Electronic Materials and Photonics
Room Ballroom BC - Session EM-ThP

Electronic Materials and Photonics Poster Session

EM-ThP-1 Comparison of Experimental Analysis and Theoretical Calculation of the Lattice Dynamics, Phonon and Vibrational Spectra Dynamics of Titanium Nitride and Oxynitride*, Ikenna Chris-Okoro*, *Sheilah Cherono, Wisdom Akande, Swapnil Nalawade, Mengxin Liu, Barbee Brianna, Brooklyn Jenkins, Ghanashyam Gyawali, Bishnu Bastakoti, Shyam Aravamudhan, J. David Schall, Dhananjay Kumar,* North Carolina A&T State University

Titanium nitride (TiN) and its isostructural oxide derivative, Titanium oxynitride (TiNO) has gained interest in industry as a cost-effective alternative material to noble metals and refractory metals with wide range of applications especially in the optoelectronics and plasmonic. However, there still remain some gaps and disagreement in the literature on specific optical and photoelectrochemical properties of TiN and TiNO, due to difficulty and the varying approach in quantifying defects, vacancies, oxidation state and direct impact of impurities in experimental results.

In this study, thin films of TiN and TiNO were synthesized via pulse laser deposition on sapphire. Structural properties of these thin films were investigated using X-ray Diffraction and Reflection (XRD, XRR), X-ray Photoelectron Spectroscopy (XPS), Rutherford backscattering spectrometry (RBS), Raman Spectroscopy and Fourier Transform Infrared Spectroscopy (FTIR). To corroborate our experimental observations, the phonon dispersions and Raman active modes are calculated using the virtual crystal approximation for rutile TiO_2 and rocksalt TiNO and molecular dynamics simulations were used to calculate the phonon density of states. The results shows that the incorporation of nitrogen atoms does not significantly alter the phonon dispersions of rutile TiO_2. However, it results in the emergence of new phonon modes at approximately 7.128 THz (237.65 cm^{-1}) at the Gamma point, which corresponds to the experimentally observed Multi-Photon Phase-MPP (240 cm-^{1}-R). From the experimental and theoretical studies, a multilayer optical model has been proposed for the TiN/TiNO epitaxial thin films for obtaining individual complex dielectric functions from which many other optical parameters can be calculated.

This work was supported by a DOE EFRC on the Center for Electrochemical Dynamics and Reactions on Surfaces (CEDARS) via grant # DE-SC0023415. Part of the work has used resources established by the Center for Collaborative Research and Education in Advanced Materials (CREAM) via NSF PREM grant # DMR-425119 PREM.ML and GG are jointly supported by the CEDARS and CREAM projects.

EM-ThP-2 Reliability Improvement for Nanostructured High Power AlGaAs/GaAs Vertical-Cavity Surface-Emitting Semiconductor Lasers*, Gwomei Wu,* Chang Gung University, Taiwan

The objective of this study has been to develop high power 850 nm vertical-cavity surface-emitting laser (VCSEL) using oxidation confinement technique. The active layer consisted of three pairs of $Al_{0.3}Ga_{0.7}As$/GaAs semiconductor nanostructures and it exhibited a photoluminance emission wavelength of 835 nm. Distributed Bragg reflector mirror nanostructures of 40 pairs in n-type and 21 pairs in p-type were designed to confine the resonance. The multi-layered epitaxial wafers were further processed by photolithography techniques. Inductively coupled plasma etching was employed to create the platform during the mesa process. Various non-oxidized aperture sizes have been achieved by a wet-oxidation method. The experimental results showed that the VCSEL device exhibited low threshold current of 0.6-0.8 mA. The optical output power was about 6.0-6.8 mW at the injection current of 6 mA. The slope of efficiency was found to be about 3.2~3.7 mW/mA. The corresponding voltage was in the range of 1.7~2.1 V. On the other hand, an eye diagram could be clearly observed under the high data rate of 25 Gbit/sec. The response frequency was measured at 17.1 GHz at -3 dB, also at the injection current of 6 mA. In addition, a high thermal conducting AlN (~230 W/m-K) dielectric bonding substrate was employed to improve device reliability. The related electro-optical characteristics would be presented and further discussed.

EM-ThP-3 Singlet Fission from Tetracene and Charge Transfer to Metal Halide Perovskites*, Yutong Ren*[1], *Antoine Kahn,* Princeton University

Metal halide perovskites (HaPs) have garnered widespread interest for light-harvesting and light-emitting applications due to their exceptional optoelectronic properties and relatively simple fabrication methods. However, like with other semiconductors, HaP-based solar cells lose excess energy through thermalization when absorbing photons with energy that exceeds the absorber bandgap.[1] A promising strategy to reduce these losses and improve photon utilization is to exploit singlet fission, whereby a high-energy singlet exciton formed in an adjacent layer splits into two triplet excitons.[2,3] By transferring these triplet excitons into a HaP film engineered with a composition that aligns the absorber's bandgap closely with the exciton energy, one can effectively harvest this otherwise wasted energy. In our work, we demonstrate that singlet fission in the molecular semiconductor tetracene (Tc) efficiently generates triplet excitons[4] that are energetically matched to the bandgap of a Sn–Pb based HaP, offering a viable pathway toward improved device performance.

In this study, we investigate the electronic structure of Sn–Pb-based HaP films and their interfaces with Tc using ultraviolet photoelectron spectroscopy (UPS) and inverse photoemission spectroscopy (IPES). Based on the work by Nagaya et al.,[5] we introduce a second molecular donor, zinc phthalocyanine (ZnPc), at the interface to engineer a more staggered energy alignment between Tc and the perovskite film, thereby promoting an energetically more favorable sequential electron transfer plus formation of a charge transfer (CT) state ($ZnPc^+$ - HaP^-). UPS/IPES measurements suggests that the CT state lies approximately between the Tc triplet energy and the HaPenergy gap, which is favorable for triplet transfer. Complementary photoluminescence (PL) and time-resolved PL (tr-PL) measurements provide guidance for selecting alternative donors with deeper or shallower HOMO levels to replace ZnPc and further refine the interfacial energetics. Moreover, optoelectronic characterization reveals insights into undesirable charge carrier recombination pathways at the organic/HaP interface. Collectively, our results underscore the potential of singlet fission to enhance the efficiency of perovskite solar cells and reduce the cost of the energy that they generate.

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EM-ThP-6 Title:Plasma-Enhanced ALD of Phase-Tunable Ternary Oxynitrides for Bandgap-Engineered Charge-Selective Contacts in Perovskite Photovoltaics*, George Kwesi Asare,* University of Science and Technlogy, Republic of Korea

We introduce a PE-ALD route for depositing aluminum-zinc oxynitride (AZON) films using alternating pulses of triethylaluminum (TEAl), diethylzinc (DEZ), oxygen plasma, and N_2/H_2 remote plasma. By precisely controlling the oxygen-to-nitrogen incorporation ratio during deposition at, we achieve continuous tuning of the AZON bandgap enable tailored alignment with both valence and conduction bands of the novel material.

In-depth structural and compositional analyses using spectroscopic ellipsometry, Rutherford backscattering (RBS), and grazing incidence X-ray diffraction (GIXRD) confirm that ALD-grown AZON films exhibit uniform density, amorphous character, and atomically sharp interfaces. Ultraviolet photoelectron spectroscopy (UPS) and in situ Kelvin probe measurements reveal controlled shifts in the work function of over 0.8 eV, enabling their application as either electron or hole transport layers depending on the ALD cycle ratio and post-deposition annealing. When incorporated as an electron transport interlayer, between the perovskite and the hole transport layer, AZON-enhanced devices exhibit a stabilized power conversion efficiency (PCE) of 23.8% with negligible hysteresis and retain over 91% of initial performance after 1500 h under continuous 1 Sun illumination. Furthermore, thermally accelerated aging tests reveal suppressed ion migration at the interface, attributed to the passivating nature of the nitrogen-rich surface.

The integration of conformal, compositionally tunable charge-selective layers remains a challenge in advancing the long-term stability and interfacial energetics of next-generation perovskite solar cells (PSCs). In this

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[1] **JVST Highlighted Poster**

work, we report a novel application of plasma-enhanced atomic layer deposition (PE-ALD) to synthesize ternary metal oxynitride (M–O–N) thin films with phase-tunable electronic properties for use as hole and electron selective interlayers for PSC applications.

EM-ThP-7 Growth of MAPbI$_3$ Single Crystals for Radiation Detection and Sensor Applications

***Basak Bagci**, Shams Noor, Ge Yang,* North Carolina State University

Hybrid halide perovskites such as methylammonium lead iodide (MAPbI$_3$) offer exceptional promise for ionizing radiation detection due to their high atomic number, strong photon absorption, low trap densities (~10^{10} cm^{-3})and excellent defect tolerance. In particular, single-crystal MAPbI$_3$ stands out for its excellent charge transport properties, including high mobility–lifetime (μτ) products ~1.2 × 10^{-2} cm^2/V and X-ray sensitivities exceeding 250 μC Gy^{-1} cm^{-2}, which are critical for achieving high-sensitivity, low-noise performance in X-ray and gamma-ray detectors.

This study focuses on the growth of MAPbI$_3$ single crystals dissolving methylammonium iodide (MAI) and lead iodide (PbI$_2$) in gamma-butyrolactone (GBL), followed by controlled heating to induce crystal formation. Experimental efforts will explore the effects of precursor concentration, temperature ramp rates, and growth dynamics on crystal size, morphology, and electronic characteristics. Theharvested crystals are intended for use in radiation detection and broader sensor applications, and they will also serve as a baseline for future comparisons with triple-cation and doped perovskite systems.

Our work builds on previous ITC reports but demonstrates a new synthesis protocol that yields centimeter-scale MAPbI$_3$ crystals with low visible defect density and improved reproducibility. Unlike earlier studies, our method carefully regulates supersaturation and convection to promote steady lateral crystal expansion. Preliminary optical and structural analyses confirm phase purity and high crystallinity, while ongoing electrical characterization is focused on quantifying μτ values under bias and assessing detector sensitivityand leakage currentunder X-ray flux. To address the well-known stability limitations of MAPbI$_3$, we are implementing post-growth annealing strategies, encapsulation and/or low-temperature storage under inert conditions to suppress decomposition. These steps aim to improve the operational durability of the material and establish a foundation for stable detector integration.

By establishing a reliable and reproducible synthesis and growth protocol, this work aims to produce high-purity, low-defect MAPbI$_3$ crystals suitable for device integration. Future steps include evaluating charge transport characteristics, assessing detector performance under radiation exposure, and exploring strategies for enhancing long-term material and device stability. The insights gained from this study are expected to contribute to the development of scalable, low-cost perovskite-based radiation detectors with improved resolution and sensitivity.

EM-ThP-8 Chemical Vapor Deposition of Uniform and Large-Scale MoS2 Using Heterogeneous Precursor

***Xiaokai Zhu*,** Duke University*; Gang Seob Jung,* Oak Ridge National Laboratory*; Jiahui Yang,* Duke University*; Xuguo Zhou,* Boston College*; Zhe Shi,* Massachusetts Institute of Technology*; Victoria Ravel, Chung-Li Lin, Xingjian Hu, Zihan Peng, Aaron Franklin,* Duke University*; Qiong Ma,* Boston College*; Tania Roy, Haozhe Wang,* Duke University

The mass production of large-scale single-layer molybdenum disulfides (MoS$_2$) is necessary for the fabrication of next-generation electronics. However, the current chemical vapor deposition (CVD) strategies are hard to produce uniform and large-scale single-layer MoS$_2$. Here, we developed a CVD strategy using heterogenous precursors for synthesizing high-quality single-layer MoS$_2$. Different from the traditional CVD strategies where the growth promoter and Mo source are mixed, our strategy employs heterogeneous precursors where the growth promoter and Mo source are positioned separately in two layers. During heating, the growth promoter initially volatilizes and condenses on the substrate to create a promoter-rich environment. In that case, a large amount of promoter accumulates and spreads uniformly on the substrate, leading to the growth of millimeter-scale single-layer MoS$_2$ on both SiO$_2$/Si and sapphire substrates. Raman spectroscopy and atomic force microscopy (AFM) imaging have confirmed the MoS$_2$ layer number. Raman and photoluminescence (PL) mapping indicated outstanding spatial uniformity of the film. Selected-area electron diffraction revealed single crystal properties within a 5 μm × 5 μm area. An array of field-effect transistors based on the as-grown single-layer MoS$_2$ demonstrated excellent electrical properties (10E-7 on/off ratio). Compared to traditional CVD strategies, the coverage ratio of single-layer MoS$_2$ increased from 66.7% to 90.3%, and the device yields increased from 6.0% to 74.0%. The growth mechanism was investigated by density functional theory (DFT) calculations concluding that the energy barrier for MoS$_2$ growth on salt is significantly lower. As a result, after the growth of the first layer, no additional layers tend to grow on top of it and all single-layer flakes merge together to form a continuous film with multiple domains which have been visualized by second harmonic generation (SHG) imaging and molecular dynamics (MD) simulation. This method provides a new understanding of the mechanism of the promoting agent in CVD MoS$_2$ growth, presents a new paradigm for high-quality MoS$_2$ fabrication, and consequently will benefit large-scale 2D semiconductor applications.

EM-ThP-9 Comprehensive Study of Tandem Cdsete Photovoltaic Devices Using Alternative Subcell Absorber Layers: Bandgap Engineering

*Chowdhury Haque, **Philip (Sanghyun) Lee**,* University of Kentucky*; Kent Price,* Morehead State University

Tandem CdSeTe thin-film photovoltaic devices represent a promising frontier in solar energy technology, utilizing innovative bandgap engineering to enhance efficiency (>30 %) by broadening absorbing spectrum of impinging light. Although CdSeTe cells have been heralded for their high conversion efficiency (23.1 %), but limitations arise when single-junction designs fail to capture the full spectrum of solar radiation. Tandem devices (dual-junction or muti-junction) address this challenge by integrating multiple subcell absorber layers, each with optimized bandgap energy to selectively absorb different portions of the solar spectrum.

The introduction of alternative subcell absorber layers in the tandem structure is pivotal for expanding device performance by overcoming the fundamental limitation of a single-layer photovoltaic device by capturing larger ranges of wavelength of sunlight. Absorber layers are carefully selected and engineered to achieve bandgap tuning that maximizes spectral overlap while maintaining material compatibility. A top cell has larger bandgap, which can absorb shorter wavelength light. A bottom cell has smaller bandgap, capturing longer wavelength light.

For dual-junction tandem device configurations, we investigated the band alignment of top and bottom subcell materials to achieve the optimized bandgap between two subcells through bandgap engineering. From the theoretical study, bandgaps of dual-junction tandem devices are 1.5 - 1.8 eV and 1.4 - 1.5 eV for top and bottom (CdSeTe) subcells, respectively. The theoretical maximum power conversion efficiency (PCE) is 33.16 %. Multiple top and bottom absorber candidates were explored, including CdZnTe (Eg = 1.75-1.8 eV) and CdMnTe (1.7-1.75 eV) for a top subcell and CdSeTe (1.4 - 1.5 eV) for a bottom subcell. To optimize tandem devices, the current matching technique is used to determine the optimal thickness of each subcell. For the top layers, the thickness of CdMnTe is 450 nm, and for CdZnTe, it is 398 nm. The thickness of the bottom layer is approximately 2.4 um to achieve the best performance in a two-terminal tandem device. With spectral filtering and current matching, CdMnTe/CdSeTe tandem devices demonstrate an open-circuit voltage (Voc) of 1.52 V, a short-circuit current density (Jsc) of 15.7 mA/cm^2, and a fill factor (FF) of 82.1%, resulting in power conversion efficiency of 19.61 %. In contrast, CdZnTe/CdSeTe tandem devices demonstrate an Voc 1.51 V, Jsc 16.2 mA/cm^2, and FF 75.52 % with PCE 18.54 %. In summary, the best PCE is MgZnTe 19.61%, indicating that these devices are promising candidates for high-performance tandem solar cells.

EM-ThP-10 Ferroelectric Tunnel Junction NVM Stability

***M. David Henry*,** Sandia National Laboratories

Ferroelectric (Hf,Zr)O$_2$-based tunnel junctions have shown significant promise as two-terminal resistive non-volatile memory (NVM) devices, exhibiting excellent area scaling capabilities and a high degree of compatibility with complementary metal-oxide-semiconductor (CMOS) technology. These devices can operate in a binary state, characterized by a high resistance state (HRS) and a low resistance state (LRS), as well as support multiple intermediate resistance states. From semiconductor physics, we describe the transport behavior using a combination of Ohmic conduction and Poole Frenkel (PF) defect mediated conduction. At low field (10^{-5}V/cm), Ohmic conduction dominates whereas at medium to high field a modified PF dominates. From the conduction mechanism, several factors can influence the stability of resistance states for a binary and multistate based devices including temperature, imprint, and even the act of reading out the state. This work will discuss these factors and demonstrate the functionality of these ferroelectric tunnel junction devices in both 5-bit and 4-bit configurations, enhancing data storage density and enabling advanced functionalities.

EM-ThP-11 Ab Initio Molecular Dynamics Modeling of Amorphous Titanium Silicon Nitride*, Somilkumar Rathi, Parag Banerjee,* University of Central Florida*;* ***Raymond Atta-Fynn,*** Los Alamos National Laboratory

Amorphous titanium silicon nitride is a ceramic material that has emerged as a strong candidate for a next-generation, ultra-thin diffusion barrier material in semiconductor device fabrication. As device dimensions shrink, TiSiN is increasingly considered a viable alternative to traditional TaN- and TiN-based barriers due to its structural tunability (crystalline to amorphous) enabled by doping. Moreover, its ease of synthesis and electrical properties are comparable to those of conventional barrier materials even at much lower thicknesses, facilitating integration into advanced device nodes. In this work, *ab initio* molecular dynamics simulations based on the quench-from-the-melt technique were employed to model amorphous titanium silicon nitride by systematically doping stoichiometric TiN with Si until clear signatures of amorphization emerged.

We observed that the onset of amorphization occurs when the fraction of Si in TiN reaches at least 25%. The distributions of various bond lengths and bond angles were analyzed to gain insight into the geometry of the structures. The angular-momentum–resolved electronic density of states was used to analyze the interactions between the Ti, N, and Si electron states. The amorphization process is explained by the reduction in ionicity and the increase in covalency induced by Si incorporation.

EM-ThP-12 Spectroscopic Characterization and Defect Identification in Wide Bandgap Semiconducting Materials*,* ***Praveena Manimunda,*** HORIBA

Wide bandgap semiconductors such as silicon carbide and Ga_2O_3, are used in power electronics, high power and high temperature devices. Achieving defect free, doped wide bandgap semiconductors are still a challenge. In this study spectroscopic characterization techniques such as photoluminescence, Raman and cathodoluminescence methods are utilized to identify microscopic defects in 3C-SiC, n-type 4H-SiC and shape engineered SnO_2 nanostructures grown on Ga_2O_3 nanowires. Semiconducting oxide nanostructures with a wide range of morphologies are emerging as a viable candidate for applications such as optical and mechanical resonators and solar cells. However, attaining effectively doped oxide nanowires with controllable conductivity is still a challenge. [1,2] Designing semiconducting oxide nanostructures requires extensive understanding of their morphology and demands efficient multimodal characterization methods. Multimodal spectroscopy is the concept of combining several different spectroscopies onto one platform, thereby expanding the range of analytical capabilities available on that single platform. Besides the obvious benefit of cost reduction, having multiple analytical spectroscopies offers the added benefit of sample colocalization so that multiple complementary measurements can be made at the same location of the sample. The benefit of colocalization is particularly important as feature sizes get smaller, from a few microns to nanometers in size. Using patterned silicon grid sample and embedded position-sensing technology, coordinates of region of interest transferred between different spectroscopic tools. Raman, Photoluminescence, cathodoluminescence and Time Resolved Photoluminescence (TRPL) techniques were used to characterize growth induced defects.

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EM-ThP-13 Flexible Perovskite Solar Cells with Reusable Stainless-Steel Foil Substrates*,* ***Pramod Baral,*** Verde Technologies Inc.

Flexible Perovskite Solar Cells with Reusable Stainless-Steel Foil Substrates

Pramod Baral[1], Vivek Babu[1], Francesca Brunetti[2]

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Perovskite solar cells (PSCs) have achieved power-conversion efficiencies (PCEs) of 27% on rigid glass substrates, yet their flexible counterparts are more attractive for lightweight, portable and roll-to-roll manufacturing applications. Conventional polymer substrates such as PET and PEN, however, are limited by low thermal tolerance, modest barrier properties, and single-use constraints. Here, we demonstrate stainless-steel (SS) foil as a multifunctional application that simultaneously serves as a flexible substrate, conductive bottom electrode, and robust barrier layer, offering high thermal and mechanical stability as well as reusability across multiple fabrication cycles. Our device stack SS/NiO_x/MeO-4PACz/PEAI/FAPI/3MTPAI/C_{60}/BCP/Cu fabricated via scalable slot-coating of the perovskite absorber and high-vacuum evaporation of the electron transport layer (ETL) and top electrode layers, achieves PCEs approaching 10% under standard 1-sun illumination. Performance is currently constrained by optical absorption losses in the semi-transparent Cu electrode, which limit photocurrent generation. To address this, we are transitioning to low-temperature high-vacuum sputtered transparent conducting oxides such as indium tin oxide (ITO) and indium zinc oxide (IZO), which offer higher transparency and lower sheet resistance while remaining compatible with roll-to-roll processing. This approach highlights a realistic pathway toward scalable flexible perovskite solar cells (FPSCs) exceeding 20% efficiency, enabling cost-effective deployment in building-integrated photovoltaics, mobile systems, and off-grid power applications.

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