Monday Morning, October 25, 2021

Live Session
Room Live - Session LI-MoM

AVS Plenary & Awards Session

Moderators: Timothy Gessert, Gessert Consulting, Dan Killelea, Loyola University Chicago, Amy Walker, University of Texas at Dallas

10:00am **LI-MoM-1 Welcome from the AVS President**, *Susan Burkett*, University of Alabama
Welcome to the AVS 67 Virtual Symposium! We hope you will enjoy our Exciting Live and On Demand Sessions this week!

10:05am **LI-MoM-2 Welcome from the AVS 67 Program Chair**, *Dan Killelea*, Loyola University Chicago
Welcome to the AVS 67 Virtual Symposium. I will review the structure of this week's program. We hope you will enjoy the event!

10:15am **LI-MoM-4 AVS Plenary Lecture: Pump-Probe Experiments with Neutral Matter: A New Approach to the Kinetics of Surface Reactions**, *Alec M. Wodtke,* Georg-August University of Göttingen and The Max Planck Institute for Biophysical Chemistry, Germany **INVITED**
Knowledge of the rates of elementary gas phase reactions has contributed decisively to our understanding of important societal problems, for example stratospheric ozone chemistry. Growing our knowledge of rates of elementary chemical reactions at surfaces is crucially important to improving heterogeneous catalysis. In comparison to gas phase reactions, there are surprisingly few known activation energies of elementary surface reactions, nor knowledge of the energies and entropies of the reactions' transition states. This situation is a result of limitations on our methods for measuring rate constants of elementary surface reactions. Furthermore, first principles theories to predict surface reaction rates remain largely un-validated. In this talk, I will present recent experimental advances yielding the rates of elementary reactions at surfaces, which rely on a stroboscopic pump-probe concept designed for neutral matter. This method is also capable of revealing surface-site-specific kinetics information. Not only is site specific reactivity an essential aspect of surface reaction mechanisms, it is essential to provide benchmarks for testing first principles methods for calculating reaction rates, another potentially powerful tool with which to investigate heterogeneous catalysis.

11:00am **LI-MoM-13 2021 Dorothy M. and Earl S. Hoffman Award Scholarship Talk: Formation and Stability of Oxygen Structures on Ag(111) Surfaces**, *Marie Turano*[1], Loyola University Chicago*; L. Juurlink,* Leiden University, The Netherlands*; E. Jamka, M. Gillum, D. Killelea,* Loyola University Chicago
We have studied oxidized Ag(111) surfaces after exposure to gas-phase O atoms using a combination of surface science techniques to determine the resultant surface structure. The total oxygen incorporation was determined with temperature programmed desorption (TPD) and the surface structures were determined with low energy electron diffraction (LEED) and scanning tunneling microscopy (STM). A long-standing challenge in the study of heterogeneously catalyzed oxidation reactions on silver surfaces is the determination of what surface species are of greatest chemical importance. This is due to the coexistence of several different oxygen reconstructions on oxidized silver surfaces. A further complication is subsurface oxygen (Osub) or O atoms dissolved into the near surface region of a metal, which alters the surface structure and reactivity of the metal. However, the effects of Osub have yet to be well characterized. Using a curved Ag(111) single crystal with two step types, we investigated the influence of terrace width and step geometry on oxidation and reconstruction formation on a well characterized Ag surface. Upon exposure of a curved Ag(111) crystal to gas-phase O atoms at 525 K, we observed a non-uniform oxygen accumulation over the crystal surface. Quantitatively, O desorption was identical to planar Ag(111) as verified by TPD. However, through STM images, we determined that A-type steps massively reconstruct with reconstruction forming at the bottom edge of steps and spreading outward. B-type steps exhibit a different growth mechanism where steps are originally pinned by initial oxidation and thus hinder the formation of reconstruction.

In addition, after oxygen exposures at low temperatures (T = 450 K) resulting in Osub formation, the surface showed the coexistence of a previously characterized stripe structure as well as an amorphous pattern. Annealing this exposure resulted in familiar surface reconstructions implying that the Osub changes the surface structure on curved Ag(111).

Based on these findings, we demonstrate the complexity of the silver surface under oxidizing conditions and the importance of Osub in resultant surface structures.

11:15am **LI-MoM-16 AVS 2021 Graduate Research Award Talk: Molecular Interactions with Frozen Ice Films: Adsorption, Oxidative Reactivity, and Isotopic Enrichment**, *Michelle Brann*[2], *S. Sibener,* University of Chicago
My research seeks to experimentally model surface-mediated processes occurring on icy-dust grains to develop a more complete understanding of the formation of planetary atmospheres, complex organic molecules, and origin of life in the universe. I use a state-of-the-art ultra-high vacuum (UHV) chamber that mimics the low-pressure conditions seen in astrophysical environments with optics for *in-situ* Reflection Absorption Infrared Spectroscopy (RAIRS). This chamber is connected to a molecular beam line that produces reactant gases with highly customizable energies for exposure onto the desired substrate. My goal is to understand how impinging molecules adsorb, react, or diffuse into frozen ice films as this is often a first step for reactions to occur resulting in new organic molecules essential for life. This talk is split into three sub-projects: (1) initial sticking probability of methane on ice films with varying porosities and crystalline structures, (2) oxidative reactivity of frozen propene films, and (3) differential condensation of methane isotopologues. For each study, changes on the surface were monitored in real time with RAIRS and mass spectrometry techniques.

I determined that more methane ended up sticking onto the porous amorphous water films, compared to the crystalline films suggesting that porous are more efficient at dissipating energy. Similarly, when examining propene oxidation, I also found that film structure was important for reactivity. In this case, I identified, through careful analysis of RAIR spectra, that I could form both an ordered as well as an amorphous propene film depending on the deposition temperature; yet, oxygen was only able to react with the ordered propene film. Lastly, I observed preferential increased sticking and condensation for CD_4 on a CH_4 film compared to CH_4, confirming an isotopic enrichment. These results suggest that there is more efficacious gas-surface energy transfer involving multiphoton excitations for the heavier isotopologue. Overall, these results are important to create accurate models of surface mediated astrophysical and terrestrial processes and understand formation of the universe.

11:30am **LI-MoM-19 2021 AVS Russell and Sigurd Varian Award Talk: Chemically Resolving Metal Supported Regioisomeric Assemblies at the Angstrom Scale using Ultrahigh Vacuum Tip-Enhanced Raman Spectroscopy: Conformations & Interactions**, *Sayantan Mahapatra*[3], *J. Schultz, L. Li, N. Jiang,* University of Illinois at Chicago
Conventional spectroscopic techniques are limited by the optical diffraction limit to about half wavelength and therefore offers about 200 nm x 200 nm microscopic zone for working in the visible light range. Tip-enhanced Raman spectroscopy (TERS) emerges as an advanced analytical technique, where the plasmonically active probe is not only used to detect the tunneling current but also to interrogate the local chemical environment of surface adsorbed molecules with angstrom scale precision. In this work, we report a topological and chemical analysis of two regioisomers (positional isomers), trans- and cis-tetrakispentafluorophenylporphodilactone (trans- and cis-H2F20TPPDL) by scanning tunneling microscopy (STM), ultrahigh vacuum (UHV) TERS on Ag(100) with the spatial resolution down to 8 Å, which has wide range of applications in various field of surface science & nanotechnology such as regioselective catalysis reaction, chemical reactions, molecular electronics etc. We have shown, it is possible to distinguish these two structurally very similar forms with high accuracy & precision. The two-component molecular junction has been identified using high resolution two-dimensional (2D) Raman mapping. In addition, the molecule-substrate interactions have been addressed at the single-molecule level by employing three different single-crystals i.e., Ag(100), Cu(100), and Au(100). Strong surface interactions at Cu(100) surface converted the flexible porphodilactone structure inverted, which was further verified by STM. Expanding upon this work, the chemical information available through STM-TERS allows me to track a complete chemical reaction, from reactant to product, with single chemical bond sensitivity. Angstrom scale chemical analysis using TERS is shown here as a broad and versatile technique in surface characterization.

11:45am LI-MoM-22 2021 AVS Graduate Research Award Talk: Investigating Surfaces, Interfaces, and their Impact on Degradation of Polymer Electrolyte Membrane Water Electrolyzers, *Sarah F. Zaccarine*[1], Colorado School of Mines*; M. Shviro,* Forschungszentrum Jülich GmbH, Germany*; M. Dzara,* Colorado School of Mines*; M. Carmo,* Forschungszentrum Jülich GmbH, Germany*; S. Pylypenko,* Colorado School of Mines

Hydrogen is an attractive option for renewable energy applications due to its ability for large quantities to be stored over a long period of time, but current H_2 production from fossil fuels is a major CO_2 emitter; consequently, there is a need for efficient, renewable H_2 production.[1] Polymer electrolyte membrane water electrolysis (PEMWE) is a promising strategy, but major degradation issues and the slow kinetics of the anodic oxygen evolution reaction (OER) limit commercialization. Ir has been shown to be the most active metal towards the OER, while IrO_2 is typically more stable in the harsh oxidizing conditions of this reaction. Both materials face high costs and limited availability, motivating studies of PEM electrolyzers with low loadings.

Commercial Ir and IrO_2 black catalysts were obtained and studied as catalyst powders, fresh membrane electrode assemblies (MEAs), and tested MEAs following durability cycling at different conditions. A variety of surface and bulk characterization techniques were employed to evaluate changes in the catalyst morphology and composition, electrode composition and structure, and various interfaces that exist in this system in order to understand their respective contributions towards degradation. Information about catalyst composition was obtained with surface-sensitive x-ray photoelectron spectroscopy (XPS) and bulk x-ray absorption spectroscopy (XAS). Scanning electron microscopy (SEM) and scanning transmission electron microscopy (STEM) combined with energy-dispersive x-ray spectroscopy (EDS) mapping of the electrode cross-sections were used to elucidate morphological and structural information as well as elemental distribution as a function of various durability conditions. Further, transmission x-ray microscopy (TXM) was used to visualize electrode structure at a larger scale than possible with electron microscopy methods. Results demonstrate that a systematic, multi-scale, multi-technique characterization approach is necessary to isolate contributions of the catalyst, ionomer, and overall CL morphology, composition, and structure on degradation of the PEM electrolyzer. These findings advance fundamental understanding towards development of more efficient electrodes, highlighting the importance of optimizing uniformity of the electrodes.

(1) Ayers, K. E. The Potential of Proton Exchange Membrane–Based Electrolysis Technology. *Curr. Opin. Electrochem.* **2019**, *18*, 9–15.

(2) Spöri, C.; Kwan, J. T. H.; Bonakdarpour, A.; Wilkinson, D. P.; Strasser, P. *Angew. Chemie Int. Ed.* **2017**, *56* (22), 5994–6021.

(3) Alia, S. M.; Stariha, S.; Borup, R. L. *J. Electrochem. Soc.* **2019**, *166* (15), F1164–F1172.

12:15pm LI-MoM-28 AVS 2021 Peter Mark Memorial Award Lecture: Novel MBE Approaches for Atomically Precise Synthesis of "Stubborn" Metal Oxides, *Bharat Jalan*[2], University of Minnesota, USA **INVITED**
Our ability to synthesize atomically-precise materials has continued to drive modern technology and fundamental study. Consider an element that is hard to oxidize and also difficult to evaporate, how do we create an atomically precise thin films of such metals, metal oxides or their heterostructures? This has been a key question in the synthesis science for many decades.

In this talk, I will present my group's effort to address this question. We have recently shown that both the low vapor pressure and difficulty in oxidizing a "stubborn" element can be addressed by using a *solid* metal-organic compound with significantly higher vapor pressure, and with the added benefits of being in a pre-oxidized oxidation state along with excellent thermal and air stability. Using this approach, we show, for the first time, the synthesis of Pt, RuO_2 and $SrRuO_3$ films with the *same ease and control* as afforded by III-V MBE. I will present a detailed MBE growth study combined with structural and transport characterizations. The effect of film thickness, orientation, strain, and defects such as cation vacancies on electronic properties will be discussed. In second part of my talk, I will present our work on the development of radical-based MBE approach for wide band gap alkaline stannates ($BaSnO_3$ and $SrSnO_3$) growth combined with their detailed structure and transport study.

12:45pm LI-MoM-34 2021 AVS Nellie Yeoh Whetten Award Talk:Efficient Near-Infrared Emission from Lead-Free Ytterbium-Doped Cesium Bismuth Halide Perovskite Thin Films, *Minh Tran*[3], *I. Cleveland, G. Pustorino, E. Aydil,* New York University
All-inorganic metal halide perovskites have attracted significant attention for applications as solar cells, light-emitting diodes, and photodetectors because they have strong and tunable absorptions and emissions. Lead-based perovskites have been the focus of many studies because they perform well in these applications, but lead is toxic. Bismuth-based halide perovskites are non-toxic alternatives to widely researched lead-containing halide perovskites for optoelectronics. Cesium bismuth bromide, in particular, may have suitable optical properties, but optical absorption and photoluminescence (PL) data reported to date are contradictory. We resolved these literature discrepancies and showed that $Cs_3Bi_2Br_9$ thin films deposited by physical vapor deposition (PVD) via coevaporation of CsBr and $BiBr_3$ show absorption and emission peaks at 433 and 472 nm, respectively. Peak location and lineshapes of blue-shifted absorption and emission previously reported and attributed to quantum confinement in $Cs_3Bi_2Br_9$ nanocrystals could be reproduced in $BiBr_3$ solutions in different solvents even without any $Cs_3Bi_2Br_9$. This suggests that high photoluminescence quantum yield (PLQY) and blue-shifted emissions reported below 472 nm may be originating from unreacted precursors and impurities in nanocrystal dispersions rather than from $Cs_3Bi_2Br_9$. We also doped $Cs_3Bi_2Br_9$ films with Yb to investigate the possibility of quantum cutting, generation of *two* near-infrared (NIR) photons (1.25 eV) from each ultraviolet or blue photon absorbed at energies >2.5 eV. Coating silicon solar cells with a material that can achieve quantum cutting with PLQY approaching 200% (2 photons for every high energy photon) has the potential to increase the silicon solar cell efficiencies above the Queisser limit, 33%. The addition of Yb that can substitute up to 50% of the Bi in $Cs_3Bi_2Br_9$ leaves the $Cs_3Bi_2Br_9$ structure unchanged and results in NIR $Yb^{3+2}F_{5/2} \rightarrow {}^2F_{7/2}$ emission (1.25 eV) with 14.5% quantum yield. A PLQY of 14.5% from Yb-doped $Cs_3Bi_2Br_9$ is promising because undoped $Cs_3Bi_2Br_9$ is otherwise not emissive due to rapid nonradiative recombination: the highest reliably measured visible PLQY in the literature is only 0.2%. Despite this, energy transfer from $Cs_3Bi_2Br_9$ to Yb appears to compete efficiently with nonradiative recombination and results in a 14.5% quantum yield. Moreover, NIR emission decreases sharply when the perovskite host's bandgap is reduced below 2.5 eV, twice the Yb^{3+} emission energy, by substituting bromine with iodine, raising the possibility that the emission mechanism may involve quantum cutting. This also raises the tantalizing possibility that $Cs_3Bi_2Br_9$ could be a potential lead-free quantum cutting material for solar spectrum shaping to increase solar cell efficiency.

1:00pm LI-MoM-37 AVS 2021 John Thornton Memorial Award Lecture: Oxide MBE Rocks! Reflections on 35⁺ Years of *Oxide* MBE, *Darrell Schlom*[4], Cornell University **INVITED**
Molecular-beam epitaxy (MBE) is the "gold standard" synthesis technique for preparing semiconductor heterostructures with high purity, high mobility, and exquisite control of layer thickness at the atomic-layer level. Its use for the growth of multicomponent oxides got off to a rocky start 36 years ago, but in the ensuing decades, it has become the definitive method for the preparation of oxide heterostructures too, particularly when it is desired to access metastable polymorphs of oxides and the novel properties they possess. In this talk I will highlight a few examples from our* work over the past >30 years demonstrating how the atomic-layer control made possible by oxide MBE can be used to break synthesis rules and create metastable compounds and heterostructures with intreguing properties. Many important growth tricks, first developed for the growth of compound semiconductors by MBE, are equally applicable to the growth of oxides. Examples include the use of strain engineering, interface engineering, epitaxial stabilization, or dimensional confinement. These can be used to transmute oxides that are usually "vegetables" into metastable polymorphs that are ferroelectric, ferromagnetic, both at the same time (multiferroic), or superconducting. A key element of this modern alchemy is the availability of substrates with appropriate structural motifs to strain these complex oxide thin films by several percent—far beyond where they would crack or plastically deform in bulk—or to stabilize metastable polymorphs. I will also discuss some of the technical challenges to the controlled synthesis of oxides in thin film form that have been overcome. The ability of MBE to customize oxide structures with atomic-level control and impart controlled strain have made oxide MBE the technique of choice

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[1] **National Student Award Finalist**
[2] **Peter Mark Memorial Award Winner**
[3] **National Student Award Finalist**
[4] **John A. Thornton Memorial Award Winner**

for precisely preparing epitaxial oxide heterostructures to understand and exploit their novel properties.

*The work reported was performed in collaboration with superb students, postdocs, colleagues, and collaborators from around the world. Although it is only possible to acknowledge a small fraction, I celebrate the achievements being honored by this award with the pioneering contributions of Jim Eckstein and Ivan Bozovic—with whom I began this journey and continue to work—together with the contributions and advice from leading collaborators: Long-Qing Chen, Chang-Beom Eom, Craig J. Fennie, Venkat Gopalan, Stanislav Kamba, Lena F. Kourkoutis, Jeremy Levy, Jochen Mannhart, David A. Muller, Nate Orloff, Xiaoqing Pan, Karin M. Rabe, Ramamoorthy Ramesh, Kyle M. Shen, Dmitri A. Tenne, Susan Trolier-McKinstry, Nicola A. Spaldin, Reinhart Uecker, and Xiaoxing Xi.

1:45pm LI-MoM-46 2021 AVS Graduate Research Award Talk: Versatile Polymer Nanoparticle Synthesis Using Initiated Chemical Vapor Deposition (iCVD), *Trevor Donadt[1], D. Streever, R. Yang,* Cornell University
Polymerization of monomers to form nanoparticles (i.e. bottom-up synthesis) is commonly performed in liquid environments which confers restrictions to monomer chemistries and particle shape based on solubility and procedures that are commonly driven by surface tension. Here we report the synthesis of polymer nanoparticles (PNPs) through a technique performed in a chemical vapor deposition apparatus that traditionally forms thin film polymer coatings. By utilizing an initiated chemical vapor deposition (iCVD) reactor, the synthesis process is afforded the advantages of an all-dry process, enabling PNPs made of insoluble polymers (e.g., hydrophobic and heavily cross-linked) and a variety of chemistries (zwitterionic, fluorinated, functionalizable, etc.) using the same technique. Furthermore, the solvent-free process enables control of the PNP diameters across an impressively broad range, from below 10 nm to above 1 μm. This approach delivers unprecedented synthetic capability for PNPs with nanoscale control over particle size without relying on laborious nanofabrication of templates, which are commonly required for particle size control in existing procedures. The approach is also substrate-independent, such that it can be performed on any type of material, turning PNPs into nanostructured thin films in situ. This technique is compatible with a library of over 70 functional monomers developed to date for iCVD. The chemical versatility, combined with the broad yet precise control of particle sizes, renders this approach a promising route to generating PNPs from materials inaccessible in liquid-based methods, thus opening new avenues for PNP applications.

2:00pm LI-MoM-49 2021 Dorothy M. and Earl S. Hoffman Award Scholarship Talk: Tunable Photonics Based on Thin-Film Vanadium Dioxide, *Chenghao Wan[2],* University of Wisconsin - Madison; *Z. Zhang,* Purdue University; *D. Woolf,* Physical Sciences Inc.; *J. Rensberg, M. Hafermann,* Friedrich Schiller University Jena, Germany; *J. Salman, Y. Xiao,* University of Wisconsin - Madison; *M. Park,* Purdue University; *C. Ronning,* Friedrich Schiller University Jena, Germany; *S. Ramanathan,* Purdue University; *M. Kats,* University of Wisconsin - Madison
Vanadium dioxide (VO_2) is a prototype strongly correlated material that undergoes a first-order insulator-to-metal transition (IMT) at ~70 °C. This reversible IMT in VO_2 has drawn decades-long research attention because it can result in orders-of-magnitude changes in carrier density accompanied by a dramatic change in the refractive index, which has advanced various applications in electronics and optics. Recently, improvements in deposition techniques have enabled synthesis of high-quality VO_2 thin films (with thickness of tens of nanometers), boosting the utilization of thin-film VO_2 in nanophotonics.

In this talk, we will first present our characterization and analysis of optical properties of thin-film VO_2 for wavelengths from the ultraviolet to the far infrared. Both ellipsometry data and effective-medium modeling will be presented, for VO_2 films grown using different methods, on different substrates, and with different thicknesses. Based on ellipsometry measurements, we have concluded that VO_2 films synthesized via different conditions generally feature consistent and large refractive-index contrast in the mid-infrared, but distinguishable (or even significantly different) optical properties in the visible and far infrared. Our data is freely available for anyone to use in their own design and simulations.

In the second part of the talk, we will give specific illustrations of tunable photonic devices by incorporating thin-film VO_2 into two kinds of nanophotonic geometries—metasurfaces and thin-film assemblies. For the metasurface-based design, we demonstrated an ultrathin reflective optical limiter comprising a VO_2 thin film and metallic aperture antennas. Our design can feature intensity-dependent modulation of transmission for a broad wavelength range (>2 μm at 10 μm) and angle of incidence (up to 50° away from the normal, for all polarizations). For the thin-film design, we demonstrated a tunable broad-to-narrow bandpass filter by introducing a VO_2 film into a dielectric stack of alternating Ge and ZnSe layers. The fabricated filter can switch between a broadband transmission window in the long-wave infrared (8 – 12 μm) and a narrow passband centered around 8.8 μm, which has potential uses for thermal-imaging enhancement.

In the end, we will also briefly discuss our engineering of the IMT temperature in VO_2 films by defect engineering via ion implantation, which can enable applications close to room temperature.

2:15pm LI-MoM-52 2021 AVS Dorothy M. and Earl S. Hoffman Award Talk: Strain Engineering of Magnetism and Topological States in Rippled Heusler Membranes, *Dongxue Du[3], S. Manzo, C. Zhang, V. Saraswat,* University of Wisconsin - Madison; *K. Genser, K. Rabe,* Rutgers, The State University of New Jersey; *P. Voyles, M. Arnold, J. Kawasaki,* University of Wisconsin - Madison
Single-Crystalline Membranes of Functional Materials Enable the Tuning of Properties via Extreme Strain States; However, Conventional Routes for Producing Membranes Require the Use of Sacrificial Layers and Chemical Etchants, Which Can Both Damage the Membrane and Limit the Ability to Make Them Ultrathin. Here We Demonstrate the Epitaxial Growth of the Cubic Heusler Compound Gdptsb on Graphene-Terminated Al_2O_3 Substrate. Despite the Presence of the Graphene Interlayer, the Heusler Films Have Epitaxial Registry to the Underlying Sapphire, as Revealed by X-Ray Diffraction, Reflection High Energy Electron Diffraction, and Transmission Electron Microscopy. The Weak Van Der Waals Interactions of Graphene Enable Mechanical Exfoliation to Yield Free-Standing Gdptsb Membranes, Which Form Ripples When Transferred to a Flexible Polymer Handle. Whereas Unstrained Gdptsb Is Antiferromagnetic, Measurements on Rippled Membranes Show a Spontaneous Magnetic Moment at Room Temperature, With a Saturation Magnetization of 5.2 Bohr Magneton Per Gd. First-Principles Calculations Show That the Coupling to Homogeneous Strain Is Too Small to Induce Ferromagnetism, Suggesting a Dominant Role for Strain Gradients. We Will Also Describe Preliminary Magnetotransport Measurements Aimed at Tuning the Topological Properties of Gdptsb, Since This Compound Shares a Similar Electronic Structure as the Weyl Semimetal Gdptbi. Together, Our Results Point to Strained Membranes as a Powerful Platform for Tuning Magnetism and Topological States in Quantum Materials.

2:30pm LI-MoM-55 AVS 2021 Medard W. Welch Award Lecture: Probing and Controlling Excitons in 2D Semiconductors, *Tony Heinz[4],* Stanford University and SLAC National Accelerator Laboratory **INVITED**
One of the key features of the optical response of 2D semiconductors is the dominant role of excitonic interactions. The strong influence of these many-body effects reflects the reduced dimensionality combined with the reduced dielectric screening of atomically thin crystals. In this paper, we will review progress in understanding the nature of optically excited states in 2D monolayers and heterostructures. We will describe how excitonic states can be tuned and probed be altering the Coulomb interaction within the layer by various approaches, including through changes in the external dielectric environment. We will particularly emphasize recent advances in applying time-resolved ARPES (angularly resolved photoemission spectroscopy) to examine the momentum-space character and dynamics of excitons in transition metal dichalcogenide semiconductors. In these studies, carried out in collaboration with the group of Keshav Dani, we have been able not only to determine the valley characteristics of both bright and dark excitons, but also to image directly the wavefunction of excitonic states in momentum space. Examples of this approach will be presented both for monolayers and for vertical heterostructures.

3:00pm LI-MoM-61 Closing Remarks and Thank You's, *Amy V. Walker,* University of Texas at Dallas
Thank you for attending the AVS 67 Plenary and Awards Session. We look forward to seeing you tomorrow at 10:00 am EDT for a full day of Live Parallel Sessions. Remember to check out the AVS 67 On Demand Sessions which are now available in the mobile app and online scheduler.

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[1] **National Student Award Finalist**
[2] **National Student Award Finalist**
[3] **National Student Award Finalist**
[4] **Medard W. Welch Award Winner**

Tuesday Morning, October 26, 2021

Live Session
Room Live - Session LI-TuM1

Tuesday Morning Live Session I: New Frontiers in Interfaces
Moderators: Ashleigh Baber, James Madison University, Erin Iski, U. Tulsa

10:00am LI-TuM1-1 Welcome and Opening Remarks, *Ashleigh Baber*, James Madison University
Welcome to the AVS 67 Virtual Symposium! We hope you will enjoy the event!

10:05am LI-TuM1-2 Electrochemical Surface Science of Platinum, *Marc Koper*, Leiden University, Netherlands **INVITED**
Platinum is the most used electrocatalyst in electrochemical energy conversion devices such as fuel cells and electrolysers. In this talk I will highlight the recent work of my group on understanding the surface chemistry of platinum in an aqueous electrolyte, by combining single-crystal electrochemistry, density functional theory calculations, ultra-high-vacuum modeling, in situ spectroscopy and in situ electrochemical scanning tunneling microscopy. I will challenge some existing explanations and interpretations of platinum electrochemistry, and show the sometimes surprising surface disordering of platinum that happens at both positive (anodic) and negative (cathodic) potentials.

10:25am LI-TuM1-6 Manipulating Electrochemical Reactions in Van Der Waals Heterostructures, *Kwabena Bediako*, University of California at Berkeley **INVITED**
Molecular-scale manipulation of electronic and ionic charge accumulation in materials is the backbone of electrochemical energy storage. Layered van der Waals (vdW) crystals are a diverse family of materials into which mobile ions can electrochemically intercalate into the interlamellar gaps of the host atomic lattice. The structural diversity of such materials enables the interfacial properties of composites to be optimized to improve ion intercalation for energy storage and electronic devices. However, the ability of heterolayers to modify intercalation reactions, and their role at the atomic level, are yet to be elucidated. In this talk I will discuss the electrointercalation of lithium at the level of individual atomic interfaces of dissimilar vdW layers. In this work, electrochemical devices based on vdW heterostructuresof stacked hexagonal boron nitride, graphene and molybdenum dichalcogenide ($MoCh_2$; $Ch=$ S, Se) layers were constructed. Transmission electron microscopy, in situ magnetoresistance and optical spectroscopy techniques, as well as low-temperature quantum magneto-oscillation measurements and ab initio calculations, were used to resolve the intermediate stages of lithium intercalation at heterointerfaces. The formation of vdW heterointerfaces between graphene and $MoCh_2$ layers was found to result in a more than tenfold greater accumulation of charge in the metal dichalcogenidewhen compared to $MoCh_2/MoCh_2$homointerfaces, while enforcing a more negative intercalation potential than that of bulk $MoCh_2$by at least 0.5 V. Beyond energy storage, this combined experimental and computational methodology for manipulating and characterizing the electrochemical behavior of layered systems opens new pathways to control the charge density in two-dimensional electronic and optoelectronic devices.

10:45am LI-TuM1-10 Scale-Up Manufacturing Processes for Powders: Pairing Powder Properties to Process, *Arrelaine Dameron, S. Moulton, J. DuMont , D. Lewis, T. Porcelli, R. Tracy*, Forge Nano **INVITED**
Control of surface phenomena by powder modification via atomic layer deposition (ALD) for a spectrum of technology applications has made its way to R&D literature. But commercial adoption of ALD powder modification has been perceived as slow and too expensive to consider as a realistic commercial process. Forge Nano has patented, constructed, and demonstrated a high throughput ALD powder manufacturing capability at commercial scale and is commercializing first markets with partners. The manufacturing capability for powder modification with ALD is unlocking new potential for lower-cost integration of ALD into products. We will discuss a cross-comparison of ALD manufacturing type to product application and scaling requirements. For the first time in history, a pathway for ALD-enhanced materials to be rapidly transitioned from lab-scale demonstration to commercial presentation is available for new product development. The scaleup process addresses the stepwise progression to validate engineering and materials requirements to meet the market price demands. We will demonstrate that ALD enabled materials are the state of the art. The manufacturing of consistent materials with ALD modification is a cost-competitive level and now possible. The future of material science and product development for operation at more demanding conditions is enabled by ALD for a variety of applications.

11:15am LI-TuM1-16 Batteries at Work: Ambient Pressure Photoelectron Spectroscopy for Lithium Ion Batteries, *I. Källquist, F. Lindgren, M. Hahlin*, Uppsala University, Angstrom Laboratory, Sweden*; Julia Maibach*, Karlsruhe Institute of Technology (KIT), Institute for Applied Materials (IAM), Germany **INVITED**
Rechargeable ion batteries such as Li-ion batteries generally consist of a negative electrode, a positive electrode and an ion conducting electrolyte. Today, much of our knowledge about the interactions of these components at surfaces and interfaces comes from post mortem photoelectron spectroscopy (PES) analyses. For these types of measurements, pre-cycled battery electrodes are transferred to the PES instrument to be characterized in UHV conditions.

Using ambient pressure photoelectron spectroscopy (APPES), we now have the possibility to acquire more realistic information about the interplay of electrode and electrolyte since the experiments can be conducted at elevated pressures and with liquid electrolyte present. We will firstly present our contributions to characterizing Li-ion battery electrodes [1] and electrolytes [2] using APPES as a precondition to achieve reliable in-situ and operando studies on working batteries.

Secondly, we present our work on electrode/electrolyte interfaces to investigate changes in Galvani potential using *operando* APPES [3]. For Li-ion batteries, Galvani potential differences (i.e. the electrostatic potential difference between two phases in contact) play an important role for the reaction kinetics at the functional electrode/electrolyte interphases. However, due to lack of suitable measurement techniques, so far little is known about how the Galvani potential difference behaves during Li-ion battery operation. We will show our approach on measuring how a change in Galvani potential difference can be followed as a function of applied external voltage using *operando* APPES, even without direct access to the electrode/electrolyte interface.

[1] J. Maibach, C. Xu, S. K. Eriksson, J. Åhlund, T. Gustafsson, H. Siegbahn. H. Rensmo, K. Edström, M. Hahlin, Rev. Sci. Inst. 86 (2015), 044101.

[2] J. Maibach, I. Källquist, M. Andersson, S. Urpelainen, K. Edström, H. Rensmo, H. Siegbahn, M. Hahlin, Nature Comm. 10 (2019), 3080.

[3] F. Lindgren, I. Källquist, M.-T. Lee, A. Shavorskiy, K. Edström, H. Rensmo, L. Nyholm, J. Maibach, M. Hahlin, in preparation.

11:35am LI-TuM1-20 In-Situ TEM Imaging of Nanoscale Reactions at Solid-Liquid-Gas Interfaces, *Haimei Zheng*, Lawrence Berkeley National Lab **INVITED**
Many chemical reactions involve the presence of solids, liquids and gases concurrently, for instance, heterogeneous catalysis, materials corrosion and others. Complex phenomena may occur at solid-liquid-gas interfaces. Direct monitoring the interfacial reactions at the nanoscale is significant for understanding the reaction mechanisms and developing strategies to control the reactions. By developing and applying liquid cell transmission electron microscopy (TEM), my group studies the dynamic nanoscale phenomena at solid-liquid-gas interfaces with high spatial and temporal resolution. In this talk, I will first show the observed accelerated etching of Au nanostructures with the presence of gas nanobubbles. Through tracking the evolution of local reaction profile and theoretical modeling, an understanding of the triple phase reactions and gas diffusion pathways at the interfaces is developed. I will also show that the solid-liquid-gas interfaces can play a critical role in mediating the oxidative etching by allowing the reduction reactions in a near distance. Future work on in situ TEM studies of the solid-liquid-gas interfaces and device applications will also be discussed.

11:55am LI-TuM1-24 Molecular Processes in Ultra-High Vacuum between the Stars, *Ewine van Dishoeck*, Leiden University, The Netherlands **INVITED**
Stars and planets are born in the cold and ultra-tenuous clouds between the stars in the Milky Way. In spite of the extremely low temperatures and densities, a surprisingly rich and interesting chemistry occurs in these interstellar clouds, as evidenced by the detection of more than 200 different molecules. Water and a large variety of organic molecules are found, including simple sugars and high abundances of deuterated species. What are the molecular processes by which these molecules are formed

and destroyed, both in the gas phase and on surfaces? And how do we calculate or measurerates that can be used in models of star-forming regions? Can these pre-biotic molecules end up on new planets and form the basis for life elsewhere in the universe? New data from the revolutionary Atacama Large Millimeter Array (ALMA) and the ESA-Rosetta mission to comet 67P will be presented.

12:15pm LI-TuM1-28 Closing Remarks and Thank You's, *Erin Iski*, University of Tulsa
Thank you for attending today's session! Please note that our afternoon sessions begin at 12:50 pm EDT. We also look forward to seeing you tomorrow at 10:00 am EDT for a full day of Live Parallel Sessions. Remember to check out the AVS 67 On Demand Sessions which are available in the mobile app and online scheduler.

Live Session
Room Live-2 - Session LI-TuM2

Tuesday Morning Live Session II: Current and Emerging Devices
Moderators: Adriana Creatore, Eindhoven University of Technology, Netherlands, Sebastian Engelmann, IBM T.J. Watson Research Center

10:00am LI-TuM2-1 Welcome and Opening Remarks, *Adriana Creatore*, Eindhoven University of Technology, The Netherlands
Welcome to the AVS 67 Virtual Symposium! We hope you will enjoy the event!

10:05am LI-TuM2-2 Aluminum Scandium Nitride Microdevices for Next Generation Nonvolatile Memory and Microelectromechanical Systems, *Troy Olsson*, University of Pennsylvania **INVITED**
Aluminum Nitride (AlN) is a well-established thin film piezoelectric material. AlN bulk acoustic wave (BAW) radio frequency (RF) filters were one of the key innovations that enabled the 3G and 4G smart phone revolution. Recently, the substitutional doping of scandium (Sc) for aluminum (Al) to form aluminum scandium nitride (AlScN) has been studied to significantly enhance the piezoelectric properties and to introduce ferroelectric properties into AlN based material systems. The properties achieved have profound implications for the performance of future 5G and 6G RF filters, piezoelectric sensors, piezoelectric energy harvesters, and for scaling the bit density of ferroelectric nonvolatile memories. This talk will present on the synthesis of highly Sc doped AlScN materials of the thickness and quality needed for applications in memory and microelectromechanical systems (MEMS). The material properties achieved will be reported and placed in the context of device specific figures-of-merit and competing material systems. Ferroelectric and electromechanical devices that utilize the unique properties of AlScN to achieve state-of-the-art (SOA) performance will be shown.

10:25am LI-TuM2-6 Memristive Devices and Arrays as AI Hardware, *J. Joshua Yang*, University of Southern California **INVITED**
Memristive devices have become a promising candidate as the AI hardware core due to their attractive properties(*1*). AI algorithms can be implemented on a Resistive Neural Network (ResNN) with memristor synapses and neurons or a Capacitive Neural Network (CapNN) with memcapacitor synapses and neurons(*2*).

For ResNNs as computing accelerators, we have built a dot-product engine based on a 128 x 64 1T1R crossbar array(*3*)and a 3D crossbar array with 8 layers of memristors(*4*)using traditional non-volatile memristors. With such computation accelerators, we have demonstrated efficient inference and learning with traditional Machine Learning algorithms(*5-7*), which is expected to significantly improve the speed and energy efficiency of neural networks.

For ResNNs beyond accelerator applications, we developed diffusive memristors(*8*)with diffusion dynamics that is critical for neuromorphic functions. Based on the diffusive memristors, we have further developed artificial synapses(*8*)and neurons(*9*)to more faithfully emulate their bio-counterparts. We then integrated these artificial synapses and neurons into a small neural network, with which pattern classification and unsupervised learning have been demonstrated(*9*).

For CapNNs, we have developed pseudo-memcapacitive devices based on the diffusive memristors. Capacitive synapses and neurons enabled by these memcapacitive devices have been developed and used to form a fully integrated CapNN(*10*), which can implement spiking signal classification and Hebbian-like learning.

1. 1. Z. Wang*et al.*, Resistive switching materials for information processing. *Nature Reviews Materials* **5**, 173–195 (2020).
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4. 4. P. Lin*et al.*, Three-dimensional memristor circuits as complex neural networks. *Nature Electronics* **3**, 225–232 (2020).
5. 5. Z. Wang*et al.*, Reinforcement learning with analogue memristor arrays. *Nature Electronics* **2**, 115 (2019).
6. 6. Z. Wang*et al.*, In situ training of feed-forward and recurrent convolutional memristor networks. *Nature Machine Intelligence* **1**, 434-442 (2019).
7. 7. C. Li*et al.*, Long short-term memory networks in memristor crossbar arrays. *Nature Machine Intelligence* **1**, 49-57 (2019).
8. 8. Z. Wang*et al.*, Memristors with diffusive dynamics as synaptic emulators for neuromorphic computing. *Nature Materials* **16**, 101-108 (2017).
9. 9. Z. Wang*et al.*, Fully memristive neural networks for pattern classification with unsupervised learning. *Nature Electronics* **1**, 137-145 (2018).
10. 10. Z. Wang*et al.*, Capacitive neural network with neuro-transistors. *Nature Communications* **9**, 3208 (2018).

10:45am LI-TuM2-10 Etch Processes for Enabling Next Generation Devices, *Eric Miller*, I. Seshadri, T. Kang, D. Metzler, J. Lee, S. Sieg, S. Engelmann, J. Shearer, J. Arnold, N. Felix, IBM Research Division, Albany, NY **INVITED**
While delivering industry first demonstrations of 7NM (FinFET) and 5NM (Nanosheet) technology nodes, IBM Research has encountered unique challenges that arise as a result of continued device scaling. Dimensional compression drives higher aspect ratios, which in turn drive difficulty with in-feature ion, radical, and volatile species transport during plasma etch. Dimensional scaling now approaches the single digit nanometer scale, and the need for solutions to unique problems exists now more than ever. In the world of plasma etch, which largely led the charge in dimensional scaling with anisotropic patterning, it is now critical to account for a variety of factors to deliver a successful etch process. Etch process development is truly a juggling act of selectivity, anisotropy, by-product control, sidewall profile, and throughput. The continuation of device scaling using extreme ultraviolet light lithography, self aligned double and quadruple patterning, as well as the introduction of three dimensional (nanosheet) devices has introduced a unique set of challenges to be addressed in the coming technology nodes. In this paper, a variety of etch applications, challenges, and innovations will be reviewed with respect to continued device scaling. The functional implementation of quasi-atomic layer etching, plasma etch modulation of line edge/width roughness, and etch selectivity/anisotropy challenges at high aspect ratios will all be explored with the viewpoint of how these impact future semiconductor nodes.

11:15am LI-TuM2-16 On the Low Deposition Rate and Ionized Flux Fraction in High Power Impulse Magnetron Sputtering, *Jon Tomas Gudmundsson*, H. Hajihoseini, University of Iceland; *N. Brenning,* KTH Royal Institute of Technology, Sweden; *M. Rudolph,* Leibniz Institute of Surface Engineering (IOM), Germany; *M. Raadu,* KTH Royal Institute of Technology, Sweden; *D. Lundin,* Linkoping University, Sweden **INVITED**
The deposition rate in high power impulse magnetron sputtering (HiPIMS) is often found to be somewhat lower than that obtained with dc magnetron sputtering (dcMS), generally in the range of 30 - 85 % of the dcMS rates, depending on target material when operating at the same average power [1]. Back-attraction of ions of the sputtered species to the cathode target is probably the main cause for the low deposition rate while some other mechanisms have also been suggested. This includes the nonlinear sputter yield effect, guiding effect of the magnetic field, the increased density of the deposited film, the effect of different ion species on the sputter yield and that the sputtered material are being transported radially outward in the vicinity of the cathode. Some approaches to increase the deposition rate are discussed. We discuss how the magnetic field strength |**B**| and geometry (degree of balancing) influences the deposition rate and ionized flux fraction F_{flux} in dcMS and HiPIMS operation both axially [2] and radially [3]. The measured quantities, the deposition

rate and ionized flux fraction, are then related to the ionization probability α_t and the back attraction probability of the sputtered species β_t. We find a significant transport of the film forming material radially or parallel to the target surface for both sputter techniques. This radial deposition decreases with increasing axial distance from the target surface and it is always higher in dcMS than HiPIMS. There are a significantly higher number of ions traveling radially in the HiPIMS discharge. We find that the relative radial flux of the film forming material is greater in dcMS compared to HiPIMS for almost all cases investigated. It is therefore concluded that the commonly reported reduction of the (axial) deposition rate in HiPIMS compared to dcMS does not seem to be linked with an increase in sideways material transport in HiPIMS. We discuss the tradeoff between a high ionized flux fraction of the sputtered species and a high deposition rate referred to as the HiPIMS compromise [4]. [1] M. Samuelsson, D. Lundin, J. Jensen, M. A. Raadu, J. T. Gudmundsson, and U. Helmersson, Surf. Coat. Technol. 202, 591 (2010)[2] H. Hajihoseini, M. Čada, Z. Hubička, S. Ünaldi, M. A. Raadu, N. Brenning, J. T. Gudmundsson, and D. Lundin, Plasma 2, 201 (2019).[3] H. Hajihoseini, M. Čada, Z. Hubička, S. Ünaldi, M. A. Raadu, N. Brenning, J. T. Gudmundsson, and D. Lundin, J. Vac. Sci. Technol. A 38, 033009 (2020).[4] N. Brenning, A. Butler, H. Hajihoseini, and M. Rudolph, J. T. Gudmundsson, T. Minea, and Daniel Lundin, J. Vac. Sci. Technol. A 38, 033008 (2020).

11:35am LI-TuM2-20 β-Ga₂O₃ Resonant Micro/Nanoelectromechanical Systems (M/NEMS), *Xu-Qian Zheng, P. Feng,* University of Florida **INVITED**
Beta gallium oxide (β-Ga₂O₃) is an emerging ultra-wide bandgap (UWBG) semiconductor (E_g=4.5-4.9 eV). The crystal is outstanding in sustaining high electrical field because of its UWBG, making it attractive for power electronics, high-voltage/power radio frequency (RF), and harsh-environment applications [1]. Based on its UWBG, β-Ga₂O₃ crystal has an absorption edge around 275 nm, thus the material is intrinsically suitable for solar-blind ultraviolet (SBUV, λ<280 nm) detection [2]. In addition, thanks to the capability of growth from liquid phase, bulk β-Ga₂O₃ crystals can be cost-effectively synthesized with exceptional crystal quality. Furthermore, β-Ga₂O₃ possesses excellent Young's modulus (E_Y=261 GPa) and speed of sound (c=6600 m/s), suitable for making mechanical devices. The outstanding ensemble of attributes in β-Ga₂O₃ enables new UWBG micro/nanoelectromechanical systems (M/NEMS) for future electromechanically coupled and tunable β-Ga₂O₃ electronic, optoelectronic, and physical sensing devices and systems.

Here we present an overview of the β-Ga₂O₃ mechanical properties characterization in nanomechanical device platforms and development of β-Ga₂O₃ resonant M/NEMS by describing the recent advances in engineering β-Ga₂O₃ nanostructures into functional devices and exploration of their device physics. We demonstrate a family of β-Ga₂O₃ NEMS resonators with resonance frequencies in high frequency and very high frequency (HF/VHF) bands and quality (Q) factors up to 1700 at room temperature. We extract Young's modulus of 245–261 GPa for thin film β-Ga₂O₃ in the nanomechanical resonator platform [3]. In additional to basic nanomechanical devices, we demonstrate real-time SBUV light detection using oscillators enabled by β-Ga₂O₃ resonant NEMS [4]. We demonstrate β-Ga₂O₃ vibrating channel transistors (VCTs) for electromechanical coupling of the β-Ga₂O₃ M/NEMS resonators and depict the future design and equivalent-circuit modeling of such devices for >GHz operations [5]. We investigate the operation of β-Ga₂O₃ nanomechanical resonators in high temperature environment (up to 350 °C) and study its resonance frequency response under different pressures from atmospheric pressure down to ~15 mTorr. Our study facilitates the development and integration of β-Ga₂O₃ resonant M/NEMS on-chip with β-Ga₂O₃ electronic circuits, supplementing the rapidly emerging β-Ga₂O₃ electronics and optoelectronics.

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[5] X.-Q. Zheng, *et al.*, Appl. Phys. Lett. **117**, 243504 (2020).

11:55am LI-TuM2-24 In-Depth Feasibility Study of Dual Damascene Extension: Patterning, Dielectric Etch and Metallization, *Xinghua Sun,* TEL Technology Center, America, LLC; *Y. Mignot,* IBM Research Division, Albany, NY; *C. Cole, E. Liu,* TEL Technology Center, America, LLC; *J. Church,* IBM Research Division, Albany, NY; *D. Santos, A. Raley,* TEL Technology Center, America, LLC; *S. Sieg,* IBM Research Division, Albany, NY; *P. Biolsi,* TEL Technology Center, America, LLC **INVITED**
As logic metal pitch keeps scaling aggressively, back end of line (BEOL) interconnects continue to push the limits of materials properties and integrations. Current extreme ultraviolet (EUV) single exposure limitation (28P) requires a new robust patterning scheme based on EUV multipatterning and new metallization integrations will likely be required due to the lack of liner/barrier and copper scaling at such small critical dimensions [1, 2].Alternative subtractive metallization scheme are being studied for very advanced node where resistance/capacitance (R/C) simulations shows benefit [1].

A key integration choice to make is whether to extend Damascene dielectric etch or move to subtractive metal etch. For Damascene dielectric, the key challenges are mask pattern assembly and EPE control, low k dielectric line wiggling and damage post etch, and liner/barrier induced high resistance after metallization [3, 4]. Subtractive metal etch presents cost issues, alignment concerns and will likely be implemented solely in first metal level(s) which have the most aggressive pitch scaling targets [3]. In terms of mask assembly, multipatterning is required to form line with a 3 masks level forSADP / cut / block and a 2 color Via mask (DPSAV) to meet design rules [4].

In this report, we present an in-depth study of the feasibility of Dual Damascene extension based on 24nm metal pitch. EUV self-aligned double patterning (SADP) is demonstrated for line and space patterning. With a cut and block flow, it enables an e-testable trench module. We demonstrate double patterned self-aligned via (DPSAV) for via tests. Dielectric reactive ion etch (RIE), including quasi atomic layer etch (QALE) and reduced low k damage etch, is leveraged for the trench and via formation, respectively. Finally, metallization and chemical mechanical planarization (CMP) is successfully demonstrated. This in-depth demonstration provides an important insight into Dual Damascene extension feasibility for future critical metal levels.

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12:15pm LI-TuM2-28 Closing Remarks and Thank You's, *Sebastian Engelmann,* IBM T. J. Watson Research Center
Thank you for attending today's session! Please note that our afternoon sessions begin at 12:50 pm EDT. We also look forward to seeing you tomorrow at 10:00 am EDT for a full day of Live Parallel Sessions. Remember to check out the AVS 67 On Demand Sessions which are available in the mobile app and online scheduler.

Live Session
Room Live - Session LI-TuA1

Tuesday Afternoon Live Session I: Harnessing and Understanding Interfacial Chemistry

Moderators: Donna Chen, University of South Carolina, Zhenrong Zhang, Baylor University

12:50pm **LI-TuA1-1 Welcome and Opening Remarks**, *Donna Chen*, University of South Carolina
Welcome to the AVS 67 Virtual Symposium. I will review the structure of this week's program. We hope you will enjoy the event!

12:55pm **LI-TuA1-2 High-Throughput Computational Screening of Diamond Like Semiconductors and Ordered Vacancy Compounds for Thermoelectrics**, *J. Xu,* University of Illinois at Urbana-Champaign; *C. Porter, J. Adamczyk, E. Toberer,* Colorado School of Mines; *Elif Ertekin,* University of Illinois **INVITED**
Computation-driven search for thermoelectrics (TEs) has recently shown several successes, but a principal bottleneck appears to be that predicted materials often prove to be difficult to dope in the lab. Here we will present our recent computational and experimental efforts to tailor the defect chemistry and dopability of a set of ordered vacancy compounds that are of interest for their TE potential. Ordered vacancy compounds (OVCs) are a family of materials whose structure is closely related to diamond like semiconductors, but contain an ordered array of vacancies. Diamond like semiconductors and OVCs are typically observed to be p-type, but our TE materials descriptor suggests that they would be more effective as thermoelectrics if they could be doped n-type. Therefore, we screen through a chemically-diverse set of 54 OVCs to assess their TE potential and dopability. For the most promising candidates, using calculations of phase stability defect formation energies, we comprehensively establish the achievable range of carrier concentrations achievable. Using phase boundary mapping, experimental carrier concentrations are measured and compared to the predicted values, typically showing correspondence within a few orders of magnitude. For all compounds, we find that a delicate competition between a set of dominant, competing defects governs the achievable range of carrier concentrations. For instance in the II_2-IV-VI_4 OVC structural prototype, enhancing n-type dopability requires suppressing the IV_{II} antisite and promoting the formation of the group II vacancy. Using this observation as a design strategy, we identify candidates that may be more amenable to n-type doping. The results of this search are used to generate a chemically intuitive framework for predicting dopabilities in this family of materials without the need to carry out full-scale first-principles analysis.

1:15pm **LI-TuA1-6 Towards a Mechanistic Understanding of Next-Generation Particle Accelerator Materials Growth: Nb Hydride Growth and Suppression and Nb₃Sn Formation on (3×1)-O Nb(100)**, *Rachael G. Farber, S. Willson, R. Veit,* University of Chicago; *N. Sitaraman,* Cornell University; *A. Hire, R. Hennig,* University of Florida; *T. Arias,* Cornell University; *S. Sibener,* University of Chicago **INVITED**
Niobium (Nb) is the current standard material for superconducting radio frequency (SRF) accelerator cavities due to its ultra-low surface resistance and high cavity quality factor (Q) at operating temperatures of ~ 2 K. However, prohibitively expensive operating and infrastructure costs prevent the implementation of accelerator-based technologies across a variety of sectors. Nb_3Sn is a promising next-generation material for SRF cavities and can operate at ~ 4.2 K, significantly reducing operating costs of cryogenic infrastructure. To increase the efficiency and accessibility of accelerator-based technologies, SRF materials must be developed that can reliably produce intense particle beams above 4 K.

Nb surface composition and contaminant incorporation directly affect Q. Hydrogen incorporated during Nb cavity fabrication results in the formation of Nb hydrides, which lower Q at high fields and reduce cavity performance. Nitrogen infusion of Nb cavities mitigates hydride formation, but the growth and suppression mechanisms of Nb hydrides are not thoroughly understood. Utilizing low-temperature scanning tunneling microscopy (LT-STM), scanning tunneling spectroscopy (STS), and density functional theory (DFT) calculations, we have investigated the growth and suppression mechanisms of Nb nano-hydrides on (3×1)-O Nb(100). STM and STS results identified the structural and electronic evolution of undoped, hydrogen doped, and co-doped Nb(100) resulting from Nb nano-hydride growth and suppression. DFT calculations corroborate experimental data and identified unique near-surface phases stabilized by

dopant incorporation. These results provide the first *in situ*, real-time nanoscale characterization of the effects of dopant incorporation on Nb nano-hydride growth and suppression, elucidating the interplay between nitrogen and hydrogen regarding Nb SRF materials performance.

The latter part of this presentation will focus on the interaction of Sn with Nb substrates leading to the formation of Nb-Sn alloys. Nb_3Sn films are grown *via* Sn vapor deposition on preexisting Nb cavities. Sn homogeneity, surface roughness, and alloy thickness must be well controlled for high Q film growth, but the Nb_3Sn growth mechanism resulting in optimal film formation is not well understood. In this work, we have visualized Sn adsorption and diffusion behavior on (3×1)-O Nb(100) at the nanometer scale. STM data revealed preferential adsorption of Sn along the (3×1)-O unit cell. Annealing the Sn/Nb(100) sample resulted in the formation of hexagonal and rectangular Sn adlayer structures for all Sn coverages studied. STS measurements of these adlayers demonstrated thickness-dependent electronic properties that are distinct from the underlying Nb substrate. Genetic algorithm calculations and DFT based descriptors aim to determine energetically preferred Sn binding sites on the (3×1)-O surface. This spatially resolved mechanistic information of Sn adsorption and diffusion on an oxidized Nb surface guides the development of predictive Nb_3Sn growth models needed for the further optimization of Nb_3Sn growth procedures

1:35pm **LI-TuA1-10 Phase Formation and Thermal Stability of Reactively and Non-Reactively Sputtered High-Entropy Metal-Sublattice Carbides**, *Alexander Kirnbauer,* TU Wien, Institute of Materials Science and Technology, Austria; *P. Polcik,* Plansee Composite Materials GmbH, Germany; *P. Mayrhofer,* TU Wien, Institute of Materials Science and Technology, Austria **INVITED**
High-entropy alloys (HEAs) and high-entropy metal-sublattice ceramics (HESCs) have recently gained particular attraction in the field of materials research due to their promising properties, such as high hardness, high strength, and thermal stability. Within this work, we report on the phase formation and thermal stability of high entropy metal-sublattice carbides to provide a further insight to a more extensive understanding of the high-entropy effect, according to which, based on the Gibbs-free energy, such materials should be stabilised in the high-temperature regime. Therefore, (Hf,Ta,Ti,V,Zr)C coatings were reactively and non-reactively sputtered from a single powder-metallurgically produced composite target (either metallic or consisting of the respective binary carbides). Reactively sputtered coatings were synthesised using an C_2H_2 – Ar mixture with different $C_2H_2/(C_2H_2+Ar)$ ratios (f_{C2H2}). After deposition, the coatings were investigated in as-deposited state and after vacuum annealing between 800 and 1200°C. The structure and morphology, the chemical composition, the mechanical properties, and the thermal stability of the coatings were investigated by scanning electron microscopy, X-ray diffraction, and nanoindentation.

The non-reactively sputtered as well as reactively sputtered coatings with f_{C2H2}= 20 % show a single-phased face-centred cubic (fcc) structure. The hardness for the non-reactively sputtered HESCs is with ~41 GPa higher than that of the reactively sputtered one which exhibits a hardness of 35 GPa. This indicates that due to the use of C_2H_2 also regions of amorphous carbon form, which slightly weaken the coating already in the as-deposited state. After vacuum annealing up to 1200 °C the non-reactively sputtered coatings maintain a hardness of ~40 GPa indicating retarded softening mechanisms due to sluggish diffusion. This behaviour was also observed in previous studies on different material classes such as nitrides, borides, and oxides indicating a stabilisation due to the high-entropy metal sublattice.

2:05pm **LI-TuA1-16 Electronic Structure and Dynamics of Single Atom Catalysts**, *Nuria Lopez,* ICIQ, Spain **INVITED**
Single atoms have shown different structural and catalytic properties with deep coupling between the oxide and metallic structures. This phenomenum, unraveled by theory might have a high impact in the understanding of the chemical properties of the materials and might affect our current understanding for materials included those that are active in energy-conversion proceses.

2:25pm **LI-TuA1-20 Methanol Synthesis Pathways for the Selective Conversion of C-H bonds**, *Sanjaya Senanayake,* Brookhaven National Laboratory **INVITED**
Methane remains a valuable yet underutilized resource, with great interest for the direct upgrade to valued products. Our recent studies indicate that, in spite of the high stability of methane, systems such as Ni-CeO2(111) and CeO2-Cu(111) can break C-H bonds even at room temperature, through

careful manipulation of interfaces and metal-support interactions, using light oxidants (CO_2, O_2/H_2O). the selective oxidation on the surface sites can lead to conversion steps that produce CH_3OH and $CO+H_2$. AP-XPS with the help of DFT has been essential to elucidate C-H activation and oxidation steps with high resolution C 1s and O 1s spectroscopies.

We have established a method for the direct conversion of methane to methanol building on these surface results yielding low methanol selectivity (~30%). Subsequently, and in remarkable contrast we have found that a $CeO_2/Cu_2O/Cu(111)$ inverse system is able to activate methane at room temperature and then, with the help of water, performs a highly selective (70%) catalytic cycle, for the production of methanol. The interfacial interaction between CeOx-CuOx is crucial while the concentration of water has a strong effect on the selectivity towards the production of methanol.

We have used AP-XPS to track the sequence of pathways that initially activate C-H bonds into -OCH3 surface species that leads to the production of methanol. DFT and KMC were then used to evaluate the most prevalent steps that are likely essential for such selective chemistry.

This work is funded by the U.S. Department of Energy under contract No. DE-SC0012704. XPS measurements were performed at beamline 9.3.2 at the Advanced Light Source of LBNL under contract no. DE-AC02-05CH11231.

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2:45pm LI-TuA1-24 Building Bridges Between University, National Laboratory, and Industrial Research, *Robert McCabe,* National Science Foundation   **INVITED**
From the earliest days of UHV single-crystal and thin-film research related to fundamental aspects of heterogeneous catalysis, researchers have recognized the need to address various technical gaps relating fundamental observations under pristine conditions to factors affecting the working catalyst.Some of those observations scale, and others do not, but in both cases the atomic/molecular scale understanding obtained from research bridging those divides has been invaluable to the advancement of heterogeneous catalysis as practiced.Nevertheless, significant technical gaps still exist in advancing catalyst technology through the concept, design, and development stages to commercial application.Catalyst technology often gets stuck at a particular level, characterized by a combination of factors best described as "knowledge gaps."At that point, industry tends to focus on optimization around a core (often proprietary) technology, and the academic community heads off to new pastures.Federal funding agencies and our national laboratories sit in a unique position to forge research partnerships between academic and industry researchers that bridge knowledge gaps.I will provide specific examples of key knowledge gaps in heterogeneous catalysis, and how NSF is funding partnerships between academic institutions and industry to bridge those gaps.

3:05pm LI-TuA1-28 Closing Remarks and Thank You's, *Zhenrong Zhang,* Baylor University
Thank you for attending today's session! We look forward to seeing you tomorrow at 10:00 am EDT for a full day of Live Parallel Sessions. Remember to check out the AVS 67 On Demand Sessions which are available in the mobile app and online scheduler.

Live Session
Room Live-2 - Session LI-TuA2

Tuesday Afternoon Live Session II: Novel Characterization and Modeling
Moderators: Mohan Sankaran, University of Illinois at Urbana-Champaign, Virginia Wheeler, U.S. Naval Research Laboratory

12:50pm **LI-TuA2-1 Welcome and Opening Remarks**, *Ginger Wheeler,* U.S. Naval Research Laboratory
Welcome to the AVS 67 Virtual Symposium! We hope you will enjoy the event!

12:55pm **LI-TuA2-2 Time-Resolved Photoelectron Spectroscopy of Solar Cell Materials**, *Ute Cappel,* KTH - Royal Institute of Technology, Sweden
INVITED
Solar cells have a great potential in replacing fossil fuels in electricity generation, if requirements of low production costs can be met. In the last years, much research has focused on developing new solar cells made from organic or hybrid materials, which can be fabricated by cheap methods. This includes solar cells with a hybrid organic inorganic perovskite as the active layer in the solar cell, which have now reached power conversion efficiencies of more than 25%. In a typical solar cell, the perovskite layer is sandwiched between two selective contacts, one for holes and one for electrons.

The future success of these developments crucially depends on understanding the details charge separation, charge transport and charge recombination at the interfaces between the different layers in a solar cell as well as what parameters limit solar cell stability. X-ray based techniques such as photoelectron spectroscopy (PES) are powerful tools for obtaining electronic structure information of materials at an atomic level.By varying the photon energy from soft to hard X-rays, photoelectron spectroscopy can be used for non-destructive depth profiling of the solar cell interfaces giving information about the energy alignment and chemical structure and composition at the interface.

In this presentation, I will describe how we have used photoelectron spectroscopy for time-resolved and *operando* studies of complete solar cells. I will present results, where we were able to measure PES of a complete perovskite solar cells while applying an external bias and during visible illumination. This allowed us to determine the electronic structure and energy alignment of the active layer / back contact interface of the solar cell under operating conditions. Furthermore, I will discuss how time-resolved pump-probe measurements can be used to determine electron transfer dynamics in solar cells. For this, I will give an example of measuring the electron transport times in lead sulfide quantum dots films by combining photoelectron spectroscopy with sample excitation by a visible short-pulsed laser [1]. The described methods provide new ways of gaining insights into the working mechanism of solar cells based different combinations of materials.

[1] T. Sloboda et al. ScientificReports, 10, 1-14 (2020).

1:15pm **LI-TuA2-6 Application of a Laboratory-Based Scanning XPS/HAXPES Instrument for the Characterization of Buried Interfaces**, *Kateryna Artyushkova, J. Mann, J. Newman,* Physical Electronics USA*; R. Inoue, K. Watanabe, H. Yamazui,* ULVAC-PHI, Inc., Japan*; A. Vanleenhove, C. Zborowski, T. Conard,* IMEC, Belgium   **INVITED**
X-ray Photoelectron Spectroscopy (XPS) is a widely used surface analysis technique with many well established industrial and research applications. The surface sensitivity (top 5-10 nm) of XPS and its ability to provide short-range chemical bonding information make the technique extremely popular in materials characterization and failure analysis laboratories. While its surface sensitivity is an important attribute, in some cases, the depth of analysis of XPS is not sufficient to analyze buried interfaces without first sputter etching the sample surface. However, sputter etching can often lead to alterations of the true surface chemistry. An alternative to sputter etching the sample is Hard X-ray Photoelectron Spectroscopy (HAXPES), available at some synchrotron facilities. HAXPES utilizes X-rays typically defined as having energies greater than 5 keV. By increasing the photon energy of the X-ray source, the mean free path of photoelectrons is increased, resulting in an increased information depth obtained from the sample. Depending on the energy used, these hard X-rays can provide depths of analysis three or more times than that of soft x-rays used on conventional XPS systems. HAXPES measurements are, therefore, more sensitive to the bulk, and contributions from the surface are minimized.[1,2]This presentation will describe a laboratory-based instrument,

the PHI *Quantes*, equipped with two scanning microprobe monochromated X-ray sources, Al Kα (1486.6 eV) and Cr Kα (5414.7 eV), thus enabling both traditional XPS and HAXPES experiments in the same instrument. By combining both soft and hard X-ray analyses, we can gain an even better understanding of composition with depth and information at buried interfaces.

References

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2. Fadley, C.S. Hard X-ray Photoemission: An Overview and Future Perspective. In Hard X-ray Photoelectron Spectroscopy (HAXPS); Woicik, J. C., Ed; Springer: Switzerland 2016.

1:35pm **LI-TuA2-10 Precise Ion Energy Control With Tailored Waveform Biasing: Determination of Sputter Thresholds as Input for ALE Process Design**, *Nicholas Chittock, S. Balasubramanyam, T. Faraz, Y. Verstappen,* Eindhoven University of Technology, Netherlands*; M. Verheijen,* Eurofins Materials Science , Netherlands*; J. Escandon-Lopez, E. Heijdra, W. van Gennip,* Prodrive Technologies, Netherlands*; E. Kessels, A. Mackus,* Eindhoven University of Technology, Netherlands **INVITED**

Anisotropic atomic layer etching (ALE) relies on the use of directional ions having an energy within a specific ion energy window to remove a modified surface layer.[1] The selectivity and etch control of ALE depend strongly on the ability to limit the ion energy within this window. However, tuning of the ion energy is often achieved by application of a radio-frequency sinusoidal bias voltage waveform to the substrate, which results in a relatively broad ion energy distribution leading to a loss of selectivity.[2] In this work, we report on employing tailored waveform bias voltages to accurately control the ion energy during ALE.

A prototype bias voltage generator from Prodrive Technologies was used to produce tailored bias waveforms consisting of a voltage pulse and a ramp. Narrow energy distributions (< 7 eV FWHM) were demonstrated for ion energies up to 200 eV, as measured using a retarding field energy analyzer (RFEA) in collisionless Ar plasmas.[3] By using a low-frequency (100 kHz) waveform, independent control of the ion energy and ion flux was obtained.

Tailored waveform biasing enables precise determination of sputter thresholds which can serve as an input for ALE processes with high synergy and selectivity.[1] Al_2O_3 and HfO_2 sputter thresholds were determined in an Ar plasma as 59 ± 5 eV and 81 ± 5 eV, respectively. Surface modification by SF_6 plasma exposure generated a fluorinated surface layer on the Al_2O_3 and HfO_2 films. Fluorination resulted in an increase in sputter yields as well as a reduction of the sputter thresholds to 23 ± 4 eV and 37 ± 4 eV, respectively. Evaluating the sputter yield as a function of time shows that an initially higher sputter yield returns toward that of the bulk, indicating full removal of the modified layer. Using this knowledge, an Al_2O_3 ALE process consisting of SF_6 plasma and Ar plasma exposures was evaluated. This work demonstrates that combing self-limiting surface reactions with accurate ion energy control can offer a route to precise and selective ALE.

1. K. J. Kanarik, et al., J. Phys. Chem. Lett., 9, 4814–4821. (2018)
2. S. B. Wang & A. E. Wendt, J. Appl. Phys., 88, 643. (2000)
3. T. Faraz et al., Journal of Applied Physics, 128, 213301 (2020)

2:05pm **LI-TuA2-16 Going Beyond Superficial Surface Analysis for Transforming Plants into Value-added Products**, *Robyn Goacher,* Materion Corp. **INVITED**

Preparation of biofuels and value-added bioproducts from lignocellulosic plant matter is an important part of moving away from our global reliance on fossil fuels. Surface analysis of the solid plant starting materials and end products can be complicated by residues from the required chemical or enzymatic treatments and by overlapping signals from plant components themselves. Peak pattern analysis by multivariate statistical approaches such as principle components analysis (PCA) is vital to identifying contaminants from buffers, plasticizers, tape supports, etc, and for distinguishing between fragment ions shared by extractive compounds such as waxes and the main plant biopolymers of cellulose, hemicellulose and lignin. This talk suggests best practices in sample preparation, choice of controls, collection of replicates, and data analysis for lignocellulosic analysis by ToF-SIMS. Accomplishments and gaps in our knowledge of characteristic ions for plant components are described, along with examples of how ToF-SIMS has been used to describe the activity of

purified enzymes on wood, fungal activity on wood, and chemical treatments of plant matter.

2:25pm **LI-TuA2-20 Molecular Dynamics Study on Damage Formation in Atomic Layer Etching of Si With Halogen Radicals**, *Erin Joy Capdos Tinacba, M. Isobe, S. Hamaguchi,* Osaka University, Japan **INVITED**

Atomic layer etching (ALE) has gained much attention in the past years as an essential technique in fabrication processes of nano-scale semiconductor devices. ALE is a technique to achieve an atomic-scale control of an etching process by separating it into two steps; adsorption and desorption. In the adsorption step, the surface is modified by depositing a mono-layer or thin layer of less reactive molecules. In plasma enhanced ALE (PEALE), the modified layer is removed in the desorption step with the bombardment of energetic ions such as Ar^+. Ideally these ions should not be energetic enough to continuously etch an unmodified or a clean surface. This is called a self-limiting process of ALE. However, more often than not, non-ideal ALE, i.e., ALE without a complete self-limiting process, is utilized in semiconductor fabrication. In non-ideal ALE, more than one monolayer is removed and the sub-layer of the material may be damaged by excessive ion bombardment. Such damages can be critical on some electronic properties of the materials.

In this work, molecular dynamics (MD) simulation [1] was employed to have a deeper understanding of the reaction mechanisms and damage formation during ALE of Si with F, Cl, or Br adsorption and low-energy Ar^+ ion bombardment. The Ar^+ ion energy was varied from 20 to 60 eV. Five cycles of adsorption and desorption steps were simulated and the results were compared with experimental observations [2-4]. It was found that the etch-per-cycle (EPC) value was typically lower during the first cycle compared to the succeeding cycles because the first cycle was mostly spent for the formation of a modified layer. After the first cycle, a reproducible EPC value was observed. The effects of Ar^+ ion bombardment on the modified surface as well as its Si sub-layer were also investigated. It was observed that, even at low Ar^+ ion incident energy (20 − 30 eV), the Si sub-layer is damaged in the desorption step and the extent of this damage increases with increasing energy.

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[2] H. Sakaue, *et al.*, Mat. Res. Soc. Symp. 222 (1991), 195.

[3] S.-D. Park, *et al.,* Jpn. J. Appl. Phys. 44 (2005), 389.

[4] S. Tan, *et al.,*ECS J. Solid State Sci. Technol., 4(6) (2015), N5010-N5012.

2:45pm **LI-TuA2-24 Variable Polarization, External Magnetic Field, and Spin Resolution for Buried Magnetic Materials Studied by Hard X-Ray Photoemission**, *Shigenori Ueda,* National Institute for Materials Science, Japan **INVITED**

Hard X-ray photoemission spectroscopy (HAXPES) with variable X-ray polarization is useful tool for studying the electronic structures of solids [1,2]. By using horizontal and vertical linear polarized X-ray, the valence band HAXPES spectra show the strong polarization dependence, which allows us to atomic orbital dependent electronic states [1]. For the magnetically ordered materials, HAXPES with left and right handed circularly polarized X-rays permits to probe the magnetic information form the magnetic circular dichroism in core-level photoemission in the element specific way [2]. Since HAXPES is known as a bulk-sensitive probe for electronic structures of solids due to large inelastic mean-free-path of photoelectrons with several keV, it is now possible to probe the electronic states of buried interfaces. In this presentation, the electronic and magnetic states of MgO/Fe interfaces are studied by HAXPES under an applied magnetic field using variable X-ray polarization [3]. The used samples are MgO(2 nm)/Fe(1.5 and 20 nm)/MgO(001), in which the thick and thin Fe films exhibit the in-palne and perpendicular magnetic anisotropies, respectively. For the thin Fe film, the electronic states of the top and bottom interfaces can be probed by HAXPES, while the electronic states of the Fe film inside are dominant in HAXPES. The role of the MgO/Fe interfaces and interface-induced magnetic anisotropy are discussed by comparing the density functional theory calculations. And I will show the results of high-throughput depth-resolved HAXPES combined with total reflection [4] for the MgO(2 nm)/Fe(50 nm)/MgO(001) and spin-resolved HAXPES for buried Fe films [5].

References

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[2] S. Ueda et al., Appl. Phys. Express 1 (2008) 077003.

[3] S. Ueda et al., Sci. Technol. Adv. Mater. 20 (2019) 796.

[4] S. Ueda, Appl. Phys. Express 11 (2018) 105701.

[5] S. Ueda and Y. Sakuraba, Sci. Technol. Adv. Mater. under review.

3:05pm **LI-TuA2-28 Closing Remarks and Thank You's**, *Mohan Sankaran,* University of Illinois at Urbana-Champaign

Thank you for attending today's session! We also look forward to seeing you tomorrow at 10:00 am EDT for a full day of Live Parallel Sessions. Remember to check out the AVS 67 On Demand Sessions which are available in the mobile app and online scheduler.

Live Session
Room Live - Session LI-WeM1

Wednesday Morning Live Session I: Recent Advances in Thin Films

Moderators: Svitlana Pylypenko, Colorado School of Mines, Angel Yanguas, Argonne National Lab

10:00am **LI-WeM1-1 Welcome and Opening Remarks**, *Angel Yanguas-Gil,* Argonne National Lab
Welcome to the AVS 67 Virtual Symposium! We hope you will enjoy the event!

10:05am **LI-WeM1-2 Metalorganic Vapor-Phase Epitaxy of Gallium (Aluminum) Oxide Thin Films and Heterostructures for High Frequency and Power Electronics**, *Sriram Krishnamoorthy,* University of California, Santa Barbara; *P. Ranga, A. Bhattacharyya, S. Roy,* Electrical and Computer Engineering, The University of Utah **INVITED**
Beta- Gallium Oxide (β-Ga_2O_3) is an emerging ultra-wide band gap (UWBG) material with the availability of high quality native substrates grown using potentially inexpensive melt-based techniques. In this talk, I will highlight the tremendous progress made by the Gallium Oxide research community in the last few years, in the area of metal-organic vapor phase epitaxy (MOVPE).

In the first part of the talk, I will focus on our group's first demonstration of delta doping and modulation-doped Aluminum Gallium Oxide/ Gallium Oxide heterostructures grown using metal organic vapor-phase epitaxy (MOVPE) towards achieving high electron mobility. Growth of delta-doped (010) β-Ga_2O_3 films is performed by Agnitron Agilis MOVPE reactor with TEGa, O_2 and silane as precursors and argon as carrier gas. Delta doping of β-Ga_2O_3 is achieved by interrupting the growth of β-Ga_2O_3 and supplying silane to the reactor with purge steps before and after the flow of silane. Multiple samples are grown under varying silane flows to study silicon incorporation inβ-Ga_2O_3. CV measurements are used to characterize the sheet charge density and FWHM of the silicon delta sheet. SIMS measurements are used to estimate the concentration of silicon donor atoms in β-Ga_2O_3. Sheet charge density extracted from CV measurements is in the range of 2×10^{12} cm^{-2} and 1×10^{13} cm^{-2}. Sharp delta doping profiles are achieved by controlling the surface riding of silicon donors. Using a delta-doped β-$(Al_{0.26}Ga_{0.74})_2O_3$ barrier layer, a room temperature electron sheet charge density as high as 1×10^{13} cm^{-2} is realized at the β-$(Al_{0.26}Ga_{0.74})_2O_3/\beta$-$Ga_2O_3$ heterojunction. The electron sheet charge did not exhibit freeze out at 90 K, confirming degenerate behavior. This value is the highest reported degenerate electron density in β-$(Al_xGa_{1-x})_2O_3/\beta$-$Ga_2O_3$ material system.

In the second part of the talk, I will discuss MOVPE-regrown selective area ohmic contacts with resistance as low as 1×10^{-4} ohm cm^2. This is particularly enabled by the large growth temperature window of MOVPE-grown homoepitaxial (010)-oriented Ga_2O_3, resulting in excellent material growth at growth temperatures as low as 600°C. These early results on delta doping, modulation doping and the large growth temperature window for β-Ga_2O_3 homoepitaxy show the potential of the MOVPE technique for achieving high quality UWBG thin film and heterostructures towards applications in high frequency and high power electronics.

10:25am **LI-WeM1-6 Selection Criteria for Small Inhibitor Molecules in Area-Selective Atomic Layer Deposition**, *Marc Merkx, P. Yu, J. Li,* Eindhoven University of Technology, Netherlands; *D. Hausmann,* Lam Research Corp.; *T. Sandoval,* Universidad Técnica Federico Santa Mariá, Chile; *E. Kessels, A. Mackus,* Eindhoven University of Technology, Netherlands **INVITED**
Implementing vapor-phase dosing of small inhibitor molecules in advanced atomic layer deposition (ALD) cycles is currently being considered to enable area-selective ALD. When using small inhibitor molecules, it can be challenging to completely block precursor adsorption, due the inhibitor size and the relatively short vapor-phase exposures. This work aims at providing a framework for the selection of small inhibitor molecules such that area-selective ALD with a high selectivity can be achieved. In previous work, we showed that small inhibitor molecules typically adsorb in a mixture of bonding configurations, and that not all bonding configurations block precursor adsorption equally well.[1]

Inhibitor selection requires consideration of the packing of inhibitors, inhibitor bonding configurations, the inhibitor binding strength, and intermolecular interactions. As a model system, the adsorption of acetic acid ($C_2H_4O_2$), acetylacetone (Hacac, $C_5H_8O_2$), and 2,2,6,6-tetramethyl-3,5-heptanedione (TMHD, $C_{11}H_{20}O_2$) was studied. Infrared (IR) spectroscopy shows that TMHD has the highest efficiency for blocking bis(diethylamino)silane (BDEAS) precursor adsorption. In terms of surface packing, random sequential adsorption (RSA) simulations [2] indicate that TMHD adsorbs in a lower surface density as compared to acetic acid and Hacac, but due to its larger size still covers a larger fraction of the non-growth area. Density functional theory (DFT) calculations reveal that attractive interactions with incoming BDEAS molecules, which cause a loss of selectivity when using Hacac,[1] are less likely to occur when using TMHD due to steric limitations. Correspondingly, IR spectroscopy shows less inhibitor displacement by the BDEAS precursor than for acetic acid and Hacac.

The model system suggests that using a more bulky inhibitor is beneficial for precursor blocking, as a larger size helps to shield the reactive group of the inhibitor from interacting with the incoming precursor. Overall, both the packing and stability of the inhibitor on the surface need to be as high as possible for effective precursor blocking, where the stability is affected by the bonding of the inhibitor with the surface and potential interactions with incoming precursors. The mechanisms that affect precursor blocking will be discussed within a framework for selecting small inhibitor molecules.

[1] Merkx *et al., Chem. Matter.***32**, 3335 (2020)

[2] Khan *et al., Chem. Matter.***30**, 7603 (2018)

10:45am **LI-WeM1-10 Ligand-Exchange Reactions Using Silane Precursors Containing Different Ligands: Pathways for Selective Thermal Atomic Layer Etching**, *Ann Lii-Rosales, V. Johnson, A. Cavanagh, S. Sharma, S. George,* University of Colorado Boulder **INVITED**
The ligand-exchange reaction is an effective pathway for thermal atomic layer etching (ALE) of metal oxides. The metal oxide is usually fluorinated by HF to make metal fluoride. Then, the metal fluoride can undergo ligand-exchange reactions with a precursor molecule. Depending on the choice of ligands on the precursor, ligand-exchange can produce stable and volatile etch products. Silanes are important precursors for ligand-exchange with metal fluorides because silicon forms strong Si-F bonds. In addition, silicon can bind to a variety of ligands including CH_3, Cl, H and $N(CH_3)_2$. This study examined ligand-exchange reactions with metal fluorides using various silane precursors such as $SiCl_4$, $SiCl_2(CH_3)_2$ and $SiH(CH_3)_2Cl$. The investigations were performed with *in situ* mass spectrometry experiments to detect the ligand-exchange products and etch species during temperature ramps from 30-520°C.

For the reaction of $SiCl_4$ with SnF_4 powder, $SiCl_4$ was observed to undergo complete F-Cl exchange with SnF_4 powder to produce SiF_4. The F-Cl exchange also produced $SnCl_4$ as the volatile etch species at 150°C. Calculations of the sequential ligand-exchange required to convert SnF_4 to $SnCl_4$ also confirmed the favorability of these reactions. In contrast to $SiCl_4$, $SiCl_2(CH_3)_2$ has both Cl and CH_3 ligands that can be involved in ligand-exchange. The reaction of $SiCl_2(CH_3)_2$ with SnF_4 powder produced $SiF_2(CH_3)_2$, and $SnCl_4$ and $SnFCl_3$ as etch species. No CH_3-containing Sn species were observed in the mass spectra indicating the preference of F-Cl ligand-exchange. In addition, $SnCl_4$ etch species did not appear until a much higher temperature of 300°C. This may be attributed to the lower Cl content in $SiCl_2(CH_3)_2$.

$SiH(CH_3)_2Cl$ contains Cl, CH_3 and H ligands that may be involved in ligand-exchange. The mass spectra revealed that $SiF_2(CH_3)_2$ was the ligand-exchange product with SnF_4 powder. $SiF_2(CH_3)_2$ was observed at 150°C and indicates both F-Cl and F-H exchange. In contrast, the SnH_2Cl_2 etch product was not detected until 350°C. HF was monitored throughout the temperature ramp and H_2 was also observed at T > 400°C. These products clearly indicate that H is transferred to the SnF_4 powder. Moreover, *ex situ* XPS measurements of the SnF_4 powders after ligand-exchange revealed the presence of metallic Sn. This indicates that the H on the precursor molecule can serve as a reducing agent. The reactions between silanes with SnF_4 and other metal fluoride powders are revealing the details of the ligand-exchange reactions during thermal ALE. These details can lead to pathways for selective thermal ALE by varying the temperature and ligands on the precursor molecule.

11:15am **LI-WeM1-16 Superconformal Trench Filling With $Hf_{1-x}V_xB_2$ Using Two-Precursor Chemical Vapor Deposition**, *Kinsey Canova, Z. Zhang, G. Girolami, J. Abelson,* University of Illinois at Urbana Champaign **INVITED**
Seamless filling of deep recessed features is an ongoing challenge in the fabrication of advanced microelectronic devices.We demonstrate a new CVD method that affords superconformal films (i.e., faster growth deeper

in the feature) based on the use of two precursor molecules with sharply contrasting adsorption and reaction properties.One precursor adsorbs strongly but reacts relatively slowly; the other precursor adsorbs less strongly but reacts more rapidly. The strongly adsorbing precursor inhibits the overall growth rate, but it is progressively consumed along the trench sidewalls.Consequently, the inhibition effect diminishes and fast growth from the second precursor affords an increase in growth rate with trench depth.The resulting thickness profile is superconformal (V-shaped), which leads to seamless fill.We show that the needed adsorption and reaction kinetics exist using $V(N(CH_3)_2)_4$ as the inhibiting precursor and $Hf(BH_4)_4$ as the second precursor; together, these afford films of the refractory metallic ceramic $Hf_{1-x}V_xB_2$. Under practical growth conditions, we obtain seam-free filling up to a depth-to-width (aspect) ratio of 10.

We model the kinetics based on the dependence of the film growth rate and composition x on the local pressure (flux) of each precursor, with ballistic transport of precursor between surfaces within the trench.The model uses a Langmuirian framework in which precursors compete for available adsorption sites and adsorbates have different reaction rates.The model shows that there is a limiting aspect ratio for a given set of kinetic coefficients.Here, the growth of $Hf_{1-x}V_xB_2$ facilitates comparisons with the model because the film composition varies with depth; this compositional change reflects the changes in the surface coverage and reaction rate of each precursor as the gas phase composition changes with depth.In future work, it will be desirable to use two precursors that afford the same film, so that the resulting composition will be uniform within the trench.We will suggest precursor combinations that are good candidates for superconformal trench filling with other technologically-relevant materials.

11:35am LI-WeM1-20 Pyroelectric Heat Detection for *In Situ* Measurement of ALD Reaction Heat, *Ashley R. Bielinski, E. Sprague-Klein, B. Phelan, A. Martinson,* Argonne National Laboratory **INVITED**
Atomic layer deposition (ALD) is used to deposit a wide range of materials for both academic and industrial applications, yet experimental resolution of the kinetics, thermodynamics, and mechanisms for even the most well-studied ALD half-reactions remains insufficient to test computational models.*In situ* measurements of the heat generated by ALD half-reactions could provide new insight into the complex chemical processes at play during ALD. ALD reactions have been observed to cause >10°C temperature changes on high surface area substrates like nanoparticles or metal organic frameworks, but the relatively small temperature changes (<0.1°C) predicted for planar substrates are much more difficult to accurately measure.Additionally, many reactions exhibit kinetics that are on the same order as or faster than the 10ms to 1s sampling times of *in situ* measurement techniques commonly used for ALD such as mass spectrometry, ellipsometry, or quartz crystal microgravimetry.

We present a pyroelectric calorimeter with thermal and temporal resolution down to 0.1 $\mu J/cm^2$ and 50 ns.This probe enables the time-resolved measurement of individual ALD half-cycles, enabling comparison to first-principles computational predictions.The calorimeter hardware was designed and optimized for operation under ALD conditions.Laser calibration was combined with a mathematical model of the transient thermal and electrical response to provide quantitative measurements of heat generation rates.Trimethylaluminum (TMA) was reacted with a planar, hydroxylated ALD-alumina surface to produce 96 $\mu J/cm^2$ over a reaction time of ~30 ms.Relative to other in situ measurement techniques, calibrated pyroelectric calorimetry offers a faster and more sensitive probe of ALD reactions.In addition to kinetic and thermodynamic measurements of steady state growth reactions, this technique may also provide the necessary precision to study the complexities and far sub-monolayer growth during nucleation or selective deposition.

This material is based upon work supported by Laboratory Directed Research and Development (LDRD) funding from Argonne National Laboratory, provided by the Director, Office of Science, of the U.S. Department of Energy under Contract No. DE-AC02-06CH11357

11:55am LI-WeM1-24 pH Sensor Tattoo, *Katrin Unger, A. Coclite, F. Greco,* Graz University of Technology, Austria **INVITED**
Temporary tattoo-based body sensors have gained high attention in the expanding field of tracking physiological biomarkers, such as the pH level of sweat. Because of its ultra-conformal adhesion towards the skin while providing excellent water vapor transmission, temporary tattoo sensors can react already at minimal sweat production but can also cope with large amounts of sweat. Within the presented work, a skin pH sensor tattoo is presented, made of a temporary tattoo paper, screen printed polymer electrodes and a pH responsive hydrogel. While so far tattoo papers have

been functionalized only by solution-based methods, within this study for the first time a vapor-based coating routine, named initiated chemical vapor deposition, was utilized to deliver a smart hydrogel. The resulting sensor tattoo can be easily transferred on the skin and shows an outstanding conformability to the topography of the epidermis. The measured morphology properties of the layers demonstrate excellent process controllability of the desired electrode width, hydrogel thickness and shielded areas. The pH responsive hydrogel exhibits a reversible pH responsive swelling of 24% to 37%, in respect to the dry state, at pH 4 and pH 6, respectively. With impedance spectroscopy the phase shift at 1000 Hz is identified as an excellent pH-related parameter of the sensor, which can only be ascribed to the presence of the hydrogel layer. The sensor can be triggered and read out also by a cheap and light-weight Arduino setup, verifying the applicability as a wearable sensor device.

12:15pm LI-WeM1-28 Closing Remarks and Thank You's, *Svitlana Pylypenko,* Colorado School of Mines
Thank you for attending today's session! Please note that our afternoon sessions begin at 12:50 pm EDT. Remember to check out the AVS 67 On Demand Sessions which are available in the mobile app and online scheduler.

Live Session
Room Live-2 - Session LI-WeM2

Wednesday Morning Live Session II: Biological, Environmental Interfaces and New Directions in the AVS
Moderators: Sidney Cohen, Weizmann Institute of Science, Israel, Caitlin Howell, University of Maine

10:00am LI-WeM2-1 Welcome and Opening Remarks, *Sidney Cohen,* Weizmann Institute of Science, Israel
Welcome to the AVS 67 Virtual Symposium. We hope you will enjoy the event!

10:05am LI-WeM2-2 ASSD 2021 Peter M.A. Sherwood Mid-Career Professional Award Talk: Information from complexity - Making Sense of the Mess Created by ToF-SIMS, *Daniel Graham[1],* University of Washington, Seattle*; M. Taylor,* Pacific Northwest National Laboratory*; L. Gamble,* University of Washington, Seattle **INVITED**
ToF-SIMS data from even simple surfaces is complicated. This complexity is a blessing and a curse it encodes information about the structure and composition of surface molecules and presents a massive data processing challenge to decode this information from within the hundreds of spectral peaks present in a typical spectrum. This challenge is further complicated by the fact that modern ToF-SIMS instruments can produce sub-micron resolution images where each pixel contains a full mass spectrum. This imaging modality can be combined with sputtering beams to enable depth profiles of materials which can contain multiple images acquired throughout the depth of a material. The result of this is a chemically rich, spatially mapped data matrix containing information about the chemistry, location, structure and composition of surface species. Such data matrices can contain tens of thousands (2D data) to millions (3D data) of spectra taking up 10s to 100s of GB. The challenge then becomes how to process this data and extract the gems of information encoded within the fragmentation patterns of each spectrum. To address these issues many researchers have applied a wide variety of multivariate and other advanced data analysis methods to ToF-SIMS data in order to extract useful information that can be used to aid in materials characterization.

In spite of this complexity, ToF-SIMS has found wide application in the analysis of organic and biological materials as it presents a method that can provide specific chemical information and precise localization of surface compounds.This can be particularly useful in the analysis of biomaterials, where understanding of the surface chemistry is critical to device success, and in the analysis of cells and tissues where mapping chemical changes can elucidate information that can be useful in understanding disease progression and possibly prevention.

In this talk I will demonstrate how the application of multivariate, and other advanced analysis methods, can facilitate digesting ToF-SIMS data and extracting useful information that can help solve problems in organic and biological materials characterization.Examples will be shown from spectral and image analysis (2D and 3D), along with ways we have explored

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[1] **ASSD 2021 Peter M. A. Sherwood Mid-Career Professional Awardee**

to enable the characterization of topographically challenging samples used in tissue engineering.In addition I will highlight the importance of sharing tools developed for this type of analysis and describe tools we have created to facilitate multivariate analysis throughout the scientific community.

10:25am LI-WeM2-6 High Throughput Discovery of Novel Antiviral Polymers for Reducing SARS-CoV-2 Surface Transmission and Improving PPE, *Xuan Xue*, J. Duncan, C. Coleman, J. Ball, C. Alexander, M. Alexander, University of Nottingham, UK **INVITED**

Respiratory diseases caused by viruses have become a serious global public health concern. The ongoing COVID-19 global pandemic has threatened people's lives and impacted socioeconomical development since December 2019. To date, Severe Acute Respiratory Syndrome Coronavirus 2 (SARS-CoV-2) appears to spread easily in droplets in the air and via surfaces. Following evidence of virus contamination of surfaces, the fomite transmission of respiratory viruses has been highlighted as a potential infection route in the pandemic. In addition, healthcare workers in the front line of the COVID-19 outbreak response are exposed to the risk of SARS-CoV-2 infection daily. Personal protective equipment (PPE) is their main defence against viral contamination and to eliminate viral transfer from infected patients. Antiviral effective PPE materials, that can be self-disinfected and ideally worn for prolonged time, need to be developed.

In our study, a range of commercially available PPE materials and common surface plastics have been evaluated using live virus in Biosafety Level 3 (BSL-3) laboratory to enable a recommendation of which existing polymers should be employed for optimal viral inactivation on PPE. Detachment assays using virus like particles (VLPs), which do not have an infection risk, were used to investigate secondary spreading of viruses invoked by movement and doffing of PPE with both liquid and air flow systems explored to mimic actual environmental conditions. The persistence of live SARS-CoV-2 on these surfaces were evaluated and compared under varied temperature and relative humidity conditions.

In order to develop new polymers for PPE and fomite transmission control, high throughput polymer microarrays developed at the University of Nottingham, were used to identify novel anti-SARS-CoV-2 polymer materials.

10:45am LI-WeM2-10 Machine-Learning-Assisted Photonics, Z. Kudyshev, A. Kildishev, V. Shalaev, **Alexandra Boltasseva**, Purdue University, USA **INVITED**

We coupled adversarial autoencoder deep generative network with adjoined topology optimization technique to advance metasurface design. The proposed approach speeds up the optimization search of highly efficient metasurface designs and also provides unparalleled control over the compressed design space distribution. The latter fact assures scalability of the approach to highly-constrained optimization problems.

Nanophotonics can provide solutions to interdisciplinary challenges in energy [1], quantum IT [2] and other areas. Addressing multifaceted problems require highly-constrained optimization of the device design, due to inherent complexity and multi-disciplinary nature of any practical application. Conventionally, adjoint [3] and genetic [4] optimization methods have been used to address such optimization tasks. However, the computational power requirement of these methods scales up with the number of constraints. This fact substantially limits the applicability of conventional optimization techniques to real-life applications. Within this work, we merged the adjoint topology optimization technique with adversarial autoencoders (AAE) to achieve significant improvement in the optimization search of non-trivial nano-antenna-based metasurface designs [5]. Particularly, we demonstrated that the proposed approach ensures not only the efficient optimization search of high-performance metasurface designs but also provides unparalleled control over the compressed design space distribution. The latter fact assures scalability of the approach to highly-constrained optimization problems. To showcase AAE-assisted method, we optimized a metasurface thermal emitter for thermophotovoltaic (TPV) applications. Compared to an adjoint-based topology optimized design with 92% efficiency of the thermal emission reshaping, the proposed method provides three times speed-up and gives 98% efficiency. The proposed approach can be adapted to a broader scope of the problems in optics.

References

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[5] Z. A. Kudyshev, A. V. Kildishev, V. M. Shalaev, and A. Boltasseva, "Machine-Learning-Assisted Metasurface Design for High-Efficiency Thermal Emitter Optimization," arXiv Preprint arXiv:1910.12741, 2019.

11:15am LI-WeM2-16 STM Measurements of Spin-Polarized Currents Carried by the Topological Surfaces States of SmB_6 Nanowires, *Vidya Madhavan*, University of Illinois at Urbana-Champaign **INVITED**

Incorporating relativistic physics into quantum tunneling can lead to exotic behavior such as perfect transmission via Klein tunneling, or apparent faster than light travel. In this talk I will describe an experiment that demonstrates `helical tunneling', a process where spin-polarized electrons can be transmitted in a nominally time-reversal invariant fashion. To do this we use nanofabrication techniques to attach SmB_6 nanowires to the end of scanning tunneling microscope tips. SmB_6 is a topological Kondo Insulator which has been proposed to be an ideal topological system with Dirac fermions naturally dominating the density of states near Fermi level. The SmB_6 nanowire tips are used to image the canonical spin density wave material, $Fe_{1.03}Te$, which hosts a bicollinear spin order with a Neel temperature of ~50 K. STM images show a superstructure with the periodicity of the antiferromagnetic order, indicating spin-selective tunneling from the nanowire. The antiferromagnetic order becomes invisible above 10 K, far below the Neel temperature, together with the diminishing topological surface states. We further confirm a smoking gun signature of spin current generated by Dirac fermions, i.e., the contrast reversal of the antiferromagnetic order at opposite bias voltages. These findings establish interacting topological systems like SmB_6 as ideal conduits for spin-polarized topological currents and reveal an unexpected and unexplored consequence of relativistic tunneling.

11:35am LI-WeM2-20 Molecular Nanostructures on Metals vs. Graphene: Towards Preserving Functional Properties, *Meike Stöhr,* University of Groningen, Netherlands **INVITED**

To preserve the (functional) properties of either individual adsorbates or well-ordered molecular assemblies upon adsorption on solid surfaces, the molecule substrate interactions have to be generally relatively weak. This can be achieved by introducing a decoupling layer between (metallic) surface and molecules. Among others, thin insulating layers of either NaCl or a single layer of hBN have been shown to be very useful to this end. The chemical inertness and the low density of states near the Fermi level also make graphene a good choice as a buffer layer to decouple adsorbed molecules from the underlying (metallic) substrate. Importantly, this holds the promise to preserve the intrinsic properties of the adsorbed species such as magnetic or catalytic properties. On the other hand, molecular self-assembly on graphene can be also employed as a promising method for tuning the electronic properties of graphene (doping or band gap opening) on a macroscopic scale while for this purpose, the molecule graphene interaction has to be larger than a mere physisorptive one.

Here we will discuss the structural and electronic properties for 1,3,5-benzenetribenzoic acid on graphene/Cu(111), for which different coverage dependent assemblies were observed. [1] We could demonstrate that the underlying Cu surface influences the structural arrangement of the molecules. With respect to the electronic properties, angle-resolved photoemission spectroscopy measurements showed n-doping of graphene. For parahexaphenyl-dicarbonitrile (NC-Ph$_6$-CN) on graphene, we observed the arrangement of a close-packed structure with a peculiar shift of every 4th molecule independent of coverage. We concluded that the screening properties of graphene are responsible for this effect since such a shift was neither observed for the case of metallic substrates nor for the bulk phase. [2] Adding Cu adatoms to submonolayer coverage of NC-Ph$_6$-CN resulted in the formation of metal-organic coordination networks with varying arrangements in dependence of the stoichiometry between molecules and Cu atoms. With scanning tunneling spectroscopy we characterized the electronic properties and could identify differences between the different assembly structures. [3] On the basis of the self-assembly process of tetracyanophenyl porphyrins before and after coordination with Co-atoms on Au(111), the influence of molecular coverage on decoupling could be demonstrated. [4]

[1] J. Li et al., J. Phys. Chem. C 120 (2016) 18093; N. Schmidt et al., unpublished.

[2] N. Schmidt et al., Chem. Eur. J. 25 (2019) 5065.

[3] J. Li et al., J. Phys. Chem. C 123 (2019) 12730.

[4] B.D. Baker et al., J. Phys. Chem. C 123 (2019) 19681.

11:55am **LI-WeM2-24 BID 2020-2021 Early Career Awardee Talk: Molecular-Level Insights Into Novel Wet Adhesion Systems Found in the Natural World**, *Joe Baio*[1], Oregon State University   **INVITED**
From sticky frog tongues to the superhydrophobic cuticles of springtails - the natural world is full of novel materials. Recent developments of surface analytical methods now allow provide a means of characterizing the structure and arrangement of molecules at complex biological interfaces. Many animals have adapted to a range of environmental surfaces by evolving a wet adhesion process. Previous studies of these adhesion mechanisms have focused almost exclusively on the mechanical and kinematic aspects of adhesion, and not on the molecular interactions at the fluid – substrate interface. In the work presented here, we first probe the molecular interactions between the adhesive fluid taken from lady beetles (*Cocinella septempunctata*) on two model substrates (one polar and one non-polar) with vibrational sum frequency generation (SFG) spectroscopy. The resulting SFG spectra demonstrate that during adhesion to a polar surface, fatty acids within the fluid form a highly ordered layer at the substrate surface. While on a non- polar surface, the mechanism changes and some other hydrocarbon species present within the fluid orders at the interface. The discussion will then be expanded to include some recent experiments identifying the structure of the biomolecules that make up the wet adhesive mechanism molecules present at a frog's tongue. Frogs capture their prey with a highly specialized tongue. Recent studies indicate this tongue is covered with fibril-forming mucus that acts as a pressure sensitive adhesive. However, no analysis of the interfacial chemistry of frog tongue mucus has been performed.Previous studies of mucus from other animals suggest that mucus from a frog's tongue consists of mucins—serine-, threonine-, and proline-rich glycoproteins. Therefore, the authors expect to observe chemical bonds associated with glycoproteins, as well as fibrils formed at the mucus–tongue interface. To test this hypothesis, we collected both near-edge x-ray absorption fine structure (NEXAFS) microscopy images and SFG vibrational spectra from layers of mucus left after frog tongue strikes on cleaned glass slides. NEXAFS imaging demonstrates a uniform distribution of amide, hydroxyl, and carbon–carbon bonds across the mucus surface. SFG spectra reveal that glycoproteins are well-ordered at the mucus–tongue interface.

12:15pm **LI-WeM2-28 Closing Remarks and Thank You's**, *Caitlin Howell*, University of Maine
Thank you for attending today's session! Please note that our afternoon sessions begin at 12:50 pm EDT. Remember to check out the AVS 67 On Demand Sessions which are available in the mobile app and online scheduler.

[1] **BID 2020-2021 Early Career Researchers Award**

Wednesday Afternoon, October 27, 2021

Live Session
Room Live - Session LI-WeA1

Wednesday Afternoon Live Session I: Controlling Matter at the Ultimate Limits

Moderators: Eric Joseph, IBM T.J. Watson Research Center, Arthur Utz, Tufts University

12:50pm LI-WeA1-1 Welcome and Opening Remarks, *Eric Joseph,* IBM T. J. Watson Research Center
Welcome to the AVS 67 Virtual Symposium! We hope you will enjoy the event!

12:55pm LI-WeA1-2 The Development of Atomic Layer Processes for Scaling & Future Device Architectures, *Rudy Wojtecki,* International Business Machines (IBM) - Almaden Research Center **INVITED**
A major aspect governing progress in electronic technologies is the ability to control or guide the deposition or subtraction of thin films.As the semiconductor community continues scaling, interfaces and surfaces become increasingly important. Traditional deposition and subtraction methods then may not be sufficient in future technology nodes as they may damage or amorphize surfaces to an otherwise crystalline and risk device performance or yield.Atomic layer processes present methods to preserve these interfaces by taking advantage of surface reactivities to either add or subtract a material one atomic layer at a time.Furthermore, these offer the opportunity to more broadly extend fabrication capabilities that may enable integration schemes for alternative computing architectures such as neuromorphic type devices.Within this space area selective depositions (ASD) offer a powerful tool to direct film growth from a chemically distinct surface in a self-aligned process with the potential to relax down-stream processing such as overlay requirements. There are many examples for the integration of these techniques to encapsulate and inhibit the oxidation of a metal or introduce surface topography from an underlying pre-pattern, for instance. Guiding this deposition is particularly challenging as it requires the careful interplay between deposition precursors and inhibiting (or activating) layers. Achieving this control, through judicious design and engineering of a surface affords exquisite control over the film characteristics such as composition and thickness.The development of processes that extend these capabilities will be discussed that include strategies to enable ASD with surface topography using an area selective polymerization that provides control over inhibitor thickness which acts as an effective inhibiting material.In addition, the combination of ASD with a patternable organic monolayer will be discussed that provides a versatile additive lithography platform, where a broad range of desired feature geometries can be readily generated.In the pursuit of methods to broaden the application of ASD processes fundamental insights to desirable material characteristics for these processes are useful parameters to consider in future ASD processes such as supramolecular interactions between inhibitors and chemical crosslinking.

1:15pm LI-WeA1-6 Recent Innovations in Tof-Sims and Their Industrial Applications, *Julia Zakel,* IONTOF GmbH, Germany **INVITED**
Time-of-flight secondary ion mass spectrometry (TOF-SIMS) is known to be an extremely surface sensitive analytical technique. It provides detailed elemental and molecular information about surfaces, thin layers, interfaces, and full three-dimensional analysis of the sample.In our contribution we will provide an overview on recent advances in TOF-SIMS instrumentation and data evaluation that are extending existing applications or even make new applications accessible. Among the discussed improvements are key values that are inherent for a dedicated TOF-SIMS instrument as mass resolution and lateral resolution, as well as improvements that are based on the integration of additional analytical components or due to the combination with complementary techniques.The latest technology step now pushes the standard lateral resolution of dedicated TOF-SIMS instruments to the sub 50 nm region. Best achieved values are even in the 20 nm range and therefore not far away from the physical limit given by the size of the sputter cascade. While new ion sources expanded the usability of SIMS instruments, SIMS analyzers lacked the required mass resolution and mass accuracy, required for the thorough investigation of molecular materials. One major challenge is based on the enormous number of molecules in the mass range of interest. An important step in order to reduce the number of interpretation possibilities is to improve the mass resolution and the mass accuracy. State-of-the-art TOF-SIMS instruments are reaching a mass resolution in the range of 30.000 and a mass accuracy in the range of few ppm. This improves the analytical possibilities compared to the previous instrument

generation and reduces the complexity of data evaluation and interpretation.MS/MS capabilities are required in order to further increase identification possibilities. In this respect it is also of high importance to generate the MS/MS spectra at high mass resolution and high mass accuracy. We will discuss an MS/MS approach that is fully integrated into a TOF analyzer. The benefit of this approach is that it can easily be integrated in the given analysis scheme and data format.While the discussed performance represents the limit attainable with recent TOF-SIMS instruments, further improvement is achieved by combining an Orbitrap™-based mass analyzer with a high-end TOF-SIMS system (Hybrid SIMS). The instrument provides highest mass resolution (> 240,000) and highest mass accuracy (< 1ppm) with high lateral resolution cluster SIMS imaging. We will present data acquired on a Hybrid SIMS instrument demonstrating fast and robust identification of main constituents in unknown samples.

1:35pm LI-WeA1-10 Microscopic Visualization of Electron Correlations in TMD Moiré Superlattices, *Shaowei Li,* University of California at San Diego **INVITED**
Van der Waals heterostructures of atomically thin layered materials provide an exciting new platform to design and fabricate novel electronic and optical devices. Through the precise control of the stacking order and the twist angle between two adjacent layers, the moiré superlattice can lead to tunable narrow electronic minibands. With the unique ability to image the structural and electronic properties of low-dimensional materials at the atomic-scale, scanning tunneling microscopy and spectroscopy provide an opportunity to study the strongly correlated physics with real-space visibility. In this talk, I will present the real-space visualization of the localized correlated electron states in the closely aligned WS_2/WSe_2. These correlated states have shown the promise of exotic electron transfer properties such as charge order states, electron transfer insulator, Mott insulator, and superconductivity.

2:05pm LI-WeA1-16 Characterizing Unconventional Strain and Bending in 2D Materials and Heterostructures with Aberration-Corrected STEM, *Pinshane Huang,* University of Illinois at Urbana-Champaign, USA*; E. Han, J. Yu, C. Lee,* University of Illinois at Urbana Champaign*; D. Luo,* University of Illinois at Urbana Champaign*; A. Khan,* University of Illinois at Urbana Champaign*; T. Santos,* University of Illinois at Urbana Champaign*; S. Kang, W. Zhu, N. Sobh, A. Schleife, B. Clark, E. Ertekin, A. van der Zande,* University of Illinois at Urbana Champaign **INVITED**
The properties of 2D materials can be strongly impacted by the presence of defects, strain, and out-of-plane bending.In this talk, we discuss our development of techniques that use aberration-corrected scanning transmission electron microscopy (STEM) to measure the unconventional strain and bending of 2D materials and heterostructures with unprecedented precision.

First, we will discuss our studies of defect-induced strain in 2D materials. High-precision characterization of defects in 2D materials remains challenging because they are irradiation sensitive, making it difficult to achieve high resolution and signal-to-noise structural data without modifying the intrinsic structure. Here, we apply deep learning techniques based on convolutional neural networks to process large volumes of atomic-resolution images of the 2D transition metal dichalcogenide $WSe_{2-x}Te_{-x}$. By class-averaging hundreds of nominally identical defects, we measure the local picometer-scale strain fields around single vacancies with 0.2 picometer precision, and we observe previously-unseen radial strain oscillations [1].

Second, we will discuss bending in 2D materials and heterostructures.Understanding the bending of two-dimensional materials and heterostructures is crucial for the development of next-generation electronics including deformable electronics, and nanoelectromechanical systems. Here, we show that electron microscopy can provide a powerful platform for measuring the bending of 2D materials. We use aberration-corrected STEM to image graphene and 2D heterostructures draped over atomically sharp hexagonal boron nitride steps. This approach enables atomic-resolution studies of their bending conformation, producing insight into both the bending stiffness and mechanisms of bending. We find that the bending stiffness of multilayer 2D materials is a strong function of bending angle, tuning by almost 400% for trilayer graphene [2]. This unusual behavior results from the atomic-scale bending mechanism in 2D multilayers, which is dominated by interlayer shear and slip. In combination with density functional theory (DFT) and continuum mechanics modeling, we derive a unifying model for bending in 2D materials and their heterostructures. Our findings have profound implications on 2D

heterostructures, where we demonstrate that the bending stiffness can be controlled by tailoring the interfacial interactions between individual atomic layers of 2D materials.

[1] Lee, C.-H. *et al.* Deep Learning Enabled Strain Mapping of Single-Atom Defects in 2D Transition Metal Dichalcogenides with Sub-picometer Precision. *Nano Lett.* (2020). doi:10.1021/acs.nanolett.0c00269

[2] Han, E. *et al.* Ultrasoft slip-mediated bending in few-layer graphene. *Nat. Mater.* **19**, 305–309 (2020).

2:25pm LI-WeA1-20 Chemistry in Confined Spaces: 2D-Porous Silicates on Metal Supports*, J. Anibal Boscoboinik,* Brookhaven National Laboratory **INVITED**
Confinement effects can give rise to interesting properties in the chemistry and physics of small molecules. In this talk, we will explore 2D-porous silicates on a metal support. These can trap noble gases (Ar, Kr, and Xe) at elevated temperatures (>300 K) within the silicate structure and at the interface with the metal. They can also affect chemical reactions taking place on the metal surface, and the case of water formation from H_2 and chemisorbed O will be used to illustrate this effect.

2:45pm LI-WeA1-24 Basic Science Needs for Transforming Manufacturing Through Atomically Precise Manufacturing*, Cynthia Jenks, H. Lee,* Oak Ridge National Laboratory*; J. Lewis,* Harvard University **INVITED**
In March of 2020, the Department of Energy, Office of Science, Basic Energy Sciences, ran a workshop aimed at providing strategic research directions that could ultimately transform manufacturing as we know it through a better understanding of fundamental science. The attendees at this workshop on Basic Research Needs for Transformative Manufacturing developed five priority research directions to revolutionize manufacturing. These directions include the following: (1) achieve precise, scalable synthesis and processing of atomic-scale building blocks for components and systems; (2) integrate multiscale models and tools to enable adaptive control of manufacturing processes; (3) unravel the fundamentals of manufacturing processes through innovations in operando characterization; (4) direct atom and energy flow to realize sustainable manufacturing; and (5) co-design materials, processes, and products to revolutionize manufacturing. This talk with provide an overview of these five areas with a particular emphasis on the priority research direction on atomically precise manufacturing. Atomically precise materials and molecules would lead to unparalleled structures and functions that, at the moment, are unattainable. There are several scientific questions to consider to achieve precision manufacturing of materials and molecules. W*hat are the mechanisms needed for manufacturing multiscale, atomically and molecularly precise materials? How can basic research uncover structure-function relationships across multiple scales in components and systems? How can chemical processes readily be scaled from laboratory results?*

3:05pm LI-WeA1-28 Closing Remarks and Thank You's*, Art Utz,* Tufts University
Thank you for attending today's session! Remember to check out the AVS 67 On Demand Sessions which are available in the mobile app and online scheduler until 11/30/21 and then in the AVS Technical Library for all Platinum Members. We will see you at AVS 68 in Pittsburgh, PA, November 6-11, 2022!

Live Session
Room Live-2 - Session LI-WeA2

Wednesday Afternoon Live Session II: Stop Worrying and Learn to Enable Quantum Science
Moderators: Charles R. Eddy, Jr., Office of Naval Research Global - London, UK, Rachael Myers-Ward, U.S. Naval Research Laboratory

12:50pm LI-WeA2-1 Welcome and Opening Remarks*, Chip Eddy,* Office of Naval Research Global - London, UK
Welcome to the AVS 67 Virtual Symposium! We hope you will enjoy the event!

12:55pm LI-WeA2-2 X-Rays Approaching Neutrons: RIXS with Ultrahigh Resolution and Applied Magnetic Field to Study a Magon-spinon dichotomy in β-Li₂IrO₃*, Alex Frano,* University of California, San Diego **INVITED**
The family of tri-coordinated iridates have been identified as potential candidates supporting a Kitaev quantum spin liquid, in which spins fractionalize into emergent Majorana fermions and magnetic flux excitations. These quasiparticles acquire long-range topological entanglement and are ideal for fault-tolerant quantum computers. While the presence of additional interactions usually leads to conventional ordering, a dominant Kitaev exchange leads to QSL behavior after the magnetic order is suppressed by temperature or magnetic field, with signatures appearing in thermodynamic measurements and dynamical probes.

β-Li₂IrO₃ is an intriguing example of the complex interplay between Kitaev coupling and magnetic field. At low temperatures, an applied field rapidly suppresses the incommensurate spiral order and drives the system into a uniform field-induced zig-zag state, which are strongly intertwined due to Kitaev interactions. Moreover, a magnetic anomaly has been observed at 100K, with an onset in magnetization and a crossover in the heat capacity without causing true magnetic order. Although these results have been suggested to emerge from thermal fractionalization of the spins, very little is known about the low-energy magnetic excitations.

In this work, we present a comprehensive picture of the dynamical response of β-Li₂IrO₃ in an applied magnetic field. The spin excitations were measured using a high-resolution RIXS spectrometer, which identified dispersing spin waves reaching a maximum of 16meV, in perfect agreement with semiclassical calculations of the dynamical spin structural factor for the intertwined states. The low-energy magnon is superimposed by a broad continuum of excitations centered around 35meV, which is unaffected by the low-temperature ordered states but sensitive to the high temperature anomaly. This continuum is consistent with the onset of nearest neighbor correlations emerging from a dominant Kitaev energy scale, and alludes to the long coherence time of the fractional excitations in the proximate QSL phase.

1:15pm LI-WeA2-6 X-Ray Spectroscopies With Increased Resolution: Principles and Perspectives*, Lucia Amidani,* ESRF, France **INVITED**
In was only in the early 90s that the use of hard X-ray emission spectrometers to collect X-ray Absorption spectra was first suggested [1]. X-ray emission spectrometers based on Bragg's law achieve resolutions below 2 eV, a huge improvement compared to solid-state detectors whose resolution is only $150 - 200$ eV. With this technical improvement, the characteristic fluorescence of the excited atoms is collected with a resolution below the core-hole lifetime broadening, resulting in better-resolved XAS spectra [2]. Since then, the use of X-ray Spectroscopies with improved resolution exploded and dedicated synchrotron beamlines multiplied. Nowadays, these techniques are largely exploited in many diverse fields of science.

Lanthanides and actinides are among the elements that profit the most of the improved resolution because of their large core-hole lifetime broadenings. Indeed, the demonstration of principle was done on Dy L_3 edge XANES [1]. For actinides, the resolution at L_3 edge is largely improved, but the biggest boost was given to $M_{4,5}$ edges, whose conventional XANES are almost featureless. These edges probe directly the 5f states. With better-resolved spectra, the oxidation state can be easily determined and the spectral features that were invisible before bring information about the local coordination and the charge exchange with ligands [3,4].

The information encrypted in these spectra is enormous. Improved resolution makes it more readily available by disclosing details and allowing smaller differences to be appreciated. However, the interpretation often represent the bottleneck to the extraction of relevant information. In this respect, theoretical simulations are fundamental. Nowadays, we have several user-friendly codes that interprets the spectra starting from different approaches, focusing on the intra-atomic interactions or favouring the multi-atomic picture of the system studied.

In this talk, I will briefly introduce some of the techniques exploiting the improved resolution and then focus on their application to actinide science. I will present few examples illustrating the high potential of these techniques and the approach we use in our group to interpret the data [5–7].

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[1] K. Hämäläinen et al., Phys. Rev. Lett. **67**, 2850 (1991).

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[4] K. O. Kvashnina et al., J. Electron Spectrosc. Relat. Phenom. **194**, 27 (2014).

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1:35pm LI-WeA2-10 Exploring Materials, Surface Treatments and Junctions for Superconducting Quantum Circuits, *Martin Sandberg,* IBM
INVITED

Multifunctional material stacks compatible with high coherence superconducting quantum circuits could lead to more efficient circuit implementations. One material with a multitude of applications in optics and electronics is silicon-germanium (SiGe). Here we show that a Si/SiGe heterostructure can be incorporated in superconducting quantum circuits without any coherence degradation [1]. This opens pathways for on-chip optical to microwave transduction among other highly attractive applications.

In addition to the SiGe work we will show the effect of various in-situ surface treatments on flux tunable superconducting qubits in a hermetic package [2], as well as the effect of Two Level Systems (TLSs) in large junction Al/AlOx/Al Merged Element Transmons (MET) [3]. Our studies suggest that surface treatments can reduce the 1/f flux noise without necessarily reducing energy relaxation. For the MET qubits we find that large Al/AlOx/Al junctions contains very strongly coupled TLSs and exhibit large fluctuations in energy relaxation times. Despite the large junction area we still observe energy relaxation times higher than 200 microseconds over several hours of measurements for the best performing devices.

Reference:

[1] Investigating microwave loss of SiGe using superconducting transmon qubits

Martin Sandberg, Vivekananda P. Adiga, Markus Brink, Cihan Kurter, Conal Murray, Marinus Hopstaken, John Bruley, Jason Orcutt, Hanhee Paik

Appl. Phys. Lett. **118**, 124001 (2021)

[2] Effects of surface treatments on flux tunable transmon qubits

M. Mergenthaler,C. Müller, M. Ganzhorn, S. Paredes, P. Müller, G. Salis, V. Adiga,M. Brink,2 M. Sandberg, J. Hertzberg, S. Filipp, and A. Fuhrer

arXiv:2103.07970

[3] Merged-Element Transmons: Design and Qubit Performance

H. J. Mamin, E. Huang, S. Carnevale, C. T. Rettner, N. Arellano, M. H. Sherwood, C. Kurter, B. Trimm, M. Sandberg, R. M. Shelby, M. A. Mueed, B. A. Madon, A. Pushp, M. Steffen, D. Rugar.

arXiv:2103.09163

2:05pm LI-WeA2-16 Engineering Superconducting Quantum Systems, *J. Yoder,* **Donna Ruth Yost,** MIT Lincoln Laboratory **INVITED**
Development of qubits – the fundamental logic element of a quantum processor – is transitioning from a scientific discovery phase to an engineering pursuit. In order to reach the scale needed for a broad range of quantum computing applications, key challenges now lie in engineering these quantum systems at every level from individual qubits to highly complex circuits. In this talk I will describe our quantum engineering of superconducting qubit systems, including our approach to predictive control of individual qubits and our three-tier stack platform for extending high-coherence circuits to increasing scale and complexity.

2:25pm LI-WeA2-20 Micro-Scale Fusion and Neutron Generation from Nanowire Arrays Irradiated With Ultrashort Laser Pulses of Relativistic Intensity, *Jorge Rocca, A. Curtis, C. Calvi,* Colorado State University*; J. Tinsley,* Mission Support and Test Services*; S. Wang, R. Hollinger, H. Song,* Colorado State University*; M. Capeluto,* Colorado State University, USAUniversidad de Buenos Aires, Buenos Aires, Argentina*; Y. Wang, V. Shlyaptsev,* Colorado State University*; V. Kaymak, A. Pukhov,* Heinrich-Heine-Universität Düsseldorf, Germany **INVITED**
The irradiation of arrays of aligned deuterated polyethylene nanowires (CD2) with ultra-high contrast femtosecond laser pulses of relativistic intensity was recently shown to accelerate deuterons to multiMeV energy and to efficiently produce flashes of quasi-monoenergetic fusion neutrons

[1]. The trapping of femtosecond laser pulses of relativistic intensity deep within ordered nanowire arrays can volumetrically heat dense matter into a new ultra-hot plasma regime [2,3]. Electron densities more than 100 times greater than the critical density with multi-keV temperatures are achieved using ultrashort laser pulses of only a few Joule energy focused to relativistic intensities. The number of fusion neutron produced exceeds by > 500 times that produced irradiating flat solid CD2 targets with the same laser pulses. Those experiments were conducted at irradiation intensities below 1 x 10 20 W cm-2. We also present recent results of deuteron acceleration from experiments conducted at irradiation intensities of ~ 2 x 10 21 W cm-2. The deuterons are measured to be accelerated to energies of several tens of MeVs and to be emitted in a cone of approximately 10 degrees half-angle. 3-D fully relativistic particle in cell computations are used to elucidate the mechanisms of ions acceleration in the nanowire arrays, which extend beyond target normal sheet acceleration. The fundamental physics of relativistic laser pulse interactions with nanostructures and their promising applications will be reviewed.

2:45pm LI-WeA2-24 The NIST Quantum Logic Clock and its Vacuum Performance, *David Leibrandt,* NIST-Boulder **INVITED**
Optical atomic clocks have achieved fractional measurement precision and accuracy at the 10^{-18} level, making them the lowest uncertainty measurement devices of any kind. In this talk, I will describe an optical clock based on quantum-logic spectroscopy of a single Al^+ ion co-trapped with a single Mg^+ ion in an ultra-high vacuum (UHV) environment. Collisions of the ions with background gas molecules degrade the stability of the clock, and cause a systematic frequency shift which must be characterized. By measuring the rate of collisions that cause reordering of the Al^+/Mg^+ ion pair and performing collision kinematics modeling, we determine the background-gas pressure in situ to be 38(19) nPa, where the uncertainty is dominated by the inaccuracy of the semiclassical differential cross sections we use in the model. By incorporating fully quantum scattering calculations, it may be possible to use this pressure measurement technique as the basis of a primary pressure standard for UHV and XHV.

3:05pm LI-WeA2-28 Closing Remarks and Thank You's, *Rachael Myers-Ward,* Naval Research Laboratory
Thank you for attending today's session! Remember to check out the AVS 67 On Demand Sessions which are available in the mobile app and online scheduler until 11/30/21 and then in the AVS Technical Library for all Platinum Members. We will see you at AVS 68 in Pittsburgh, PA, November 6-11, 2022!

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