## Electronic Materials and Photonics Division
## Room B116 - Session EM-WeM

### Advancements in Microelectronics and Nanotechnology by Early and Mid Career Professionals

**Moderators: Erica Douglas**, Sandia National Laboratories, **Stephen McDonnell**, University of Virginia

8:00am **EM-WeM-1 Assessment and Benchmarking of Nonvolatile Memory Devices for Analog In Memory Computing***, Matthew Marinella,* Arizona State University*; C. Bennett, P. Xiao, W. Wahby, S. Agarwal,* Sandia National Laboratories **INVITED**

Deep neural networks (DNNs) have garnered significant recent attention due to the revolutionary new capabilities they are enabling. These advancements have been made possible by the exponential increase in performance and energy efficiency of digital computing hardware over the past several decades. However, digital DNN accelerators are hitting ultimate limits of around 1-10 teraoperations per second per watt (TOPS/W) – and for progress to continue, new computing paradigms are needed.Analog in-memory computing (AIMC) is an architecture which promises to enable > 100 TOPS/W by efficiently processing the analog vector matrix multiply (VMM) operation at the heart of DNN algorithms – enabling capabilities well beyond what is possible with digital systems. The VMM operation is performed using an array of nonvolatile memory devices, which are programmed to represent a matrix of network weights through their conductance states. An input to this array is scaled to represent a vector, and each multiply is carried out using ohms law, followed by the accumulation of currents down each column. Many devices are under consideration for use with AIMC, including the flash memory cell (charge trapping and floating gate), and emerging resistive memory (ReRAM), conducting bridge memory (CBRAM), and electrochemical memory (ECRAM). The use of these devices for AIMC represents a significant departure from using the same devices for digital memory in that the neural network classification accuracy depends directly on the nuanced device-level behavior of nonvolatile memories. Device properties such as programming variability, read noise, drift, write linearity, and symmetry must be characterized in detail to form a dataset that can be used to model the accuracy of a DNN algorithm, when executed on an AIMC processor using that particular nonvolatile memory. For example, we have electrically characterized SONOS and ReRAM devices and simulated the classification accuracy for an AIMC accelerator running ImageNet on ResNet50 – which is a common machine learning benchmark. This talk will overview the process of benchmarking nonvolatile memory devices for AIMC, including electrical characterization, dataset generation, and process of modeling DNN accuracy based on this data.SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525.

8:40am **EM-WeM-3 AVS Peter Mark Memorial Award Talk: Heterostructures for Low-Power Logic and Memory Devices***, **Deep Jariwala**[1],* University of Pennsylvania **INVITED**

The isolation of a growing number of two-dimensional (2D) materials has inspired worldwide efforts to integrate distinct 2D materials into van der Waals (vdW) heterostructures. While a tremendous amount of research activity has occurred in assembling disparate 2D materials into "all-2D" van der Waals heterostructures and making outstanding progress on fundamental studies, practical applications of 2D materials will require a broader integration strategy. I will present our ongoing and recent work on integration of 2D materials with 3D electronic materials to realize logic switches and memory devices with novel functionality that can potentially augment the performance and functionality of Silicon technology. First, I will present our recent work on gate-tunable diode[1] and tunnel junction devices[2] based on integration of 2D chalcogenides with Si and GaN. After that I will present phase control growth and integration strategies for 2D In chalcogenides at back end of line (BEOL) compatible temperatures.[3]

Following this I will present our recent work on non-volatile ferroelectric memory devices based on AlScN.[4] First, I will present on Ferroelectric Field Effect Transistors (FE-FETs) made using a heterostructure of $MoS_2$/AlScN[5, 6] and also introduce our work on Ferroelectric Diode (FeD) devices also based on thin AlScN.[7] In addition, I will also present how FeDs provide a unique advantage in compute-in-memory (CIM) architectures for efficient storage, search as well as hardware implementation of neural networks.[8]

[1] **Peter Mark Memorial Award Winner**

**References:**


1. Miao, J.; et al….Jariwala, D. *Nano Letters* **2020,** 20, (4), 2907-2915.

2. Miao, J.; et al…. Jariwala, D. *Nature Electronics* **2022,** 10.1038/s41928-022-00849-0.

3. Song, S.; et al…. Jariwala, D. *arXiv preprint arXiv:2303.02530* **2023**.

4. Kim, K.-H.; Karpov, I.; Olsson III, R.; Jariwala, D. *Nature nanotechnology* **2023,** DOI: 10.1038/s41565-023-01361-y.

5. Liu, X.; et al…. Jariwala, D. *Nano Letters* **2021,** 21, (9), 3753-3761.

6. Kim, K.-H.; et al…. Jariwala, D. *Nature nanotechnology* **2023,** (in press).

7. Liu, X.; et al….Jariwala, D. *Applied Physics Letters* **2021,** 118, (20), 202901.

8. Liu, X.; et al…. Jariwala, D. *Nano Letters* **2022,** 22, (18), 7690–7698.


9:20am **EM-WeM-5 BeyondFingerprinting – Materials Discovery via High-Throughput, Low Cost, AI-Guided Materials Science***, B. Boyce, R. Dingreville, **Elliott Fowler**, N. Trask, D. Adams, J. Coleman, K. Johnson,* Sandia National Laboratories

In 1957 Richard Bellman first introduced the 'Curse of Dimensionality' – describing how the number of samples needed to estimate an arbitrary function with a given level of accuracy grows exponentially with respect to the number of input variables [1]. Almost 70 years later, the field of Materials Science is still grappling with the Curse. Despite significant advances in capability and speed in materials synthesis and characterization since Bellman's observation, most materials discovery challenges are far too high dimensional in terms of both inputs and material properties to brute force through with high throughput experimentation alone [2]. Thus, artificial intelligence (AI) and machine learning (ML) are increasingly being utilized because they allow for the rapid development of process-structure-property-performance relationships across a vast material domain. These AI/ML frameworks are designed to take high dimensional search spaces and significantly reduce them into strongly correlated latent spaces. The core question motivating Sandia's *Beyond*Fingerprinting Grand Challenge is: *How do you merge scientific data with a range of dimensionalities and uncertainties from multiple disparate sources (both experiments and high-fidelity simulations) to extract the most meaningful information through advanced machine learning algorithms?* In this talk, I will discuss how *Beyond*Fingerprinting is addressing this question with a two-fold approach, including development of high throughput, low-cost data streams and Himulaya (Hybrid-Informed Multi-Layered Algorithms), across three distinct material exemplars: Laser Powder Bed Fusion, Electrodeposition and Physical Vapor Deposition. Furthermore, I will show how this framework is enabling the acceleration of material discoveries across each of these three domains through discussion of combinatorial synthesis (100s of samples per day) and high-throughput characterization (1000s of measurements per week) strategies, as well as data management and AI/ML approaches. Perspective will be provided on how advances in *Beyond*Fingerprinting might impact the development of Electronic Materials and Devices.


[1]L. Chen, "Curse of Dimensionality," in *Encyclopedia of Database Systems*, L. Liu and M. T. ÖZsu Eds. Boston, MA: Springer US, 2009, pp. 545-546.

[2]E. J. Amis, X.-D. Xiang, and J.-C. Zhao, "Combinatorial materials science: What's new since Edison?," *MRS bulletin,* vol. 27, no. 4, pp. 295-300, 2002.


9:40am **EM-WeM-6 Tunability of the Thermal and Photophysical Properties of Blue-Emitting Fluoranthene Chromophores***, **Christopher Brewer**, J. Wheeler, A. Pyrch, F. Castellano,* North Carolina State University

Designing organic blue-emitting chromophores with properties suitable for applications in devices, such as OLEDs, is a challenging task. Organic blue-emitting chromophores often have broad emission profiles and do not sublimate cleanly for device fabrication. Consequently, organometallic blue emitters are more readily used in device applications due to their desirable thermal and photophysical properties. Despite these drawbacks, fluoranthene is a potential organic scaffold for designing blue-emitting organic chromophores. Fluoranthene's modular synthetic approach allows for nearly limitless functional group modification. Additionally, modifying its functional groups can tune fluoranthene's thermal and photophysical properties. Most notably, the volatility of the fluoranthene can be increased by installing trifluoromethyl substituents, while the volatility decreases when substituents such as methoxy are utilized. To date, our deepest blue-emitting fluoranthene chromophore (CIE 1931: 0.156, 0.111) incorporates trifluoromethyl and methoxy substituents while retaining desirable thermal properties. Ultimately, the vast array of synthetic modifications available with the fluoranthene scaffold makes this organic chromophore suitable for device fabrication, as both the emission and volatility can be controlled. This talk will discuss the photoluminescence of fluoranthene derivatives in both the solid and solution state, as well as the substituent influence on the volatility of the molecule.

11:00am **EM-WeM-10 Hf-Doping of Polycrystalline Gallium Oxide Thin-films**, ***Seth King***, University of Wisconsin - La Crosse

Hafnium (Hf) doping of $Ga_2O_3$ single crystals has shown that Hf occupies an octahedrally coordinated Ga site and behaves as an n-type dopant [1-3].However, these reports have only studied a single concentration of Hf incorporated into melt grown $Ga_2O_3$ single crystals.To gain insight into how Hf concentration impacts the optical, structural, and morphological properties of the material, polycrystalline Hf-doped $Ga_2O_3$ were deposited by RF-sputtering onto silicon and fused silica substrates at room temperature. Deposited films, with varying concentrations of Hf, were subsequently characterized by spectroscopic ellipsometry, UV-Vis spectrophotometry, x-ray diffraction, x-ray photoelectron spectroscopy, and atomic force microscopy both in the as-deposited state and upon subsequent, ex-situ annealing.

Results show that all films, regardless of Hf concentration, are initially amorphous, but crystalize as β-$Ga_2O_3$ upon annealing.Spectroscopic ellipsometry measurements show that the index of refraction of the film is altered by Hf incorporation, while UV-Vis measurements show that the optical bandgap is not significantly altered.These results suggest that Hf-doped $Ga_2O_3$ may find use in optoelectronic devices and applications.

[1]https://iopscience.iop.org/article/10.1088/1361-6641/ab75a6

[2]https://aip.scitation.org/doi/10.1063/5.0062739

[3] https://doi.org/10.1063/5.0062739

11:20am **EM-WeM-11 Composition of Chemically Treated (111) Surfaces of $Cd_{0.9}Zn_{0.1}Te$ by X-Ray Photoelectron Spectroscopy**, *H. Yuan, T. Nguyen,* ***Thomas Tiedje,*** University of Victoria, Canada; *B. Aitchison, Y. Song, M. Jackson,* Redlen Technologies, Canada; *J. Chen, H. Wang,* University of Saskatchewan, Canada

$Cd_{0.9}Zn_{0.1}Te$ (CZT) x-ray detectors have enabled high performance medical x-ray imaging systems. The surface properties of CZT are important in x-ray detector applications as they influence performance through their effects on electron-hole injection and collection. In this work, the composition of 111A surfaces of CZT single crystals were investigated following chemical etching with $Br_2$/methanol and HCl, vacuum annealing, ozone oxidation and $H_2S$ exposure. Both synchrotron and lab-based X-ray photoelectron spectroscopy (XPS) were used to investigate changes in the surface composition and interfacial band alignment of treated CZT surfaces. Chemical etching with $Br_2$/methanol was used to remove polishing damage, and leaves 4-6 monolayers of excess Te on the surface depending on the etch time and composition of the etch. HCl etching removes surface oxides formed by air exposure or by exposure to UV-generated ozone, leaving elemental Te ($Te^0$) on the surface. Residual $Te^0$ was removed by vacuum annealing at 250°C for one hour. XPS and Raman spectroscopy measurements on the vacuum annealed samples confirm the formation of a stoichiometric CZT surface. We were able to grow a mixed CZT-oxide about 8 nm thick by UV ozone exposure in air at room temperature for 1 hr. Depth profiles of the surface composition were obtained from the energy dependence of the photoelectron escape depth, accessible with the tunable x-ray energy available from the synchrotron source. We found a non-uniform vertical composition profile with CdO on the surface and $Te^0$ and $TeO_2$ underneath, suggesting that Cd out diffuses during oxidation.

Vacuum annealed and ozone oxidized surfaces were exposed to 500 ppm $H_2S$ in $N_2$ in a tube furnace at 250 °C and 280 °C for 0.5-2 hr. SEM/EDX imaging and ellipsometry measurements indicate that a 50-60 nm CdS layer is formed after 2 hr exposure to $H_2S$ at 280 °C. The ozone oxidized starting surface was found to be more reactive with $H_2S$ than the vacuum annealed surface. Sulfided surfaces were depleted in Te and O leaving a surface layer rich in CdS similar to the results of Nelson and Levi [1] with $H_2S$ plasma treatment. We are exploring the effect of the various surface treatments on x-ray detector performance.

[1] A. J. Nelson, D. Levi, Novel method for growing CdS on CdTe surfaces for passivation of surface states and heterojunction formation, JVST A, 15, 1119 (1997).

11:40am **EM-WeM-12 High Throughput Design of 2D Electronic Materials and Heterostructures**, ***Nicholas Glavin,*** Air Force Research Laboratory, Materials and Manufacturing Directorate, USA **INVITED**

2D materials represent an exciting opportunity to create tunable heterostructures for next generation electronic applications. In this talk, strategies and processes to enable high throughput design and customization of 2D materials which enable novel, multifunctional properties is presented. These techniques include rapid laser-manufacturing approaches, where high throughput structure/property evaluation can allow for rapid device design. This same process can be implemented in a roll-to-roll configuration to allow for manufacturing of ultralow cost 2D devices at scale for detection of a host of different sensing environments including detection of pathogens. Additionally, a two-step metal conversion process will be discussed that allows for direct synthesis of 2D transition metal dichalcogenide superlattices which can result in 3D heterostructures of interest to future applications.

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