## Nano and 2D Materials

## Room Naupaka Salon 4 - Session NM1-TuE

### Synthesis and Manipulation

**Moderator: Sarah Burke**, University of British Columbia

6:00pm **NM1-TuE-2 Using a Zeolite Imidazolate Framework-8 Nanomaterial for Adsorption and Removal of Thymol from Water and Heparin Recovery**, ***Deepak Ganta,*** Texas A&M International University*; Mahmood Karimi Abdolmaleki,* Texas A&M University-Corpus Christi*; Sergio Gonzalez Torres,* Texas A&M International University*; Carlos Velazquez,* Texas A &M International University

There is a strong demand for multiplex sensing and storage capabilities from nanomaterial-based biosensors. To address the limitations in the adsorption capacity of existing materials, porous zeolite imidazolate framework-8 (ZIF-8) 3D nanomaterial, with a larger surface area, was chosen to absorb and remove thymol from water. The experimental adsorption measurement results agree well with theoretical Langmuir and Freundlich isotherm models. The maximum adsorption capacity of thymol on ZIF-8 was determined to be 454.6 mg/g. Furthermore, we also demonstrated the potential of ZIF-8 in recovering heparin from porcine intestinal mucosa. A recovery of 37 mg/g of heparin was reported and verified through kinetic and thermodynamic adsorption models, along with the appropriate surface conditions for the adsorption of heparin molecules. All the characterization methods will be presented.

6:20pm **NM1-TuE-3 Interaction of Defects on Mxene Surfaces: Nonlinear and Anisotropic Effects***, **Steven Goldy***, Colorado School of Mines, USA*; Garritt Tucker,* Baylor University*; Cristian Ciobanu,* Colorado School of Mines, USA

Defects in two-dimensional (2D) materials like hexagonal boron nitride (hBN) and MXene can drastically change mechanical, electronic, and optical properties. Furthermore, surface defects specifically affect the electrocatalytic performance of the material, and their understanding and control can lead to novel materials for catalysis, photocatalysis, and gas sensing. From a fundamental standpoint, understanding the surface-mediated interactions between defects provides insight into their spatial distribution and can serve as a way to control catalytic, sensing, and transport properties. Based on molecular statics simulations, we have developed an approach to extract the formation and interaction energy of vacancies on 2D (hBN) and quasi-2D (MXene, MoS2) materials. We have found that the interaction of defects on 2D and quasi-2D materials shows significant anisotropy, as well as marked departures from the well-used inverse cube distance-dependence associated with linear elasticity. The divergence from linear elasticity is more apparent in MXenes due to their complex, thickness-dependent scaling behaviors and out of plane displacement. Due to highly variable surface chemistries, understanding surface defects on MXenes is critical to their application. These scaling laws inform defect separation distributions that assist in design on 2D composites and catalytic applications.

6:40pm **NM1-TuE-4 Synthesis of Uniform Borophene: In Situ Spectroscopic Analysis and Ex Situ Macroscopic Transfer***, **Marko Kralj,*** *Sherif Kamal, Borna Radatovic, Valentino Jadrisko, Dino Novko, Natasa Vujicic, Marin Petrovic,* Center for Advanced Laser Techniques, Institute of Physics, Croatia

Borophene (Bo), a recently realized polymorphic monoelemental two-dimensional (2D) material, holds promise for diverse applications, including metal-ion batteries, supercapacitors, hydrogen storage, gas sensors, and freshwater production. We present a study of Bo fabricated via segregation-assisted chemical vapor deposition (CVD) epitaxy, where an Ir(111) substrate was exposed to borazine vapors in ultra-high vacuum (UHV) at elevated temperatures. This process yielded structurally uniform and high-coverage χ6 polymorph of Bo, as evidenced by electron diffraction and scanning probe microscopies. Such Bo samples were further subjected to extensive spectroscopic analysis and post-synthesis manipulation, both of which are scarce due to experimental challenges posed by sample inhomogeneity and significant chemical reactivity of epitaxial Bo systems.

In the first part of this talk, we characterize Bo on Ir(111) (Bo/Ir), focusing on electronic properties influenced by the nanoscopic modulation of the Bo sheet. X-ray photoelectron spectroscopy (XPS) and scanning tunneling spectroscopy (STS) data reveal inhomogeneous binding of Bo to Ir, creating a stripe-like structure. This structure acts as a one-dimensional (1D) grating, causing Umklapp scattering of photoelectrons detected in ARPES experiments [1]. Density functional theory (DFT) calculations support our findings, providing insights into the pristine electronic structure of Bo, unaffected by the Ir substrate.

In the second part, the challenges of developing large-area Bo applications are addressed. We demonstrate large-area growth followed by electrochemical transfer of macroscopic single-layer Bo sheets from the growth substrate to a target Si wafer [2]. Our results show that deterministic manipulation of Bo layers is feasible despite their inherent chemical and mechanical instability, advancing Bo research and utilization. Post-transfer Bo displayed minimal mechanical defects, such as cracks and holes, mostly inherited from the synthesis substrate. Successful Bo transfer was further confirmed by Raman spectroscopy, which showed very good overlap of Raman peaks before and after the transfer, indicating preservation of Bo's original crystal structure.

References:

[1] ACS Appl. Mater. Interfaces 14 (2022) 21727–21737

[2] ACS Appl. Mater. Interfaces 15 (2023) 57890–57900

7:00pm **NM1-TuE-5 Design at Nanoscale of Thermostable Hybrid Sol-Gel Bondlayer to Functionalize Aeronautical CFRP by Thermal Spray***, **Sophie Senani-de Monredon,*** SAFRAN TECH, France*; Laurence Rozes,* Sorbonne Université, France*; Guillaume Penvern,* SAFRAN TECH, Sorbonne Univ., France*; Aurélien Joulia,* SAFRAN TECH, France*; Simon Bonebeau,* SAFIR, France

Composite Fibers Reinforced Parts (CFRP) are widely used in aeronautic since more than 40 years to contribute to decrease the aircrafts environmental footprint. Indeed $CO_2$ and NOx emissions have been considerably decreased by lightweighting correlated to significate fuel consumption reduction (15% for last LEAP aircraft engines). Nevertheless to go further and reach the new ambitious target of 20% reduction for the next aircraft engine, functionalization and metallization of CFRP is mandatory to extend them to more aggressive use cases than fuselage, by resistance against high temperature, erosion or icing. To reach this goal, thermal spray coatings are widely studied, even if it remains very complex to implement.

Metallization of CFRP, especially by coldspray is favored by numerous teams [1,2,3], with interesting results but not sufficient to fit performance required for aeronautic qualification. Our approach aims to design a thermostable sol-gel hybrid bondcoat. We will discuss how we succeed to control of the chemical composition, the nanostructuration of this bondlayer and the nature of the substrate/bondlayer/topcoat interfaces to influence the thermomechanical bondcoat's properties and thus the building and the thickness increase of the thermal sprayed topcoat layer linked to the adhesion of the stack. Understanding the relation between nanostructuration of the hybrid sol-gel layer and their mechanical and thermal properties is essential to optimize the whole system. Finally, this will widely open the variety of materials (from metals to oxydes) reachable to functionalize CFRP part and allow new use cases unthinkable up to now.

**References**

*1*- Cold spray of metal-polymer composite coatings onto carbon fiber-reinforced polymer (CFRP). V. Bortolussi, F. Borit, A. Chesnaud, M. Jeandin, M. Faessel, *et al*. International Thermal Spray Conference 2016 (ITSC 2016)., DVS, May 2016, Shanghai, China. p.7 - hal-01337696

*2*-Metallization of polymers by cold spraying with low melting point powders [https://scholar.google.com/scholar?oi=bibs&cluster=18020247034159663012&btnI=1&hl=fr]. H Che, AC Liberati, X Chu, M Chen, A Nobari, P. Vo, S. Yue, Surface and Coatings Technology, 2021, 418, p 127229

3- CO3 Project– F. Delloro et al (https://www.projectco3.eu/fr/ )

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