2D Materials

Room 304 - Session 2D-ThM

2D Materials Devices and Applications

Moderators: Dr. Kai Xiao, Oak Ridge Natinal Laboratory, **Huamin Li**, University at Buffalo

8:00am **2D-ThM-1 Morphology and Adhesion of Carbon Nanowalls Grown via Microwave Surface Wave Plasma on Various Substrates**, ***Parker Hays,*** *Dhruval Patel, Dren Qerimi,* University of Illinois at Urbana-Champaign*; Michael Stowell,* Lyten*; David Ruzic,* University of Illinois at Urbana-Champaign

Carbon nanowalls (CNWs) have a wide range of applications in energy storage, sensing, and other technologies due to their high surface area, electrical conductivity, and mechanical strength. However, their deposition remains challenging, particularly on substrates such as aluminum where adhesion is poor, limiting their integration into practical devices.

In this work, a microwave surface wave plasma (MSWP) is used to deposit CNWs on aluminum, copper, and silicon substrates. Growth is performed via plasma-enhanced chemical vapor deposition (PECVD), using methane and hydrogen as precursor gases and argon to enhance plasma ionization. The high-density microwave plasma promotes methane dissociation into reactive carbon species, while hydrogen radicals preferentially etch amorphous or sp^3-bonded carbon. A heated sample stage is employed to promote surface mobility and favor growth pathways associated with nanowall formation.

CNWs are grown while varying experimental parameters, including gas composition, pressure, and substrate temperature. Resulting CNW morphology is characterized using scanning electron microscopy (SEM) and Raman spectroscopy, while adhesion is evaluated via triboindentation. Aluminum is expected to exhibit significantly lower adhesion compared to copper and silicon, motivating future efforts to incorporate adhesive interlayers for improved film stability. These results provide insight into substrate-dependent growth mechanisms and inform strategies for improving CNW adhesion in device-relevant systems.

8:15am **2D-ThM-2 Orientation-Independent Strong TERS Response in Anisotropic ReS_2 on Gold**, ***Andrey Krayev,*** HORIBA Instruments Incorporated*; Pavel Valencia-Acuna, Oliva Primera-Pedrozo, Chih-Feng Wang,* PNNL

Rhenium disulfide (ReS_2) crystallizes in a distorted 1T‘ lattice with triclinic symmetry arising from Re–Re dimerization, which produces in-plane anisotropic properties and a dense set of Raman-active modes with mixed atomic displacements. Prior conventional Raman microscopy studies in this material showed strong dependence of absolute and relative intensities of some Raman bands on the mutual orientation of the optical electric field and the in-plane crystalline axii. In presented study we show strongly enhanced (at least 10 times over the far field background) tip enahnced Raman scattering (TERS) response from 1-4 L ReS_2 on gold which not only enables high spatial resolution in the TERS maps, but also remains to great extent indifferent to the in-plane orientation of the ReS_2 crystals. We attribute this orientation indifference to the fact that in the gap mode TERS configuration optical electric field is normal to the crystal plane. Additionally, we demonstrate in our TERS spectra presence of low frequency bands the spectral position of which correlates with the local crystal layer number and matches very well previously published conventional Raman data which allows a straightforward nanospectroscopic assessment of the layer number even in sub-micron sized crystals.

8:30am **2D-ThM-3 Optical properties of 2D chiral perovskite thin films (R-MPA)2PbI4 and (R-BrPEA)2Pb2I4 from near infrared to Ultraviolet**, ***Suresh Chaulagain,*** The University of Toledo, USA*; Tingting Zhu, Zhaoning Song, Nikolas J. Podraza,* The University of Toledo

Two-dimensional (2D) chiral perovskites have drawn significant attention due to promising optoelectronic properties like tunable bandgap, high absorption coefficients, robust quantum confinement effects, circular dichroism, and prolonged environmental stability. 2D chiral perovskites are anticipated to exhibit the benefits of both lead halide-based perovskites and chiral materials. These attributes of 2D chiral perovskites make them suitable for light-emitting diodes, photovoltaics, photonic lasers, and circularly polarized light detection. Despite a wide range of potential applications, limited studies have been conducted on the optical properties of 2D chiral perovskites. In this work, we studied the optical properties of $(R\text{-}MPA)_2PbI_4$ and $(R\text{-}BrPEA)_2Pb_2I_4$ perovskite thin films on soda lime glass (SLG), single crystal (100) oriented $SrTiO_3$, and in a stack suitable for electrical characterization using spectroscopic ellipsometry to extract and compare their complex dielectric function spectra, band-to-band critical point transitions, and bandgap energies.Optical response of 2D chiral perovskite $(R\text{-}MPA)_2PbI_4$ and $(R\text{-}BrPEA)_2Pb_2I_4$ thin films have been extracted in the form of complex dielectric function ($e = e_1 + ie_2$) spectra and compared over the photon energy range from 0.73 to 5.89 eV. For the $(R\text{-}MPA_2PbI_4$ thin film, seven direct critical points are identified at 2.462, 2.541, 2.782, 2.83, 3.44, 4.12, and 5.69 eV, with their dimensionalities from critical point analysis. For the $(R\text{-}BrPEA)_2Pb_2I_4$ thin film, seven critical points are determined at 2.49, 2.638, 2.690. 3.15, 3.79, 4.17, and 5.86 eV with their dimensionalities from critical point analysis. The direct bandgaps for $(R\text{-}MPA)_2PbI_4$ and $(R\text{-}BrPEA)_2Pb_2I_4$ thin films are determined from Tauc plots to be 2.4323 ± 0.0003 and 2.453 ± 0.001 eV, respectively.

Acknowledgement

Public Affairs release approval #_____.

8:45am **2D-ThM-4 Molecular Dynamics Simulation of Plasma-Surface Interactions for Transition Metal Dichalcogenides**, ***Jaehong Kwon,*** Princeton University, Republic of Korea*; Jeremy Mettler, Vincent Donnelly,* University of Houston*; David Graves,* Princeton University

Transition metal dichalcogenide (TMD) semiconductors such as WS_2 are enabling a variety of new 2D devices that serve as complementary building blocks for alleviating challenges in silicon integrated circuits (ICs), owing to their atomically thin geometry, layer-tunable bandgap, and dangling-bond-free interfaces [1]. Because the electronic structure of TMDs is strongly thickness-dependent [2], device performance hinges on atomic-precision control of layer count. Plasma atomic layer etching (ALE), in which alternating O_2 and BCl_3 plasma steps thin the film one monolayer at a time, is a candidate process. To understand the atomistic mechanism of the O_2 modification step, we combine experiment and molecular dynamics (MD) simulation. In the experiments, WS_2 samples are exposed to a 20% O_2/Ar inductively coupled plasma, and the resulting surface chemistry is characterized by in-vacuum X-ray photoelectron spectroscopy (XPS).

To create an MD potential tailored to plasma–surface interactions on WS_2, we fine-tune the Universal Models for Atoms (UMA), a graph neural network (GNN)-based foundation machine-learning interatomic potential (MLIP) recently released by Meta FAIR [3]. Although GNN-based MLIPs incur higher computational cost than other MLIP architectures, they often deliver higher accuracy and accommodate additional element types without modification [4]. After fine-tuning, UMA reaches near-DFT accuracy on the W–S–O system (energy MAE ~5 meV/atom, force MAE ~80 meV/Å). Simulating 15 eV O_2^+ exposure of WS_2 at cumulative doses up to ~20×10^{15} cm^{-2}, we observe layer-selective modification: the topmost layer takes up chemisorbed oxygen, while physisorbed molecular O_2 and sulfur-containing species (in the form of SO_x) accumulate between the layers, and the layer immediately beneath shows only minor modification. The simulated dose-dependent oxygen uptake reproduces the trend measured experimentally by XPS. These results provide an atomistic baseline for the self-limiting selectivity needed in WS_2 plasma ALE and a template for applying GNN-based foundation MLIPs to other plasma–surface interaction problems.

References

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9:00am **2D-ThM-5 Operando SEM Study of WS_2 Growth**, ***Shaoliang Guan,*** *Stephan Hofmann, Jinfeng Yang, Hao Yu,* University of Cambridge, UK

Salt enhanced chemical vapor deposition of WS_2 and related 2D materials is widespread, and while many mechanisms including vapor-liquid-solid (VLS) mediated growth have been suggested, gaining a more detailed understanding remains challenging. We employ operando scanning electron microscopy to resolve the entire process of salt-assisted CVD of WS_2, focusing on a model system of individual, small (<100 μm), sapphire supported sodium tungstate (Na_2WO_4) salt particles. We reveal support interactions that lead a salt particle to develop a lateral halo interface, driven by surface eutectic melting above 630 °C. This halo dictates the salt

wetting as well as Na and W transport, and thus upon gaseous sulfur precursor exposure dominates the spatiotemporal WS_2 nucleation and mono- and multilayer domain expansion kinetics, all of which we can directly track by secondary electron (SE) contrast with a conventional InLens SE detector. Unlike for a conventional VLS mechanism, large (>20 μm) monolayer WS2 formation does not involve the salt droplet directly attached to the growth facets, rather the salt droplet drives WS_2 layer growth in the contiguous halo interface region with a continuous supply of W. We compare this to SiO_2 and NaOH treated sapphire where corrosive surface roughening dictates the salt wetting, and critically discuss our findings in the context of the connected wider literature.

References

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2. Hofmann, et al. *Nat. Mater*. 2008, 7(5), 372-375.

9:15am **2D-ThM-6 *in-situ* Characterization of Thermal Atomic Layer Deposition Process for Extrinsic P-Type MoS_2 Thin Films***, Sungjoon Kim, Jeffrey Elam,* Argonne National Laboratory

Computational energy consumption is increasing exponentially, making energy-efficient microelectronics and computing an urgent need. Three-dimensional integrated circuits (3D ICs) and neuromorphic computing promise to revolutionize information technology by drastically reducing the energy consumption of computers, and two-dimensional (2D) semiconductors like molybdenum disulfide (MoS_2) can enable such technologies. However, the development of complementary p-type MoS_2 is needed to fully leverage the benefits of 2D semiconductors. Moreover, thermal processes for thin film deposition are preferred over plasma-based techniques in high aspect ratio applications such as vertical gate-all-around transistors and 3D NAND.Here, we demonstrate the uniform and controlled deposition of extrinsically doped p-type MoS_2 using thermal atomic layer deposition (ALD). By varying the dopant cycle ratio, the final MoS_2's resistivity and charge carrier concentration can be precisely tuned. The resulting p-type MoS_2 was characterized using techniques including *in-situ* spectroscopic ellipsometry, *in-situ* FTIR, Raman spectroscopy, X-ray photoelectron spectroscopy, and Hall measurements. This work offers a pathway to deposit p-type 2D materials with tailored material properties.

9:30am **2D-ThM-7 Nanostructured TiS_2@TiO_2 Nanotube Arrays Fabricated by Magnetron Sputtering for Efficient Energy Storage***, Raman Devi,* IIC, Indian institute of technology Roorkee, India*; Ramesh Chandra,* Indian institute of technology Roorkee, India

The development of advanced electrode materials with high surface area, excellent electrical conductivity, and superior electrochemical stability is essential for next-generation energy storage applications. In the present work, anodized TiO_2 nanotube arrays are proposed as a binder-free electrode platform for enhanced energy storage performance. Titanium foil will be anodized to fabricate highly ordered TiO_2 nanotubes with large active surface area and efficient ion transport pathways. Subsequently, a TiS_2 thin film will be deposited over the nanotubular architecture using magnetron sputtering to improve the electrical conductivity and electrochemical activity of the electrode. The hybrid TiO_2 nanotube/TiS_2 structure is expected to combine the structural stability of TiO_2 with the high conductivity and pseudocapacitive behaviours of TiS_2, thereby enhancing charge transfer kinetics and electrolyte accessibility. The synthesized electrodes will be characterized using X-ray diffraction (XRD), field emission scanning electron microscopy (FESEM), and electrochemical techniques including cyclic voltammetry (CV), galvanostatic charge–discharge (GCD), and electrochemical impedance spectroscopy (EIS). The proposed hierarchical nanostructured electrode is anticipated to exhibit improved specific capacitance, rate capability, and cyclic stability, making it a promising candidate for high-performance supercapacitor applications and future energy storage technologies

Keywords: Anodization, TiO_2 nanotube arrays, Magnetron sputtering, Binder-free electrode, Energy Storage

9:45am **2D-ThM-8 Low-Temperature Deposition and Annealing of NbXW1-XSY Thin Films for Photolithography-Compatible Processing***, Gia Rivers,* University of Michigan, Ann Arbor*; Rebecca A. Dawley,* University of Michigan*; Anil Adhikari, Steven J. Koester,* Notre Dame University*; Ageeth Bol,* University of Michigan, Ann Arbor

Two-dimensional transition metal dichalcogenides (2D-TMDs) are promising class of layered materials for next-generation metal-oxide semiconductor field effect transistors (MOSFETs). Tungsten diselenide (WSe_2) is one 2D p-type semiconductor that has generated interest as a channel material for scaled MOSFETs. However, device performance is limited by high contact resistance at the metal/semiconductor interface. Prior work has shown that a plasma-enhanced atomic layer (PEALD) deposited $Nb_xW_{1-x}S_y$ film grown at 300°C can serve as a doped contact interlayer and reduce contact resistance.[1,2] However, the elevated deposition temperature complicates integration with photoresist-based lithographic processing. Here, we report a supercycle PEALD process for $Nb_xW_{1-x}S_y$ deposition at 120°C to improve compatibility with certain photolithography fabrication flows. Initial $Nb_xW_{1-x}S_y$ thin films of a ~10nm thickness were deposited onto SiO_2/Si substrates and characterized using Raman spectroscopy, X-ray photoelectron spectroscopy (XPS, and four-point-probe measurements. Raman and XPS indicate that the as-deposited films are amorphous and sulfur rich, with S/(W+Nb) ≈ 3.5, and exhibit a high sheet resistance of $4.63x10^9$ μΩ*cm. To recover material quality after depositing at low temperatures, we investigate post-deposition annealing at 450°C and 900°C. After optimization of annealing conditions, XPS shows that the films approach more ideal stoichiometry with S/(W+Nb) ≈ 1.9, while Raman indicates improved crystallinity with the emergence of the characteristic A_{1g} and E^1_{2g} modes. Additionally, there is a large reduction in the sheet resistance to $4.88x10^3$ μΩ*cm after 450°C annealing and $3.04x10^3$ μΩ*cm after 900°C annealing. Finally, deposition on PMMA-patterned samples is used to assess process compatibility with resist-patterned device structures, demonstrating the viability of integrating low-temperature PEALD $Nb_xW_{1-x}S_y$ contact interlayers into lithography-based device workflows.

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(2) Schulpen, J. J. P. M.; Lam, C. H. X.; Dawley, R. A.; Li, R.; Jin, L.; Ma, T.; Kessels, W. M. M.; Koester, S. J.; Bol, A. A. Nb Doping and Alloying of 2D WS2 by Atomic Layer Deposition for 2D Transition Metal Dichalcogenide Transistors and HER Electrocatalysts. *ACS Appl. Nano Mater.* **2024**, *7* (7), 7395–7407.

11:00am **2D-ThM-13 Hierarchical Heterostructure of 2D Nicob@Co_3O_4 for Energy Saving Hydrogen Generation***, Krishna Modi, Anand Joshi,* Micro-Nano Research & Development Center, Parul University, India

The development of efficient and low-cost two-dimensional electrocatalysts for hydrogen generation is crucial for clean energy technologies.Herein, the rational engineering of two-dimensional Co_3O_4 and NiCoB heterostructure is studied for the energy-saving hydrogen production coupled with the methanol oxidation reaction. Initially, cobalt oxide (Co_3O_4) nanoflowers are deposited on Ni foam using a facile hydrothermal synthesis approach. Subsequently, NiCoB nanosheets are homogeneously deposited onto Co_3O_4 through a dip-coating-assisted chemical reduction strategy, resulting in the formation of a hierarchical nano-heterostructure. A fabricated nano-heterostructure was characterized using various characterization techniques, such as SEM, elemental mapping, and XPS. The SEM image suggests that the successful growth of NiCoB nanosheets on Co_3O_4 nanoflowers offers hierarchical heterostructure formation. Furthermore, XPS analysis suggests the presence of Ni 2p, Co 2p, B 1s, and O 1s elements. Electrochemical study demonstrates that the as-fabricated Co_3O_4@NiCoB nano-heterostructure exhibits excellent HER and OER performance, achieving an overpotential of 0.247 V vs RHE and 1.52 V vs RHE, respectively, at 100 mA/cm^2. Furthermore, introducing methanol into the electrochemical reaction has resulted in an overpotential of 1.33V at a current density of 100 mA/cm^2. Furthermore, the two-electrode NiCoB/Co_3O_4||NiCoB/Co_3O_4 cell provides a cell voltage of 2.03V for water electrolysis and 1.74 V for methanol-based electrolysis at a current density of 100 mA/cm^2, showing a significant reduction in energy consumption for the hydrogen generation. Additionally, NiCoB/Co_3O_4||NiCoB/Co_3O_4 provides the stability of 80 hrs at a higher current density of 100 mA/cm^2 in the methanol electrolysis configuration, and the formation of value-added formate species is confirmed from the NMR analysis. Overall, this study represents an important development of highly active, stable, and highly conductive metal oxide-metal boride-based nanocomposites for energy-saving hydrogen generation.

11:15am **2D-ThM-14 Hybrid Pd@Graphene Oxide–Magnetite Nanozyme Materials: Design, Properties, and Theranostic Potential***, Davide Patti, Giulia Lacanea, Giuseppe Attinasi, Luisa D'Urso, Giuseppe Forte,* University of Catania, Italy*; Irina Naletova,* National Council of Research, Italy*; **Cristina Satriano**,* University of Catania, Italy

Hybrid nanozyme materials that combine catalytic and functional properties are becoming increasingly interesting for advanced theranostic

applications. In this study, we present the design, synthesis and characterisation of a novel material consisting of palladium–graphene oxide–magnetite (Pd@GO–Fe_3O_4). Palladium nanoparticles were immobilised on graphene oxide sheets decorated with nanomagnetite to yield multifunctional hybrid architectures with combined catalytic, magnetic and biointerfacial properties. The physicochemical characteristics were systematically investigated using UV–visible, XPS, Raman and FTIR spectroscopies, as well as dynamic light scattering, zeta potential measurements, atomic force microscopy and electron microscopy. Nanozyme activity was evaluated through catalytic and light-assisted redox reactions, which revealed the pivotal role of interfacial interactions and Pd dispersion in catalytic performance. Magnetic responsiveness enabled efficient manipulation and recovery, while GO provided structural stability and enhanced surface functionality. Biointerface interactions were assessed in cancer cell models via cytotoxicity and intracellular ROS generation, revealing dose- and structure-dependent responses. Under light irradiation, the hybrid nanozymes exhibited photothermal and photocatalytic activity, demonstrating multimodal functionality. Overall, Pd@GO–Fe_3O_4 nanozyme hybrids represent a versatile nanocatalyst platform with tunable catalytic efficiency and theranostic potential.

11:30am **2D-ThM-15 Taguchi-Based Analysis of Wear Performance in SLA Printed Boron Nitride Composites***, **Swathi Bale**,* Government Engineering College, Hassan, Karnataka, India

This work uses the Taguchi technique to optimize wear behaviour in hexagonal boron nitride-reinforced stereolithography (SLA) composites. Cylindrical wear samples based on the ASTM G99 standard were created utilizing an Anycubic SLA printer and photosensitive resin reinforced with hexagonal boron nitride (h-BN) particles at different weight percentages (0, 0.5, 1.0, and 1.5 wt%). The following process characteristics were taken into account: Material composition (Mc), Build angle (Ba), Post-curing time (Pc), and Lift speed (Ls). Wear experiments were carried out using a pin-on-disc apparatus with a constant load of 10 N, sliding speed of 200 rpm, and sliding distance of 502.72 m/s. Scanning Electron Microscopy and Energy-Dispersive X-ray Spectroscopy (EDAX) were used to assess h-BN particle dispersion for the developed samples. The signal-to-noise (S/N) ratio and analysis of variance (ANOVA) were used to identify the best process parameters and their relative contributions to wear rate. The findings showed that material composition had the greatest impact on wear rate (49.724%), followed by lift speed (27.075%), post-curing time (16.934%), and build angle (6.266%). The morphology of the worn surface was studied by SEM analysis. The ideal combination of parameters for producing the lowest wear rate was found to be 1.5 wt% BN, 90° construction angle, 30 minutes post-curing period, and 15 mm/min lift speed. The outcomes of this work show that the Taguchi technique has the ability to optimize the wear behaviour of h-BN reinforced SLA composites, which can be useful in a variety of applications that need improved tribological features.

11:45am **2D-ThM-16 Advanced Nanostructured Graphene Devices for Real-Time Environmental and Agricultural Sensing***, **RAPTI GHOSH**,* University of Chicago, India

Sustainable agriculture requires continuous monitoring of nutrients and air quality to improve crop growth, reduce fertilizer waste, and increase resource efficiency. However, conventional nutrient analysis methods, such as ICP-MS, ion chromatography, and colorimetric assays, are expensive, laboratory-based, and unsuitable for real-time monitoring. Commercial CO_2 and O_2 sensors also face limitations because they are bulky, costly, and sensitive to humidity. To address these challenges, we propose an integrated platform of advanced printable devices and nanostructured materials for sensing and photonic applications. The system combines plant-derived graphene thin-film transistors (FETs) with curvature-engineered nanostructures for real-time monitoring of macronutrients and greenhouse gases in hydroponic and aeroponic systems. The sensor platform uses eco-friendly graphene ink synthesized from plant-derived carbon materials. The devices are fabricated using scalable inkjet or aerosol-jet printing to produce flexible and low-cost FET sensor arrays. The graphene channels are functionalized with selective receptors, such as ferritin for phosphate sensing and amine-containing molecules for CO_2 detection. These functional layers enable selective sensing through charge-transfer interactions at the transistor surface. In addition, curvature-engineered 2D heterostructures improve surface reactivity and electronic properties, enabling ultrasensitive detection of contaminants. This work integrates advanced materials, nanoelectronics, and intelligent sensing into a single multifunctional platform. The proposed system provides a scalable and sustainable approach for autonomous environmental monitoring, precision nutrient mapping, and next-generation smart agriculture technologies.

12:00pm **2D-ThM-17 Xenon Trapping in Two-Dimensional Silicate Nanocages under Air-Containing Gas Environments***, **Laiba Bilal**,* XenCage Technologies

Previous studies demonstrated that plasma-assisted ionization enables xenon trapping within two-dimensional silicate nanocages supported on metal powders. These investigations established the feasibility of noble gas confinement in scalable nanocage materials under controlled xenon environments. An important remaining question is whether xenon trapping can be maintained in the presence of atmospheric species introduced through air-containing gas mixtures.

In this work, we investigate xenon trapping in silicate nanocage powders exposed to xenon-air gas mixtures under near-ambient-pressure conditions. Silicate nanocages supported on transition metal powders were exposed to plasma-activated xenon in the presence of air and subsequently characterized using ambient-pressure and ultra-high-vacuum X-ray photoelectron spectroscopy. The experiments were designed to evaluate the influence of air-containing gas environments on xenon trapping and retention within the nanocage structure.

Preliminary results reveal clear Xe photoemission features following exposure and evacuation, indicating successful xenon trapping despite the presence of atmospheric gas components. These observations suggest that the confinement mechanism remains active in mixed-gas environments and that competing species do not completely suppress noble gas trapping under the investigated conditions. Ongoing analysis is focused on quantifying trapping behavior and evaluating the influence of gas composition on noble gas retention.

This work extends previous studies of noble gas trapping in two-dimensional silicate nanocages and provides new insight into trapping behavior under mixed-gas conditions. The results support future investigations of xenon and krypton capture, retention, and recovery in nanocage-based materials relevant to isotope production, nuclear technologies, and environmental applications.

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