedical Sciences, University of Padua, Padua, Italy
[2]A. J. Drexel Nanomaterials Institute and Department of Materials Science and Engineering, Drexel University, Philadelphia, PA, USA
[3]Department of Systems Pharmacology and Translational Therapeutics, University of Pennsylvania, Philadelphia, PA, USA
[4]School of Biomedical Engineering, Science and Health Systems, Drexel University, Philadelphia, PA, USA
[5]Department of Neurology, University of Pennsylvania, Philadelphia, PA 19104, USA
[6]Department of Biological Sciences, Khalifa University, Abu Dhabi, UAE

Laura.fusco@unipd.it

Abstract

Transition metal carbides, nitrides, and carbonitrides (MXenes) are emerging as promising candidates for a growing list of biomedical applications [1-5], including skin-related uses such as artificial skin, wound healing dressings, and skin sensors. However, there is limited data available regarding the potential skin toxicity of newly synthesized MXenes such as Nb_4C_3.
Here, we investigated the interactions of Nb_4C_3 MXene with human skin cells, utilizing both immortalized HaCaT cells and primary normal human epidermal keratinocytes (NHEK). To this end, we applied LINKED, our recently proposed label-free single-cell detection strategy based on single-cell mass cytometry by time-of-flight (CyTOF) [1], enabling nanomaterial detection and simultaneous measurement of multiple cell markers. We detected Nb_4C_3 in the ^{93}Nb channel and demonstrated its ability to be internalized by skin cells and its biocompatibility on the two skin cell models used, regardless of the extent of interactions. Our analysis detected Nb_4C_3 in the ^{93}Nb channel, demonstrating its ability to be internalized by skin cells and confirming its biocompatibility across both skin cell models, regardless of the extent of interactions. Additionally, we employed reconstructed human epidermis tissue models (EpiDerm, EPI200) to evaluate potential irritation effects.
Our findings demonstrate that Nb_4C_3 exhibits favorable uptake and maintains high cell viability across both cell types, while irritation assessments using the EpiSkin model indicated no adverse reactions. These results suggest that Nb_4C_3 is a safe material with promising implications for cutaneous applications, supporting its potential use in dermatological products and therapies.

Acknowledgements

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Biocompatibility of Water-Dispersible Pristine Graphene and Graphene Oxide Using a Close-to-Human Animal Model: A Pilot Study on Swine

Giro Linda8, Paola Nicolussi1, Giovannantonio Pilo1, Maria Giovanna Cancedda1, Guotao Peng2, Ngoc Do Quyen Chau3, Alejandro De La Cadena Perez Gallardo4, Renzo Vanna5, Yarjan Abdul Samad6,7, Tanweer Ahmed6, Jeremia Marcellino6, Giuseppe Tedde1, Acelya Ylmazer9, Federica Loi1, Gavina Carta1, Loredana Secchi1, Silvia Dei Giudici1, Simona Macciocu1, Dario Polli4,5, Yuta Nishina10,11, Ciriaco Ligios1, Giulio Cerullo4,5, Andrea Ferrari6, Alberto Bianco3, Bengt Fadeel2, Giulia Franzoni1* and Lucia Gemma Delogu8*

(1) Istituto Zooprofilattico Sperimentale della Sardegna, Sassari, Italy
(2) Institute of Environmental Medicine, Karolinska Institutet, Stockholm, Sweden
(3) CNRS, Immunology, Immunopathology and Therapeutic Chemistry, UPR 3572,University of Strasbourg ISIS, 67000 Strasbourg, France
(4) Dipartimento di Fisica, Politecnico di Milano, Milan, Italy
(5) Istituto di Fotonica e Nanotecnologie - CNR, Milan, Italy
(6) Cambridge Graphene Centre, University of Cambridge, Cambridge, United Kingdom
(7) Department of Aerospace Engineering, Khalifa University of Science & Technology, UAE
(8) ImmuneNano Laboratory, Department of Biomedical Sciences, University of Padua, Padua, Italy
(9) Department of Biomedical Engineering, Ankara University, Ankara, Turkey
(10) Graduate School of Natural Science and Technology, Okayama University, Tsushimanaka, Kita-ku, Okayama, 700-8530, Japan
(11) Research Core for Interdisciplinary Sciences, Okayama University, Tsushimanaka, Kita-ku, Okayama, 700-8530, Japan

linda.giro@unipd.it

Graphene-based materials (GBMs) are of considerable interest for biomedical applications, and our pilot study on the toxicological and immunological impact of pristine graphene (GR) and graphene oxide (GO) using swine as a close-to-human provides valuable insights. First, *ex vivo* experiments were conducted on swine blood cells, then GBMs were injected intraperitoneally (i.p.) into swine. Hematological and biochemical analyses at various intervals indicated that neither GO nor GR caused systemic inflammation, pro-coagulant responses, or renal or hepatic dysfunction. Importantly, no systemic toxicity was observed. Analysis of a panel of 84 immune-related genes showed minimal impact of GO and GR. The animals were sacrificed 21 days post-injection, and transient absorption imaging and Raman mapping showed the presence of GO and GR in the mesentery only. Histological evaluation revealed no signs of alterations in other organs. Thus, clusters of both materials were detected in the mesentery, and GO aggregates were surrounded only by macrophages with the formation of granulomas. In contrast, modest local reactions were observed around the GR clusters. Overall, these results reveal that i.p. injection of GBMs resulted in a modest local tissue reaction without systemic toxicity. Our study, performed in swine, provides essential guidance for future biomedical applications of graphene.[1]

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Effective Removal Of Antibiotics From Wastewater Using Deep Eutetic Solvent- Grafted On Graphene Oxide Adsorbents

Anjali Goyal,[1,2] Tarek Lemaoui, [1,2,3] Shadi W. Hasan,[1,2,3] and Inas M. AlNashef [1,2,3,] *

[1] Department of Chemical Engineering, Khalifa University of Science and Technology, Abu Dhabi, PO Box 127788, United Arab Emirates

[2] Center for Membranes and Advanced Water Technology (CMAT), Khalifa University of Science and Technology, Abu Dhabi, PO Box 127788, United Arab Emirates

[3] Research & Innovation Center for Graphene and 2D Materials (RIC-2D), Khalifa University, Abu Dhabi, PO Box 127788, United Arab Emirates

Email: enas.nashef@ku.ac.ae

Abstract

The escalating prevalence of antibiotic residues in wastewater constitutes a grave environmental concern, contributing to antibiotic resistance and negatively impacting aquatic ecosystems. Current treatments are often energy-intensive or ineffective at removing low concentrations of antibiotics[1]. This study investigates an innovative, cost-effective approach to tackle this problem by using adsorbents[2] created from deep eutectic solvents (DES) grafted on graphene oxide (GO).

We synthesized the GO-based adsorbents using eco-friendly green solvents-based thymol for employing surface modification techniques to enhance hydrophobic interactions between the antibiotic molecules and the adsorbent. The synthesized adsorbents were characterized through Fourier-Transform Infrared Spectroscopy (FTIR), UV-Vis Spectroscopy, Total Organic Content (TOC) ,Scanning Electron Microscopy (SEM), and X-ray Diffraction (XRD). Batch adsorption experiments were conducted using different classes of antibiotics such as Meropenem and Ciprofloxacin at various concentrations. The study thus presents a viable, environmentally benign method for antibiotic removal from wastewater, opening avenues for large-scale applications in wastewater treatment facilities.

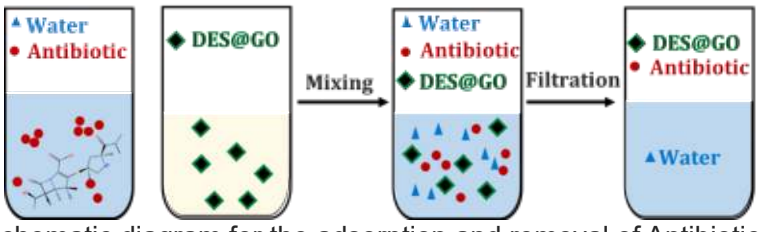

Figure 1: Schematic diagram for the adsorption and removal of Antibiotic from waste water by using DES@GO adsorbent.

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Fabrication and Microstructural Analysis of SiC-Al IPCs for Enhanced Mechanical Properties

Abdul-Rahman Kharbatli[1], Kin Liao[2], Andreas Schiffer[1]
[1] *Department of Mechanical and Nuclear Engineering, Khalifa University, Abu Dhabi, United Arab Emirates*
[2] *Department of Aerospace Engineering, Khalifa University, Abu Dhabi, United Arab Emirates*
100052992@ku.ac.ae

Abstract

Interpenetrating Phase Composites (IPCs) represent a groundbreaking class of materials that combine the benefits of ceramics and metals by deploying both high-temperature stability and wear resistance with enhanced ductility and toughness. IPCs integrate two or more continuous phases that contribute to unique interlinked microstructure design that imparts superior properties beyond those of conventional composites. This makes IPCs ideal for demanding applications such as surgical instruments, grinding tools, defense, aerospace, and components in extreme environments [1]. Recent advancements have introduced IPCs with tailored porosities and novel structures, such as 3D interconnected porous matrices and layered configurations [2]. In this study, silicon carbide (SiC) IPCs was fabricated by infiltration with aluminum alloy to further optimize their mechanical performance. Using a pressureless infiltration method in an atmospheric furnace, aluminum blocks were introduced into SiC foams (10 ppi and 20 ppi) contained within graphite molds. The furnace was filled with N_2 gas and gradually heated to 1100 °C over four hours, then held at this temperature for an additional three hours, and subsequently cooled. Optical microscopy confirmed a well-interconnected Al-SiC structure that revealed an absence of voids or cracks, thus indicating robust metal-ceramic interconnection.

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Figures

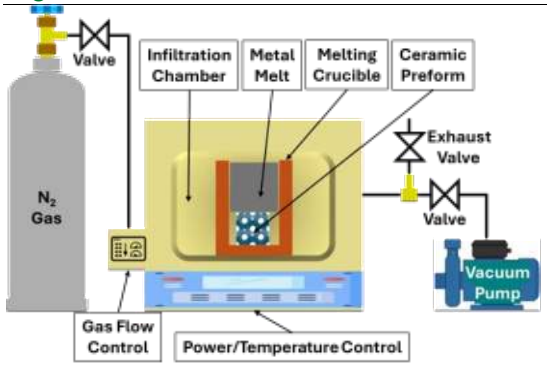
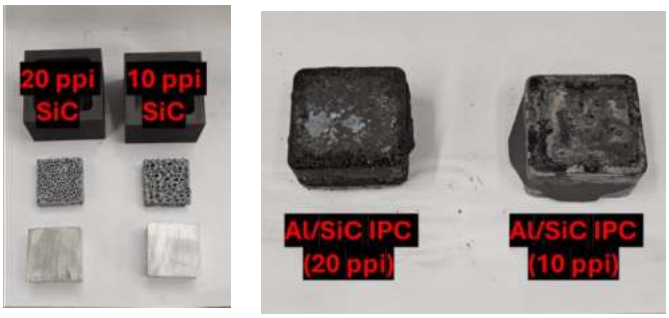
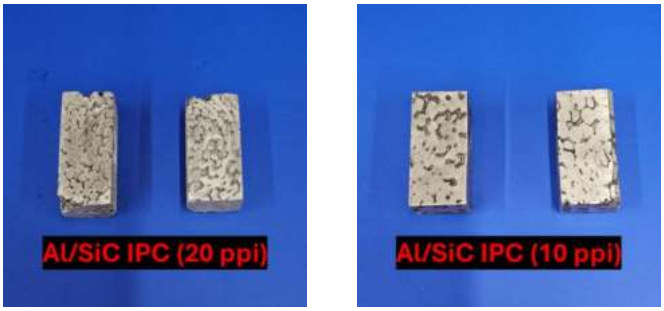


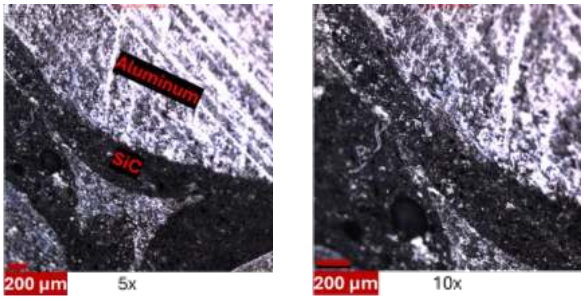
Figure 1: Schematic illustrating the metal infiltration process



(a) **(b)**
Figure 2: Photographic Images showing **(a)** Infiltration tools and **(b)** IPCs after infiltration



(a) **(b)**
Figure 3: Post-machining of IPCs using **(a)** 20 ppi SiC preform and **(b)** 10 ppi SiC preform



(a) **(b)**
Figure 4: Optical microscopy images of Al/SiC interface at magnifications of **(a)** 5× and **(b)** 10×

MXenes as Pioneers in Immune Modulation and Tissue Regeneration for Spaceflight Health

Olla Elkhatib[1*], Maha Alhosani[1*], Benjamin Chacon[2*], Linda Giro[3,5], Immacolata Greco[4], Carlo Iorio[4], Laura Fusco[2,3], Marco Orecchioni[5], Antonio Bencomo [6], Jiranuwat Sapudom [7], Jeremy Teo [7], Yarjan Abdul Samad [8], Yury Gogotsi [2], and Lucia Gemma Delogu [1,3]

1. *Department of Biological Sciences, Khalifa University of Science and Technology, Abu Dhabi, UAE.*
2. *J. Drexel Nanomaterials Institute and Department of Materials Science and Engineering, Drexel*
3. *University, Philadelphia, PA, United States*
4. *Department of Biomedical Science, University of Padua, Padua, Italy*
5. *Centre for Research and Engineering in Space Technologies, Universite Libre de Bruxelles, Brussels, Belgium*
6. *Immunology Center of Georgia, Augusta University, Augusta, Georgia*
7. *Abu Dhabi Stem Cells Center (ADSCC), Abu Dhabi, UAE*
8. *Laboratory for Immuno Bioengineering Research and Applications, Division of Engineering, NYU Abu Dhabi, Abu Dhabi, UAE*
9. *Department of Mechanical Engineering, Khalifa University of Science Technology and Research, Abu Dhabi, UAE*

lucia.delogu@ku.ac.ae

MXenes, a novel family of 2D nanomaterials, are gaining attention for their biocompatibility, antimicrobial properties, and applications in cancer therapy, diagnostics, and tissue engineering [1-3]. However, their biological effects under microgravity conditions remain unexplored. Astronauts face compromised immune systems and impaired wound healing during spaceflight, largely due to the sensitivity of immune cells like peripheral blood mononuclear cells (PBMCs) to gravitational changes[4-6]. To address these challenges, we are investigating whether MXenes can modulate immune function and promote tissue repair under microgravity conditions.

Based on the nanoimmunity-by-design approach[7], we assessed the impact of MXenes on PBMC populations in simulated microgravity using random positioning machine. Additionally, we explored MXenes' potential to enhance skin regeneration, addressing critical health concerns for astronauts on long-duration space missions.

Preliminary results from our analysis in simulated microgravity show that this environment does not affect the viability of PBMCs treated with MXenes. Monocytes and dendritic cells demonstrate significantly higher uptake of MXenes under microgravity conditions, indicating a gravity-dependent impact on cellular interaction. Furthermore, Nb_4C_3 MXene is non-irritating and non-toxic to skin cells, promoting regeneration in a dose-dependent manner up to 200 µg/mL.

Further data from parabolic flight experiments are currently under analysis to validate these results. This research could lead to novel strategies for enhancing astronaut health and open new biomedical applications for MXenes in both space and terrestrial environments.

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Robust Self-Supporting MoS_2@Ni_2B Electrode for Enhanced Hydrogen Evolution

Shubra Lalwani, Maryam AlNahyan, TieJun Zhang, Amal AlAGhaferi, Faisal Almarzooqi
Khalifa University of Science & Technology, P.O. box 127788, Abu Dhabi, United Arab Emirates
Contact@shubra,lalwani@ku.ac.ae

Abstract
The production of hydrogen via electrolysis employing efficient and durable electrocatalyst is highly desirable as a fuel for the future global energy. [1,2] As platinum (Pt) remains the top-performing catalyst in acidic media, the high cost restricts its scalability. [3-5] Therefore, it is imperative to look out for non-noble metal catalysts as an alternative to replace the expensive platinum. Molybdenum sulphide(2D-MoS_2) as a hydrogen evolution catalyst (HER) promises great potential especially, when, combined with conductive carbon supports like graphene oxide (GO) and carbon nanotubes (CNT). Though, the hydrophobicity of these carbon supports significantly limits the catalytic potential of MoS_2. To enhance the hydrophilicity, we incorporated hydrophilic Nickel boride (Ni_2B) into GO/CNT electrodes (Ni_2B-GO/CNT). [6] The incorporation of Ni_2B significantly reduced the water contact angle from 116.6 (GO/CNT) to 25.3° (Ni_2B-GO/CNT) enhancing the wettability. Subsequently, hydrothermal deposition of MoS_2 as an active HER catalyst onto hydrophilic Ni_2B-GO/CNT electrode generated a self-supporting MoS_2@Ni_2B-GO/CNT electrode. This MoS_2 deposition facilitates multi-interfaces among MoS_2-GO/CNT, MoS_2-Ni_2B and Ni_2B-GO/CNT, favoring interfacial electronic redistribution to improve the HER activity significantly. Proposed MoS_2@Ni_2B-GO/CNT electrode exhibits an overpotential of 224 mV at 10 mA cm^{-2} with an excellent durability of 97% for 100 h in acidic medium.

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Figures

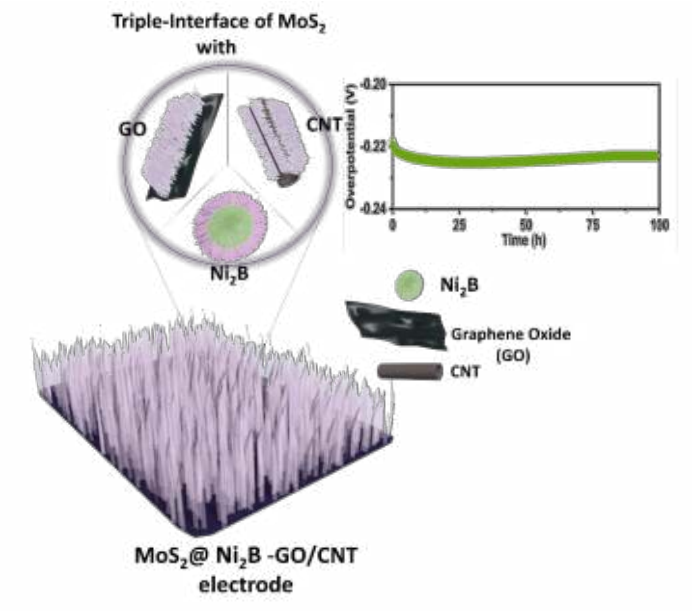

Figure 1: MoS_2@Ni_2B-GO/CNT electrode for enhanced hydrogen evolution reaction in acidic medium

Machine Learning-Assisted Prediction of Proton Permeation Barriers in 2D Materials

Yuting Li[1], Daniel Bahamon[1,2], Lourdes F. Vega[1,2]
[1]*Research & Innovation Center for Graphene and 2D Materials (RIC-2D), Chemical and Petroleum Engineering Department, Khalifa University of Science and Technology, PO Box 127788. Abu Dhabi, UAE*
[2]*Research and Innovation Center on CO2 and Hydrogen (RICH), Khalifa University of Science and Technology, PO Box 127788. Abu Dhabi, UAE*

yuting.li@ku.ac.ae, lourdes.vega@ku.ac.ae

Abstract
Proton Exchange Membranes (PEM)[1], often referred to as proton-conductive membranes or proton-conducting electrolytes, are specialized materials designed to facilitate the flow of protons (H^+) while blocking the passage of electrons and other gases, and they are important in a variety of fields, including fuel cells, gas separation and energy storage. The two-dimensional (2D) crystals hold the potential to significantly advance the field of PEM technology, characterized by exceptional molecular permeability and selectivity. Previous research has proved that understanding the energy barriers involved in proton permeation on 2D materials is essential for designing efficient proton-conductive materials[2,3]. This study employs ab-initio molecular dynamics (AIMD) simulations[4] and machine learning (ML) techniques[5] to predict and analyse proton permeation barriers in non-metal two-dimensional (2D) materials as shown in **Figure 1**. Utilizing structures sourced from online databases[6], we calculated permeation barriers on around 500 2D materials through AIMD, thereby establishing a dataset that correlates 9 simple structural and electronic properties with proton permeation capacity, shedding light on the key determinants of proton permeation, which includes pore diameter, pore size and atomic electron affinity in modulating proton transport, offering insights into the design of advanced 2D materials for proton exchange membranes and fuel cells. The final step involves further assessing the selected potential 2D materials through AIMD simulations to evaluate their selectivity towards hydrogen molecules and protons. This step aims to ensure that the screened 2D materials not only exhibit low proton permeation barriers, but also demonstrate high selectivity for PEM. The integration of AIMD and ML accelerates the discovery of high-performance proton-conducting membranes and provides a deeper understanding of the fundamental mechanisms underlying proton permeation in non-metal 2D materials.
This work is financially supported by the RIC2D centre through project 2DMat4H2 (D0001). Computational resources from the RICH Center at Khalifa University are also gratefully acknowledged.

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Figures

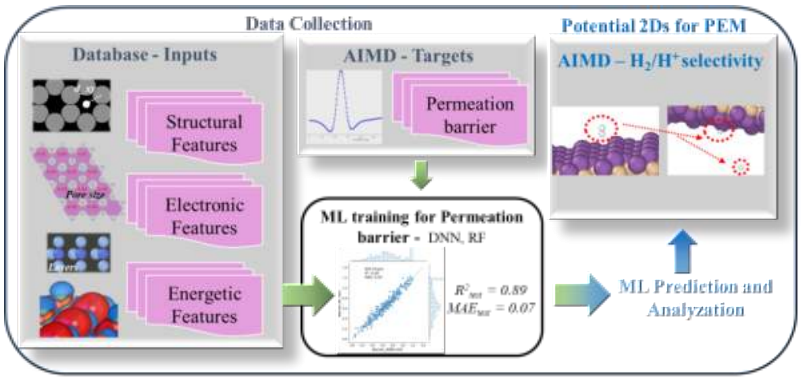

Figure 1: Schematic illustration of predicting of permeation barriers in non-metal 2D Materials using AIMD and ML.

Decoding the Etching Protocols for Conversion of MAX Phases into 2D MXene structures

Mehya Mansoor[1, 2], Mubashir Mansoor[1], Maryam Mansoor[1], Yahya Sorkhe[1], Kamil Czelej[3], Mustafa Ürgen[1] Sebahattin Gürmen[1], Onur Ergen[4*]

[1]*Department of Metallurgical and Materials Engineering, Istanbul Technical University, Istanbul 34450, Türkiye*
[2]*Department of Geological Engineering, Istanbul Technical University, Istanbul 34450, Türkiye*
[3]*Department of Electrical and Communication Engineering, Istanbul Technical University, Istanbul 34450, Türkiye*
[4]*Faculty of Chemical and Process Engineering, Warsaw University of Technology, Waryńskiego 1, 00-645, Warsaw, Poland*

mansoor18@itu.edu.tr

Abstract

MXenes, a group of 2D materials with layers of transition metal carbides/nitrides/borides, and hold significant potential in energy storage, catalysis, and a wide range of applications. Synthesis of MXenes typically involves etching A-layer atoms from MAX phases using acid, alkali, or molten salt etchants [1], however the atomistic mechanisms behind this process are not fully understood [2-4]. We used ab-initio calculations to explore the thermodynamic drive and defect formation energies for 11 MAX phases; Ti_2AlC, Ti_3AlC_2, Ti_2AlN, Ti_4AlN_3, Ta_2AlC, Ta_4AlC_3, Cr_2AlC, V_2AlC, V_4AlC_3, Nb_2AlC and Nb_4AlC_3. Contrary to conventional wisdom, we find that the etching mechanism is not limited by thermodynamic feasibility, and that the inability to synthesize many compositions is due to kinetic constraints. We demonstrate, as a proof of concept study, the applicability of defect engineering approach for development of etching protocols in the broader MXene compositional phase space to pave the way for accelerated and commercial scale MXene synthesis.

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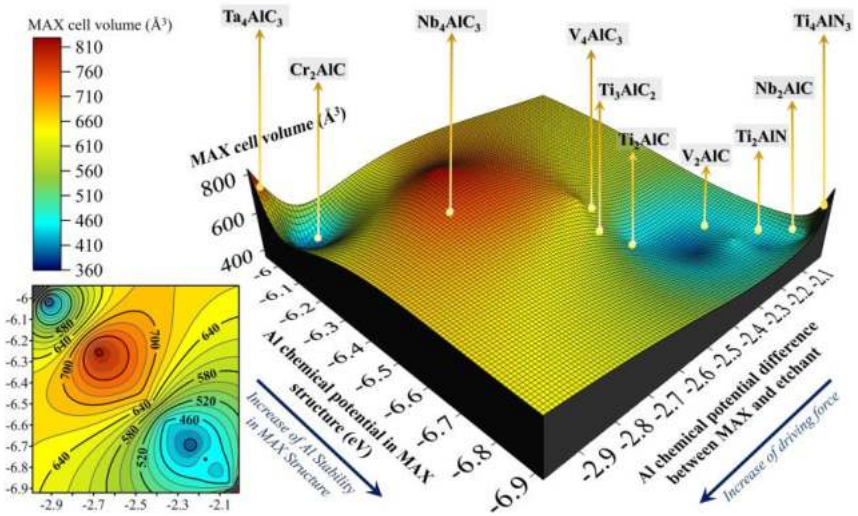

Figure 1: 3D representation of the etching driving force and its correlation with MAX cell volume, and Al chemical potential

TRANSPARENT HYDROPHOBIC MXENE: DE-ICING AND SELF-CLEANING COATINGS FOR SOLAR PANELS

Ezrah Mariam, Lois Damptey, Ajay Kumar, Irwing Ramirez, Nicholas Power, Ravi Silva, Satheesh Krishnamurthy
Advanced Technology Institute, University of Surrey, Guildford, United Kingdom, GU2 7XH
e.mariam@surrey.ac.uk

Photovoltaic (PV) devices play a vital role in addressing global sustainability issues like climate change, as a renewable source of energy which can help achieve net zero carbon emissions. However, soiling of the PV panel surface restricts solar radiation from reaching the solar cells leading to irregular generation of output power and hence decreasing their efficiency significantly. This poses environmental and sustainability challenges due to output losses and high usage of clean water required for their maintenance. Self-cleaning coatings provide an automated alternative for cleaning glass surfaces of solar panels while reducing abrasion damage as well as expenditure on workforce and water usage.

Current self-cleaning coatings have certain drawbacks like reflectivity and durability issues [1]. In our work, we propose the study of transparent and de-icing self-cleaning coatings which can assist in maintaining the effectiveness and reliability of PV panels. 2D materials like MXenes are studied for their extraordinary photothermal properties for inducing an anti/de-icing effect in the self-cleaning coatings [2][3][4]. MXenes are also known for their good mechanical durability making them an efficient candidate for coatings [5][6]. A comparison of HF etching and molten salt synthesis method is done to study the surface functionalities and their effect on the photothermal property of MXene. A non-thermal atmospheric pressure plasma jet printing of MXene to glass has been used and tuned for its hydrophobicity, thickness, and durability. Last but not the least, methods to promote environmental friendliness and reduce the toxicity and risks of the coatings are explored.

Various characterisation techniques are used to analyse the coating properties. Contact angle measurements show that after the Ti_2C MXene coating on glass, the hydrophobicity increased significantly with the highest average contact angle of 138.91°. Furthermore, MXenes show interesting photothermal properties upon plasma printing onto glass slides. A de-icing and self-cleaning coating with high photothermal temperature which goes up to 85°C was achieved. The structural and morphological characterisation techniques were used to confirm the etching of MAX phase and subsequent formation of MXene. The electronic properties were studied using monochromatic XPS and it was found that chemical bond formations and functionalities play a key role in defining the surface and photothermal properties of MXene. Further investigation and analysis are in progress to understand the mechanisms of these materials. Alternative greener methods to synthesise MXenes, including molten salt synthesis using $CuCl_2$, are explored.

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High-Efficiency Supercapacitor with Graphene/ Vanadium oxide Nanocomposite Electrodes

Mahmoud Moussa, Rhys Phillips, Dusan Losic
Technology Innovation Institute. P.O.Box: 9639, Masdar City Abu Dhabi, UAE
School of Chemical Engineering and Advanced Materials, University of Adelaide, Adelaide, Australia
mahmoud.moussa@tii.ae

Abstract
Supercapacitors, also known as ultracapacitors, are energy storage devices with significant potential to replace conventional batteries across a wide range of applications. This is due to their high-power density, rapid charge–discharge rates, extended cycle life, enhanced safety, cost-effectiveness, and environmental sustainability. In this study, a CO_2 laser beam was employed as a clean, low-cost method to synthesize graphene/Vanadium oxide nanocomposite films in a single-step process. The CO_2 laser treatment produced mechanically robust films characterized by high electrical conductivity and large specific surface area, making them suitable for direct use as supercapacitor electrodes without the need for additional binders or current collectors. The choice of metal oxides was optimized to facilitate effective intercalation with graphene, thereby enhancing the performance of the supercapacitors. The fabricated supercapacitors were systematically evaluated using cyclic voltammetry (CV), galvanostatic charge/discharge (CD) testing, and electrochemical impedance spectroscopy (EIS).

Graphene Enhanced Concrete Roads for Runoff Management

Murugan Muthu
RIC-2D Research Center, Khalifa University, PO 127788, Abu Dhabi, UAE
murugan.muthu@ku.ac.ae

Abstract

Pervious concrete pavement is a unique and effective means to address environmental problems and support sustainable growth. By capturing stormwater and allowing it to seep into the ground, pervious concrete is instrumental in recharging groundwater, reducing stormwater runoff, and meeting United States Environmental Protection Agency (EPA) stormwater regulations. In this experimental research, crushed granite aggregates were coated with reduced graphene oxide (RGO) and incorporated into a pervious concrete (PC) mix to enhance its capacity for removing heavy metals. The RGO in aqueous form, at concentrations of up to 0.03 wt%, was introduced into the PC mixture. The aggregate and binder interfaces were strengthened by the RGO, improving the concrete compressive strength by 25%. The addition of RGO reduced the formation of capillary pores in the cement matrix by 33%, resulting in much better resistance to the leaching of calcium ions from cement matrix in strong acids. The average removal of copper, zinc, lead, and cadmium from the desecrate water in this RGO decorated concrete reached 98%, 92%, 96% and 94%, but this removal was reduced when these ions were mixed in the wastewater and passed at the same time. Immobilized heavy-metal ions were detached from cement sites when a strong acid was passed through the concrete samples, but this desorption was reduced in the RGO-treated samples. Overall, the nano-engineering exhibits multiple benefits, and the increased use of graphene-decorated PC as a permeable road surface can remediate heavy metal pollution from urban runoff.

Characterization of Additive Manufactured SiCN ceramics

Adam Otabil[1], Kin, Liao[2], Andreas Schiffer[1]
1 Department of Mechanical and Nuclear Engineering, Khalifa University, Abu Dhabi 127788, United Arab Emirates
2 Department of Aerospace Engineering Khalifa University, Abu Dhabi 127788, United Arab Emirates

100062562@ku.ac.ae

Abstract

Polymer-derived ceramics (PDCs) are ceramic materials produced via the thermal degradation of polymeric ceramic precursor which can used in a wide range of applications, such as aerospace, defense, electronics, photonics, and biological purposes [1]. In this study, 3D printed polymer derived ceramics lattice structures were produced using the Digital Light Processing technique and pyrolyzed at 900 ℃, 1100 ℃ and 1300 ℃ as seen in Fig. 1. With increasing pyrolysis temperature, the ceramic yield decreased as the linear shrinkage increased which could be ascribed to either the reorganization of the microstructure of the ceramic material or the crystallization process. As seen in Figure 2, the XRD pattern of the pyrolyzed sample at 1300 ℃ depicted phases of SiO_2, β-SiC and carbon indicating the sharpness of the peaks at higher temperature. The carbon phases were confirmed with the Raman analysis. As shown in Figure 2, the Raman spectra exhibited two characteristic attributes of disordered graphitic carbon at 1332 cm−1 and 1620 cm−1, which correspond to the D and G bands, respectively [2]

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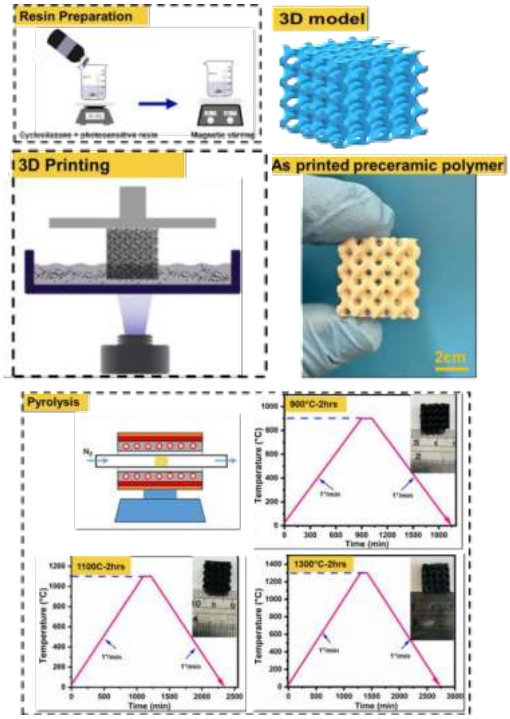

Figure 1: Experimental set-up

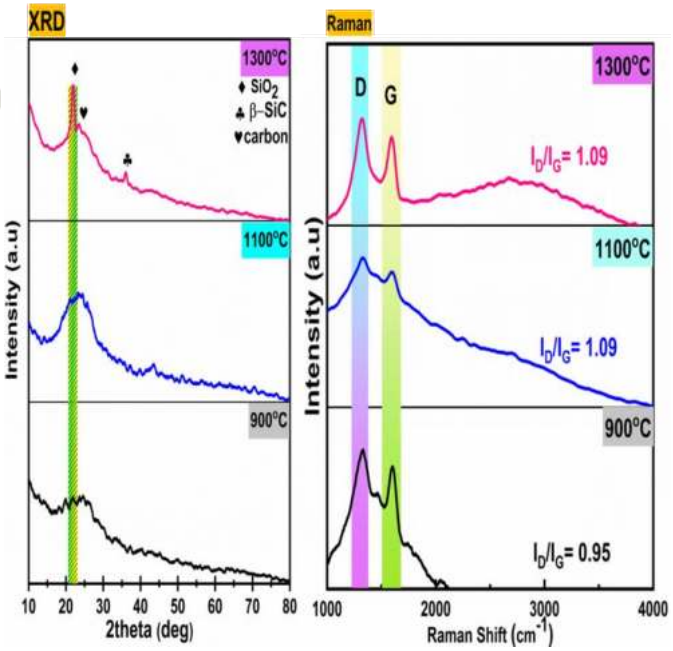

Figure 2: XRD and Raman Spectra of samples

Versatile Perforated MXene for Enhanced Water Purification

Desani Ramadhan, Shashikant P. Patole
Applied Quantum Materials Laboratory (AQML), Department of Physics, Khalifa University of Science and Technology, Abu Dhabi, United Arab Emirates
100065797@ku.ac.ae
shashikant.patole@ku.ac.ae

Perforated MXene, a novel variant of the two-dimensional (2D) transition metal carbide, has emerged as a promising material for water purification [1]. This work explores the unique properties and potential applications of perforated MXene in water purification. By introducing controlled perforations into the MXene structure, researchers have significantly enhanced its surface area and porosity. This increased surface area-to-volume ratio allows for more efficient adsorption and filtration of contaminants from water. Additionally, the perforations can be tailored to specific applications, enabling selective removal of various pollutants. This review summarizes the methods used to fabricate perforated MXene and the factors influencing its performance. It also highlights the potential advantages of perforated MXene over traditional MXene in terms of adsorption capacity, filtration rate, and selectivity. Applications of perforated MXene in water purification include the removal of heavy metals, dyes, organic pollutants, and even salts for desalination [2]. The ability to selectively target specific contaminants makes perforated MXene a valuable tool for addressing complex water quality issues. In conclusion, perforated MXene represents a significant advancement in water purification technology. Its unique properties and versatility offer promising solutions to the challenges posed by water scarcity and pollution. Further research and development in this area are expected to lead to even more innovative and effective applications of perforated MXene in water treatment.

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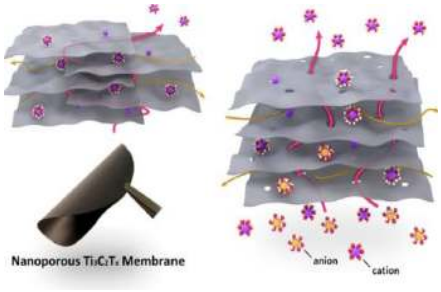

Figure 1: Mxene-based Nanoporous Membrane with in-plane porosity

Density Functional Theory Insights into Electro-Hydrogenation of Furfural on CoxMoOy-Decorated Activated Carbon Catalysts

Ashraf Sabri*, Seba Zakaria Al-Areeqi*, Daniel Bahamon Garcia*, Fawzi Banat, Lourdes Vega*
**RICH Center*
Khalifa University, Abu Dhabi, United Arab Emirates
Lourdes.vega@ku.ac.ae

Abstract:
The electrochemical hydrogenation (ECH) of biomass-derived furfural (FF) into valuable chemicals, such as furfuryl alcohol (FA) and tetrahydrofurfuryl alcohol (THFA), is a promising pathway for sustainable chemical and fuel production. However, large-scale ECH applications are limited by the complexity of reaction mechanisms and a lack of understanding regarding optimal catalytic parameters. This study employs density functional theory (DFT) to investigate the reaction mechanisms and energetics of FF electro-hydrogenation on activated carbon (AC) electrodes enhanced with CoxMoOy catalysts. These catalysts, including MoO2, MoO3, and MoCoO4, were selected based on their electrochemical potential for improved wettability and FF adsorption on AC surfaces. Activated carbon was chosen for its high surface area, tunable porosity, and role as a sustainable electrode support derived from biomass processing byproducts like bio-char [1]. Using the Vienna Ab initio Simulation Package (VASP), DFT calculations assessed the adsorption energy of FF with and without solvation across the four catalyst configurations (pure AC, MoO2/AC, MoO3/AC, and MoCoO4/AC) [2]. MoCoO4/AC exhibited the highest adsorption energy for FF, attributed to the unique interaction facilitated by cobalt's addition, which enhances both wettability and electron transfer efficiency on the electrode surface. This configuration offers an energetically favorable pathway for FF conversion, with implications for optimizing faradic efficiency and selectivity toward FA production [3]. The DFT results suggest that MoCoO4 on AC improves FF conversion efficiency by maximizing electron transfer and creating a surface conducive to reactant adsorption. The strong affinity of MoCoO4 for FF, combined with favorable reaction pathways, highlights its potential for scalable electrocatalyst applications. These findings offer a predictive framework for designing efficient electro-catalysts in sustainable biomass valorization, presenting a pathway for bio-based chemical materials that can be used as raw material for sustainable fuel production as FF can further be hydrogenated to fuel formulations. Further investigations, including nudge elastic band (NEB) calculations, were performed to explore selectivity and yield optimization, aiming to bridge laboratory findings with industrial feasibility.

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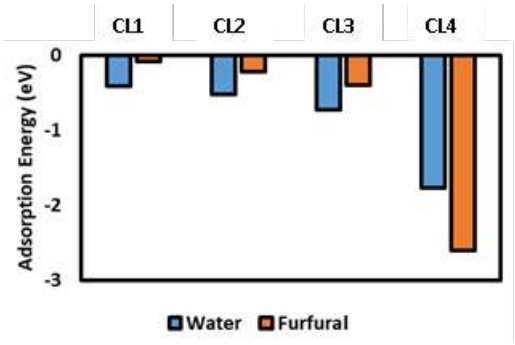

Figure 1: Adsorption energies of water (H_2O) and furfural (FF) on various electrode surfaces: carbon layer (CL1), AC layer with MoO_2 (CL2), AC layer with MoO_3 (CL3), and AC layer with $MoCoO_4$ (CL4).

Understanding the effect of ripples and electric fields on the catalytic activity of graphene by Density Functional Theory calculations

Nuha Sahir[1, 2], Daniel Bahamon[1, 2, 3], Marcelo Lozada-Hidalgo[2, 4], Nirpendra Singh[2, 5], Lourdes F. Vega[1, 2, 3]*

[1]*Department of Chemical and Petroleum Engineering, Khalifa University of Science and Technology, Abu Dhabi, UAE*
[2]*Research and Innovation Center on Graphene and 2D Materials (RIC2D Center), Khalifa University of Science and Technology, Abu Dhabi, UAE*
[3]*Research and Innovation Center on CO2 and Hydrogen (RICH Center), Khalifa University of Science and Technology, Abu Dhabi, UAE*
[4]*Department of Physics and Astronomy, University of Manchester, Manchester, UK*
[5]*Department of Physics, Khalifa University of Science and Technology, Abu Dhabi, UAE*

100053809@ku.ac.ae

Abstract:

Hydrogen (H2) is an important energy vector that can be used in fuel cells to produce carbon-free energy or as a clean fuel. In fuel cells, the dissociated H atoms react with oxygen (O2) to produce energy and water. However, the H2 dissociation reaction is an energy-expensive process and requires the usage of precious metals such as Platinum (Pt). These noble metals are expensive and are present in limited quantities. Therefore, alternative solutions need to be found to facilitate H2 dissociation.

Previous studies have shown that introducing ripples into the structure of graphene can help with increasing its activity as a catalyst and decreasing the energy barrier for H2 dissociation [1], [2]. Ripples can occur intrinsically in graphene and other 2D materials due to thermal fluctuations or they can be induced by applying a strain. Other studies [3], have explored the effect of the potential energy field of a material on the catalytic activity of graphene. In this work, first-principle density functional theory (DFT) is used to study the effect of the ripple and electric field on the graphene-H2 system and how they affect the energy barrier. The stability of the system and the energy barriers are obtained for different ripple heights and electric field magnitudes to fine-tune the best conditions for hydrogen dissociation.

Acknowledgements:

This work belongs to a long-term collaborative project between the University of Manchester and Khalia University of Science and Technology through the Research & Innovation Center for Graphene and 2D Materials (RIC2D center), aiming at exploring and developing 2D-crystals as a disruptive technology addressing some of the challenges faced by hydrogen energy conversion.

Financial support for this work from the RIC2D Center through project 2DMat4H2 is gratefully acknowledged.

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Mechanism of Proton Permeation Through Graphene Monolayer

Mohd Rafie bin Shaharudin, Daniel Bahamon, Lourdes F. Vega, Nirpendra Singh
Khalifa University of Science and Technology,127788, Abu Dhabi, United Arab Emirates
mohd.shaharudin@ku.ac.ae

Research from The University of Manchester has shown that graphene is permeable to protons while hindering other single-charge ions, such as Lithium [1, 2], which is a breakthrough in developing graphene as a 2D membrane for fuel cell application. In this study, we modelled the proton permeation through a pristine graphene monolayer to bring to light the mechanism of permeation that has been hypothesized: i) direct penetration, ii) flipping penetration, and iii) H3O+ penetration. [3] Mechanism 3 is less likely to occur due to the large size of the hydronium ions, leading to a high energy barrier for it to pass through the graphene ring. Besides, our study includes the permeation flux of proton influenced by the electric field at a temperature range between 300 K and 350 K. All Molecular Dynamics (MD) with ReaxFF force field simulations are conducted using the LAMMPS package.

Our results demonstrate that the permeation of proton through graphene follows Mechanism 1 and Mechanism 2, with Mechanism 2 having a higher occurrence than Mechanism 1. Hydrogenation of graphene is observed as proton shuttles via vehicular and Grotthus's hopping mechanism through the reservoir under the influence of an electric field. Our results agree with the experiment on single-gated graphene. [2] Due to the high tendency of hydrogenation on the graphene, Mechanism 2 is the most probable and observed at higher frequencies in our simulation, where protons are adsorbed on the graphene atom before flipping to the other side through the graphene ring. The results of Mechanism 2, as the most probable pathway for proton permeation, also hold at higher temperatures up to 350 K. During permeation, the graphene ring expands, leading to a larger ring size with a broader bond distribution (see Figure 1b). The larger ring size does not have a significant impact on the proton permeation mechanism, as protons are more likely to be trapped within the hydrogenation well as they approach the graphene. With increasing temperature, a higher flux (see Figure 1a) of proton permeation is observed. This could be attributed to the lower charge density on the graphene plane (see Figure 1c) having a weaker electrostatic interaction with the proton and the thermal energy added to the proton to escape the hydrogenation well. Besides, it is also observed that most permeations occur in saturated areas with hydrogen. These results again agree with previous DFT reports [4, 5] that show a higher local saturation of hydrogen on graphene reduces the energy barrier for proton permeation. In this study, we demonstrate the permeation mechanism of protons through defect-free graphene and the influence of temperature on the flux of proton permeation.

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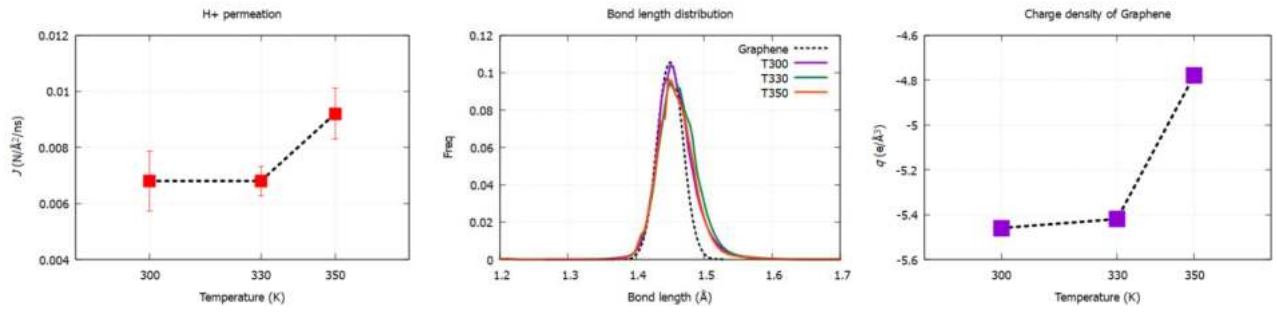

Figure 1: a) Permeation flux of proton. b) Bond distribution of Graphene. c) Charge density on Graphene XY plane.

Solar Assistant Liquid Phase Exfoliation of Graphene and its Thermal Properties

Shanavas Shajahan[1,2*], Rami Elkaffas[1], Dhinesh Babu Velusamy[1,2,] Yarjan Abdul Samad[1,2,3*]
[1]*Department of Aerospace Engineering, Khalifa University of Science and Technology, 127788, Abu Dhabi, United Arab Emirates.*
[2]*Research & Innovation Center for Graphene and 2D Materials, Khalifa University of Science and Technology, 127788, Abu Dhabi, United Arab Emirates.*
[3]*Cambridge Graphene Centre, Department of Engineering, University of Cambridge, Cambridge, UK*
Shanavas.shajahan@ku.ac.ae

Abstract
Graphene generally exhibits exceptionally high thermal conductivity (~2000 W/mK). This is due to its unique two-dimensional structure, where carbon atoms are arranged in a honeycomb lattice, allowing for efficient phonon transport [1,2]. Hence, it can be used as an efficient thermal management material in high-power-density batteries (e.g., Li-ion batteries), mobile communications, consumer electronics, and automotive industries [3-6]. We produced graphene sheets with a lateral size of about ~4 microns through a novel solar light-assisted liquid phase exfoliation technique. The production of few-layer graphene sheets is confirmed by Raman analysis Figure 1 [7]. The SEM image (Fig.1b) confirms the production of graphene sheets in large lateral sizes around ~4 µm. The graphene sheets exhibit an in-plane thermal conductivity (λ) of about 220.3 W/mK, which is almost similar to a traditional heat transfer material aluminum (237 W/mK) [8,9]. The thermal management capability of graphene is demonstrated by recording the difference between the temperature of a bare electrothermal plate and an electrothermal plate with graphene film stuck on it (Fig. 1c). The temperature of the bare electrothermal plate is around 89.7 °C after 150 s. While placing the graphene film on the electrothermal plate, the maximum temperature of the electrothermal plate after 150 s is around 69.3 °C; it is due to the rapid heat dissipation through the graphene film. Our work demonstrates that graphene sheets with large lateral size (~4 µm) play a significant role in achieving high thermal conductivity and diffusivity similar to aluminum, which makes it a potential candidate for thermal management applications.

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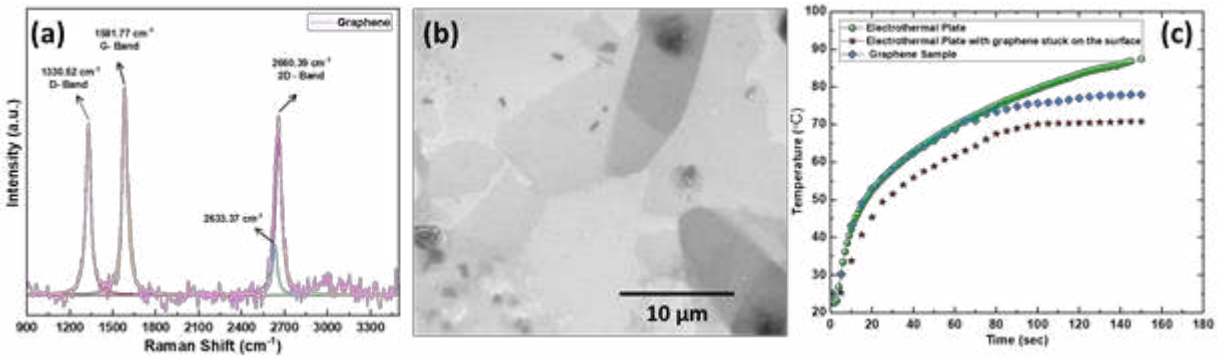

Figure 1: (a) Raman graph of produced graphene; (b) SEM image of produced graphene; (c) Time-dependent temperature profile on electrothermal plate and graphene sheets.

EVALUATION OF THE EFFECT OF GRAPHENE IN MORTARS PRODUCED WITH BLAST FURNACE SLAG

Tarcizo Souza, Paloma Soares, Xavier Yves Roger Raby, Rafael da Silva, Valdirene Peressinotto
Gerdau Graphene, 3200 Engenheiro Miguel Gemma Av., Mogi das Cruzes, Brazil.
tarcizo.souza@gerdaugraphene.com

This work focuses on utilising granulated blast furnace slag (GGBFS), a supplementary cementitious material, in synergistic effect with graphene, as an alternative to reduce CO_2 emissions. GGBFS is commonly used in the production of composite cement [1] but has limitations in performance at early ages due to its low reactivity. On the other hand, researchers have been studying the incorporation of graphene to improve performance in cementitious nanocomposites due to its exceptional physical properties, [2-4]. To evaluate performance, mortars were produced using the replacement of pure cement by 20% and 40% of GGBFS along with graphene at ratios of 0.015%, 0.030%, and 0.050% (wt). These were compared to a reference mortar without substitution and graphene.

There were no significant changes in the fresh state. However, graphene effectively improved compressive strength in the hardened state, even at early ages. Additionally, it increased the elastic modulus and durability-related parameters. This creates a new method to boost the use of GGBFS in cementitious composites without sacrificing performance, alongside the potential to help reduce carbon emissions from cement production.

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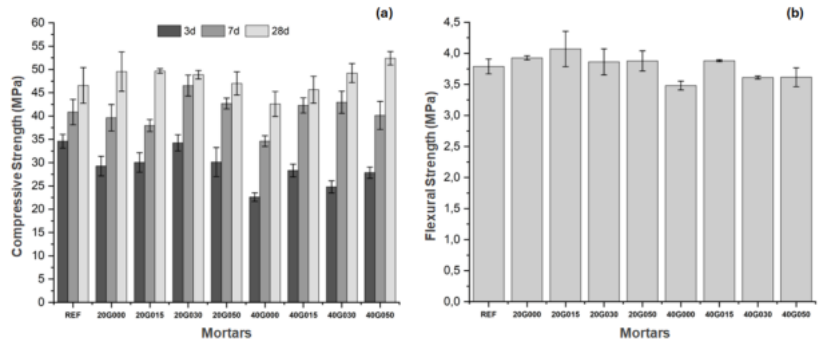

Figure 1: (a) Compressive strength evolution; (b) Flexural strength at 28 days.

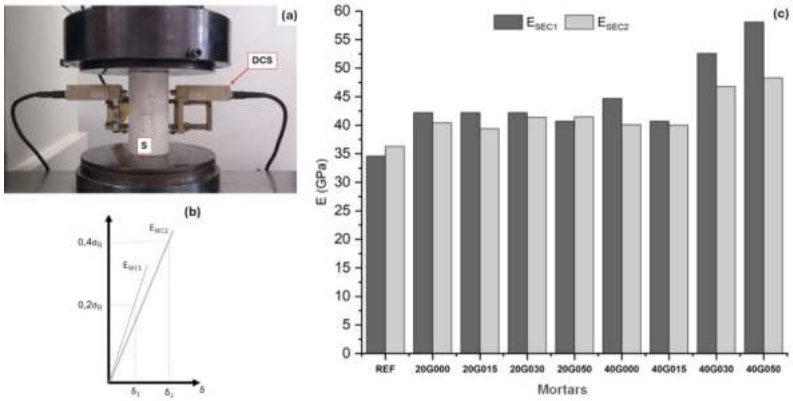

Figure 2: (a) Apparatus to obtain Young´s Modulus (S- sample; DCS – Data collection system); (b) Stress-strain curve; (c) Secant Modulus values.

Band Tuned Enhanced Photodetection in 2D $CuInP_2Se_6$ Interfaced Silicene for NIR photodetectors

Amutha Subramani, Luxa Jan, Kalyan Jyoti Sarkar, Sedmidubsky David, * and Zdeněk Sofer*
The University of Chemistry and Technology, Technická 5, 160 00 Praha 6-Dejvice
subramaa@vscht.cz

Abstract

Photodetectors used in current electronic devices to convert optical impulses into electrical signals, have recently been explored for NIR variations [1-2]. Combination of unique narrow-bandgap electronic and optical properties, along with van der Waals (vdW) surface in 2D materials makes them valuable for advancing the capabilities of non-linear near-infrared (NIR) photodetectors. Emerging 2D van der Waals materials have gained additional interest to develop devices with an improved performance, paving the way for innovations in optoelectronics and information technologies. Here, we use first-principles calculations to examine the structural, electronic, and vibrational features of the as-synthesized 2D non-centrosymmetric van der Waals material, $CuInP_2Se_6$. The study comprehensively investigates various phases, encompassing 2D bulk paraelectric, ferroelectric, and paraelectric monolayer configurations of $CuInP_2Se_6$. Notably, the narrow energy band spectra of $CuInP_2Se_6$ exhibit tunability through phase transitions and layer thickness. The results imply that the paraelectric monolayer phase not only displays a notable response in second harmonic generation (SHG) but also demonstrates lower thermal conductivity, suggesting promising applications in nonlinear optics. Near-infrared silicon photodetectors based on two-dimensional paraelectric monolayer $CuInP_2Se_6$ material with suitable interfacial encapsulation layer is relatively a new design. Furthermore, ab-initio simulations of monolayer silicene demonstrated the appearance of linear band dispersion in planar and low buckling structures of silicene that was stable [3], used here as an encapsulating layer. The designed Au/ $CuInP_2Se_6$/Silicene/SiO_2 photodevice for NIR applications exhibited a significant increase in photoconductive gain due to highly efficient pathway for photocarriers as well as an interfacial encapsulation layer. The optoelectronic device studied using a finite element method had a maximum photoresponsivity of 0.23 A/W at 760 nm. This research reveals the potential to revolutionize integrated nano NIR optoelectronic devices, leading the way for future developments.

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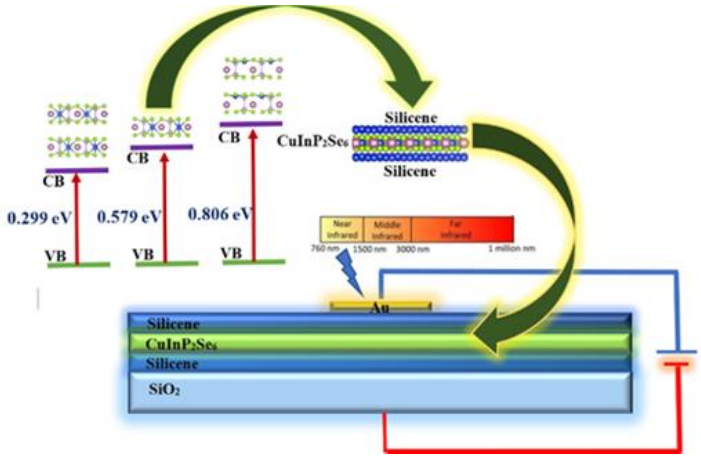

Figure 1: Schematics of the NIR Photodetector employing silicene, $CuInP_2Se_6$, and SiO_2

Enhancing the Performance of Double Perovskite Cathode for Protonic Ceramic Fuel Cells with Mo-doping

Wenkai Yang, Timileyin Aworinde, Lakshya Mathur, Lourdes Vega, Sivaprakash Sengodan
Research and Innovation Center on CO2 and Hydrogen (RICH), Khalifa University, Abu Dhabi, UAE
100050023@ku.ac.ae

Abstract

Protonic ceramic fuel cells have attracted more interest than solid oxide fuel cells due to their potential to be operated at lower temperatures and therefore address the limitation for SOFC commercialization. Double perovskite materials with triple conductivity such as $PrBa_{0.5}Sr_{0.5}Co_{1.5}Fe_{0.5}O_{5+\delta}$ (PBSCF) has demonstrated outstanding performance as cathode in PCFCs [1]. Recent studies have identified high valence Molybdenum (Mo) doping as an effective strategy in increasing the surface oxygen reduction activity and reducing thermal expansion coefficient [2]. Here we enhance cathode performance by incorporating Mo into PBSCF and synthesized $PBSCFM_x$ (x = 0, 0.01, 0.03, 0.05). Results indicate that Mo-doping increases the formation of oxygen vacancies, which facilitates oxygen ion mobility. Furthermore, Mo-doping increase adsorbed oxygen which suggests more oxygen-active sites formed and the catalytic activity enhanced. Last but not least, Mo doping reduced polarization resistance of cathode, suggesting that it facilitates better charge transfer and ion mobility, leading to more efficient oxygen reduction reaction. PBSCFM01 exhibits the best performance among these three materials, which makes it promising candidate for cathode in PCFCs.

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Study of charge transport mechanisms in 2D/3D junctions

R. Yatskiv, S. Tiagulskyi, O. Černohorský, J. Grym
Institute of Photonics and Electronics, Czech Academy of Sciences, Chaberská 1014/57, Praha, Czech Republic.
yatskiv@ufe.cz

Abstract

Unique properties of graphene-semiconductor junctions offer a great opportunity to investigate new fundamental phenomena taking place at the interface between a two-dimensional (2D) semimetal and a three-dimensional (3D) bulk semiconductor and make this junction extremely attractive for a new generation of graphene-based devices. One of the key issues in these junctions is to understand the charge transport mechanisms. In this work [1-3], we focus on a systematic analysis of charge transport mechanisms in the junctions formed by a 3D oxide semiconductor (Ga_2O_3 and ZnO) and 2D graphene. We further attempt to deeply understand how the interaction between graphene and different crystallographic planes of oxide semiconductors affect the charge transport.

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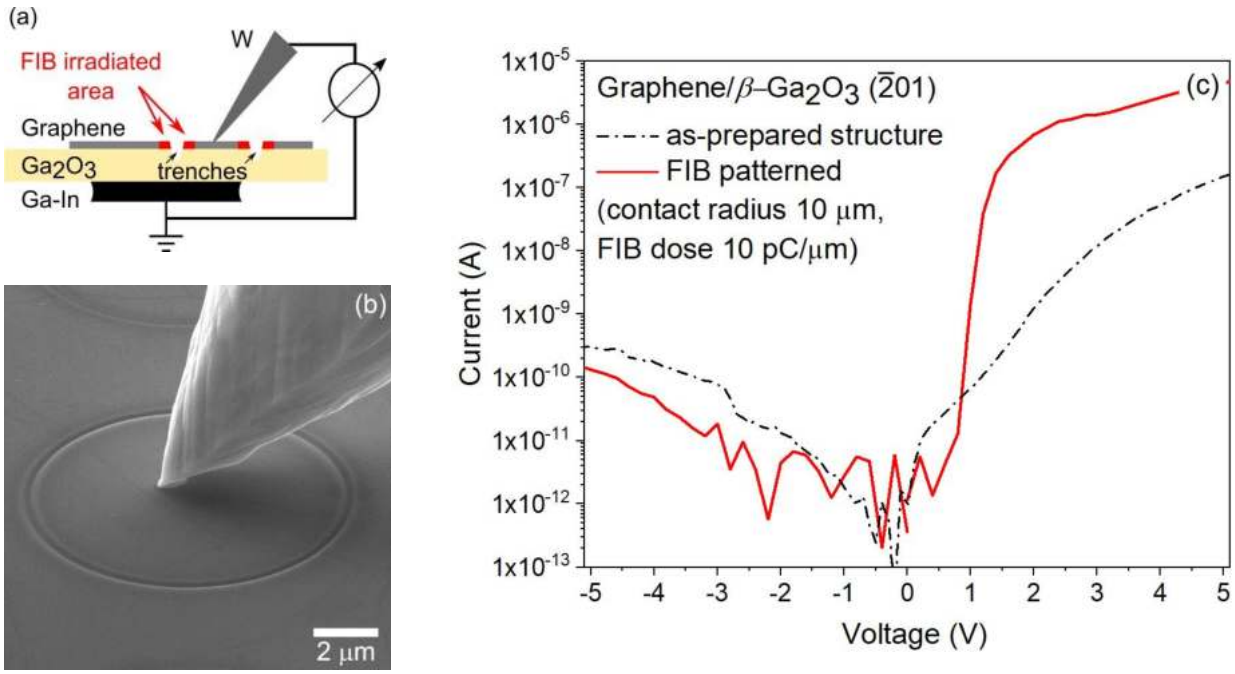

Figure 1: (a) The cross-sectional view of the graphene/β-Ga_2O_3 structure under the in-situ SEM I-V characterisation. The graphene surface is contacted by the W tip of nanomanipulator and β-Ga_2O_3 is grounded via the In-Ga bottom contact. The circular trench was milled by the focused Ga^+ ion beam; (b) An SEM image of the nanomanipulator needle contacting the graphene surface carved by FIB milling; (c) I-V characteristics of the as-prepared and the FIB-patterned graphene/β-Ga_2O_3 structures on the ($\bar{2}01$) surfaces of β-Ga_2O_3 substrates.

Viscoelastic Behaviour of Freestanding Cellular Lattices Made of $Ti_3C_2T_x$ MXene

Abdallah Kamal, Baosong Li, Abdullah Solayman, Lianxi Zheng and Kin Liao
Khalifa University of Science and Technology, 127788, Abu Dhabi, UAE.
100062640@ku.ac.ae

Two-dimensional (2D) materials, such as graphene and MXenes, exhibit multifunctionality due to their wide range of outstanding properties. Thus, they represent appropriate solutions for many technological challenges [1]. Investigating the various properties of such materials in various freestanding three-dimensional (3D) architectures is essential. The mechanical properties of rGO lattices showed high sensitivity toward the relative density, lattice's architectures, and the number of unit cells [2]. Similarly, gyroidal cellular lattices made of $Ti_3C_2T_x$ MXenes exhibit ultrasensitive micromechanical sensing applications [3]. High sensitivity (139 Pa-1) was achieved by refining the dip coating process which makes it an appropriate candidate for multifunctional application. Additive manufacturing (AM) of customized architecture, made of freestanding 2D materials, showed a high capability to acquire preferable properties [4]. Accordingly, investigating the mechanical performance and viscoelastic behaviour of such lattices is of interest. Additionally, optimizing the structural parameters to get robust lattices for multifunctional applications is crucial.

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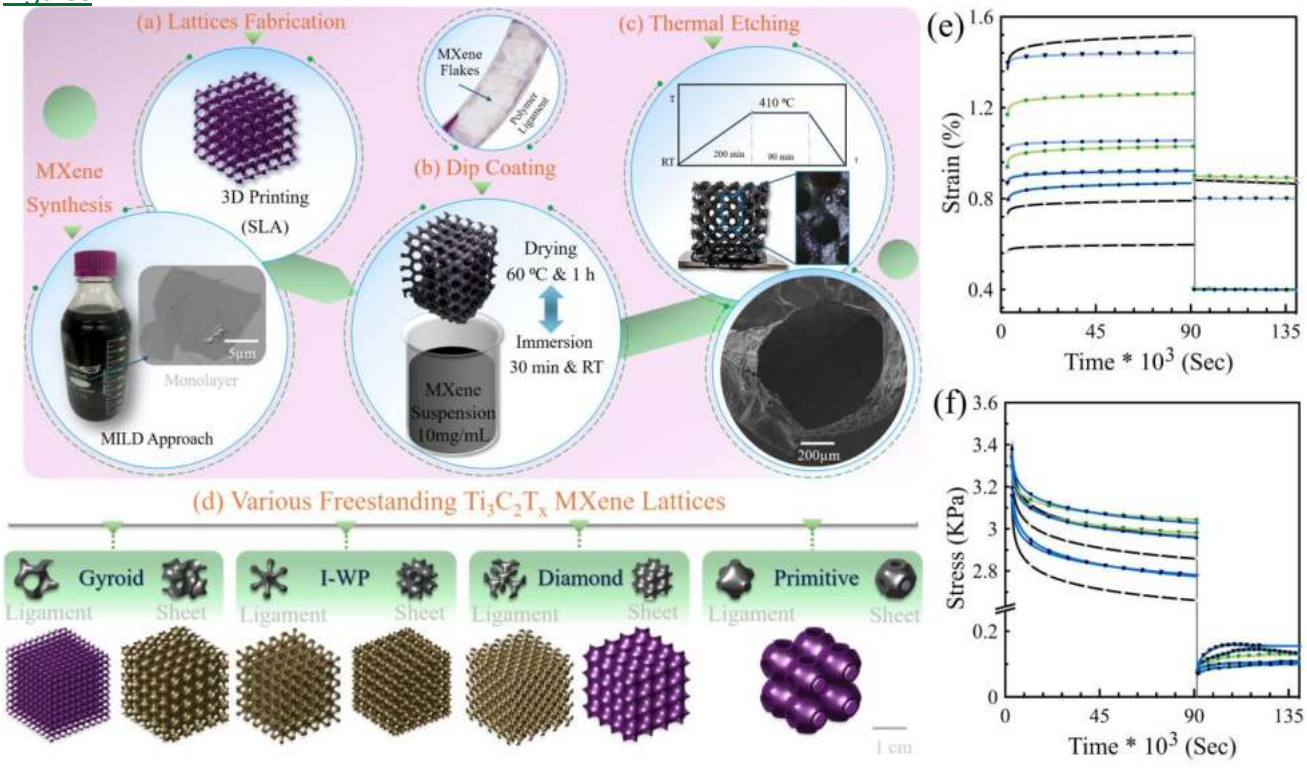

Figure 1: Fabrication of free-standing MXene lattices via dip-coating approach, starting by (a) Fabrication of the castable wax scaffolds then, (b) Dip coating in MXene suspension, and (c) Thermal etching. (d) Images of the fabricated MXene Lattices with various architectures. (e) Creep behaviour, and (f) Stress relaxation curves of MXene lattices.

Processing and applications of MXenes at the MXene Innovations Lab (MIL)

Faisal Shahzad, Hassan A. Arafat
Research and Innovation Center for Graphene and 2D Materials (RIC2D), Khalifa University, Abu Dhabi, United Arab Emirates
faisal.shahzad@ku.ac.ae

Abstract

The MXene Innovation Lab at RIC2D, Khalifa University is at the forefront of advancing MXene-based technologies through innovative synthesis, processing, and application development. Our multidisciplinary research explores the versatile potential of MXenes in areas such as water remediation, biosensing, electromagnetic interference (EMI) shielding, energy storage, and energy conversion. By tailoring the chemical composition and surface functionalization of MXenes, we engineer novel hybrid structures with enhanced properties. We process MXenes into films, composites, fibers, and inks, enabling their integration into diverse platforms. Our pioneering efforts in high-resolution printing methods aim to revolutionize flexible electronics, establishing a foundation for next-generation devices and sustainable technologies [1-5].

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Figure

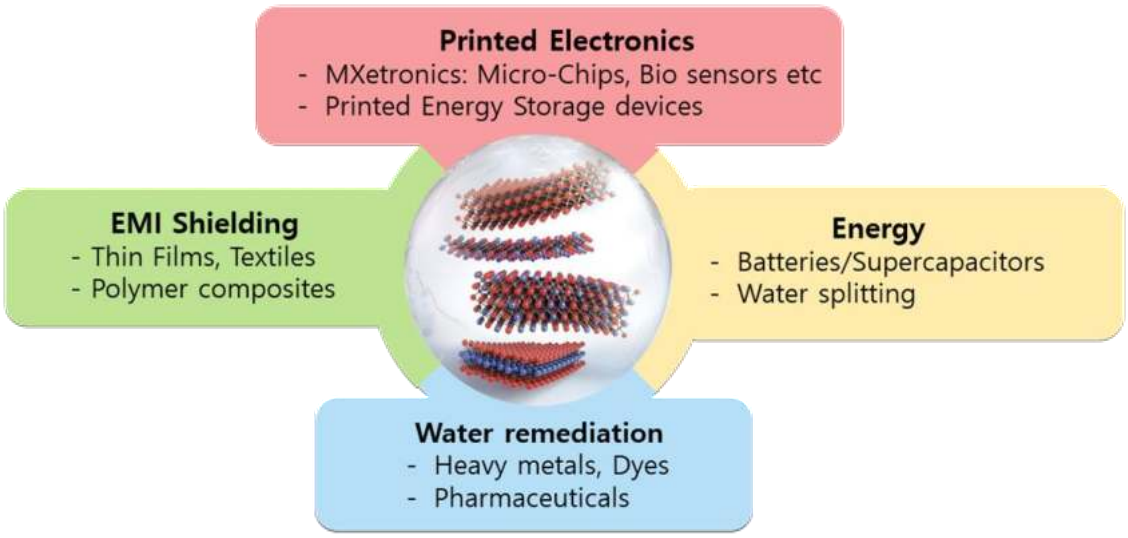

Figure 1: Processing and applications of MXenes

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