PCSI
Room Keahou I - Session PCSI-SuA1

Materials for Novel Information Systems
Moderator: Michelle Simmons, UNSW

2:30pm PCSI-SuA1-1 Interfacing Biomolecules with Coherent Quantum Sensors, *Peter Maurer,* University of Chicago **INVITED**
Quantum metrology enables some of the world's most sensitive measurements with potentially far-reaching applications in the life sciences. Although the ultrahigh sensitivity of qubit sensors has spurred the imagination of researchers, implementation in actual devices that enable monitoring cellular processes or detecting diseases still remains largely elusive. Overcoming limitations that hold back wider application of quantum technology in the life sciences, requires advances in both fundamental science and engineering. In this talk, I will discuss our research group's recent results on addressing one of these long-standing research challenges, namely, how to interface highly coherent quantum sensors with biological target systems.

My discussion will start with the development of a novel biocompatible surface functionalization architecture for highly coherent diamond crystals. I will then continue with discussing a new approach to engineering spin coherence in core-shell structured diamond particles, which can be readily chemically modified and delivered to intact biological systems. Finally, I will conclude my talk with an outlook on a novel class of protein-based qubit sensors that will overcome many of the fundamental challenges associated with current diamond-based quantum sensors. The unifying theme of these advances are the convergence of techniques from single-molecule biophysics, material science, and quantum engineering. Specific applications of the developed sensing platforms to questions in the life sciences will be discussed throughout this talk.

3:10pm PCSI-SuA1-9 Magnetoresistance Spectroscopy of Near-Surface Defects in Semiconducting Hosts, *Stephen McMillan,* Donostia International Physics Center, Spain **INVITED**
Components for quantum information processing and quantum sensing require localized spin-coherent states. These states can be realized in isolated magnetic dopants embedded in a non-magnetic semiconducting host. A critical requirement for utilizing a dopant-based system is an understanding of how the complex host environment influences the coherent spin dynamics at an individual site. Resolving these faint dynamics against a strong incoherent background is a challenge that is typically solved by exciting the system via ac fields. In this work we propose a method that leverages non-equilibrium spin correlations in the presence of dc magnetic fields to probe coherent interactions in individual near-surface magnetic dopants. In previous work, we calculate the dc magnetoresistance through a spin-1/2 dopant that is addressed by a spin-polarized scanning tunneling microscope (SP-STM) and exchange coupled to an inert spin-1/2 center [1]. This work is then extended to the technologically relevant case of an individual spin-1 center [2]. In particular we use the stochastic Liouville formalism to calculate the current through a divacancy in 4H-SiC. We predict distinct few-milli-tesla-dc magnetoresistance signatures that identify a single spin-triplet center's character and reveal the orientation of the spin triplet's zero-field splitting axis relative to the magnetic contact's polarization. For example, in 4H-SiC the single (hh), (kk),(hk), and (kh) divacancies are all distinct. Spin-polarized current flow efficiently polarizes the spin, potentially electrically initializing spin-triplet-based qubits without the use of ac fields or optical hardware.

3:50pm PCSI-SuA1-17 Development of 'Artificial' Memristive Synapses Using Various Sp2 C (Graphene-Like) -Sp3 C (Diamond) Heterojunctions as Neuromorphic Devices, *Sanju Gupta,* Gdansk University of technology and Penn State University; *R. Bogdanowicz,* Gdansk University of Technology, Poland
The integration of allotropic sp^2-/sp^3-bonded carbon (sp^2C/sp^3C) interfaces and devices has evoked increasing attention since they offer a versatile and rich playground for carbon-based electronics, electrochemical sensing platforms, and optoelectronic neuromorphic computing attaining enhanced performance [1-5]. Moreover, inspired by human brain functionality and its low power consumption of only 10W, memristors for neuromorphic computing have gained significance for implementing solid-state neurons and 'artificial' synapses due to their nanoscale footprint and reduced complexity. In this talk, we present the fabrication of various carbon-based heterojunctions comprising graphene-like (sp^2C)-diamond (sp^3C) architectures using microwave plasma-assisted chemical vapor deposition on nanodiamond seeded p-Si (100), SiO_2/p-Si (100) and Fz-Si (001)

substrates. These are the key elements emulating the characteristics of biological synapses and memory functions which are game-changing energy-saving computing devices. The resulting heterojunctions behave as memristors (*i.e.,* resistors with tunable memory) having multiple resistance states and nonvolatile memory functions, a phenomenon that refers to the ability of synapses (neuronal links) to adapt in response to an increased or decreased activity, essential to human memory and learning. The resulting heterojunctions behave as memristors (*i.e.,* resistors with tunable memory) having multiple resistance states and nonvolatile memory functions, a phenomenon that refers to the ability of synapses (neuronal links) to adapt in response to an increased or decreased activity, essential to human memory and learning. We performed *I–V* characteristics with temperature (up to 250 °C) and in response to photoirradiation at 365 nm, 532 nm, and 633 nm in addition to comprehensive microstructural properties. Interestingly, high or low resistance states (equivalently, short-term, and long-term potentiation) can be controlled by combined applied bias and light irradiation, giving a resistive switching ratio of $\sim 10^6$, observed in sparse materials and/or heterostructures. They exhibit quasi-linearity and symmetry when subjected to identical input pulses, essential for their role in the online training of neural networks. The linearity holds for a range of pulse width, amplitude, and applied pulse number. We ascribe the observed behavior to redox reaction (or reorganization of carbon orbitals) at the sp^2-sp^3 interfaces and the role of hydrogen and oxygen movement by applied bias. Finally, heterostructure arrays could be designed for better memristive devices and memory functions and photo sensing (image sensors) applications.

3:55pm PCSI-SuA1-18 In-Situ Transmission Electron Microscopy of Hafnium Zirconium Oxide for Phase Identification in Memristor Devices, *Krishnamurthy Mahalingam,* BlueHalo-UES Inc; *S. Asapu,* Department of Electrical and Computer Engineering, University of Massachusetts; *L. Blank,* ARCTOS Technology Solutions; *D. Winner,* University of Dayton; *C. Bowers,* Blue Halo-UES Inc; *S. Ganguli, A. Roy,* Air Force Research Laboratory, Materials and Manufacturing Directorate, USA; *J. Yang,* Department of Electrical and Computer Engineering, University of Southern California
Hafnium zirconium oxide (HZO) has attracted much attention for the development of memristive technologies essential for neuromorphic computing, which is based on ferroelectric switching behavior attributed to orthorhombic polar phase (OPP) formation. This phase is stabilized by thermal strain induced by electrode type and process conditions. However, due to the polymorphic nature of HZO, formation of other stable polycrystalline phases with monoclinic, tetragonal and cubic structure is also possible. The identification of the crystalline phases by standard techniques is achallenge due to the similarity of lattice parameters and symmetry along some orientations, making it difficult for insightful optimization of OPP formation in these devices.

Herein we performed in-situ transmission electron microscopy, combining electron energy loss spectroscopy (EELS) and position averaged convergent beam electron diffraction (PACBED) to directly examine amorphous to crystalline phase transformation in HZO films under rapid thermal annealing. In EELS the signatures to identify the different phases was investigated by a detailed examination of the fine structure near the O_k edge. In PACBED we combine dynamical diffraction simulations with neural network based machine learning (ML) to examine distinction between the different phases. A high resolution TEM image of the crystalline phase formation is presented in Fig. 1(a) along with an inset showing its digital fast Fourier transform after rapid heating to 700°C (at 50°C/sec). Figure 1(b) is an EELS profile comparing the O_k edge from an amorphous region (Blue) before and the crystalline region (Red) after the annealing operation. Noticeable shift in peak-B position and a reduction in the B/A peak ratio are evident. While conventional diffraction analysis confirmed the formation of OOP, application of ML was inconclusive. Further details on the interpretation of changes in the O_k edge fine structure based on EELS modeling, and challenges with the ML approach to electron diffraction data analysis will be presented.

4:00pm PCSI-SuA1-19 Quantum Sensing Using Two-dimensional Hexagonal Boron Nitride, *Hailong Wang,* Georgia Institute of Technology, USA
Emergent color centers with optically accessible spins have attracted tremendous research interest in recent years due to their significant potential for implementing transformative quantum sensing technologies. Spin defects hosted by hexagonal boron nitride (hBN) are emerging candidates in this catalog due to their remarkable compatibility with solid-state nano device integration and multimodal sensing of proximal two-

dimensional quantum materials/devices [1]. Taking advantage of boron vacancy spin defects in hBN, we report nanoscale quantum imaging of low-dimensional ferromagnetism sustained in Fe_3GeTe_2/hBN van der Waals heterostructures [2]. Exploiting quantum spin relaxometry methods, we have observed spatially varying magnetic fluctuations in exfoliated Fe_3GeTe_2 nanoflakes, whose magnitude reaches a peak value around the Curie temperature. Using optically detected magnetic resonance measurements, we further show that ferromagnetic resonance and parametric spin excitations in a magnetic insulator $Y_3Fe_5O_{12}$ (YIG) can be effectively detected by boron vacancy spin defects under various experimental conditions through the off-resonant dipole interaction between YIG magnons and boron vacancy spin defects [3]. Our results highlight the opportunities offered by novel quantum spin defects in layered vdW materials for investigating microscopic spin behaviors in magnetic solid-state matters.

[1]A. Gottscholl et al., Nature Materials **19**, 540 (2020).

[2]M. Huang et al.,Nature Communications**14**, 5259 (2023).

[3]J. Zhou et al., Science Advances **10**, eadk8495 (2024).

PCSI
Room Keahou I - Session PCSI-SuA2

Semiconductor Heterostructures: Growth, Nanostructures, & Interfaces I
Moderator: Kirstin Alberi, National Renewable Energy Laboratory

4:20pm **PCSI-SuA2-23 Correct Treatment of Spontaneous Polarization at Polar Wurtzite Interfaces**, *Chris Van de Walle*, University of California Santa Barbara **INVITED**
Herbert Kroemer's famous statement, "the interface is the device," also applies to polar interfaces in nitride-based devices; but in wurtzite-structure materials we additionally have to reckon with polarization fields. Sometimes these fields are a nuisance, suppressing efficiency of light emitters, sometimes they provide functional enhancement, by increasing the density of two-dimensional carrier gases in transistors. Accurate knowledge of polarization constants is critical for analysis of experiments and for device design. Some time ago we identified deficiencies in the calculation of polarization fields in simulation tools, related to the choice of the zinc-blende phase as a reference for the spontaneous polarization of wurtzite. However, since the current implementations contain *two* errors that to some extent cancel, most modeling has continued to use the zinc-blende-referenced approach.This has, unfortunately, led to major confusion in the analysis of polarization in AlScN alloys. Correct referencing of spontaneous polarization (relative to a layered-hexagonal phase) is essential for consistent interpretation of ferroelectricity.

Correct referencing of polarization also allows for an intuitive visualization of the origins of polarization, in which the electron cloud within the unit cell is shifted relative to the positive ionic cores. Different shifts in GaN and (strained) AlN then produce the polarization discontinuity at the interface, and lead to the insight that the electrons in the two-dimensional electron gas (2DEG) at a GaN/AlN [0001] heterojunction are *intrinsic* to the interface; i.e., they do not need to be provided by doping or surface states. The surface actually acts as a *sink* for electrons; proper surface engineering should prevent interfacial carriers from leaking away to the surface. The majority of the compensation charge on the surface is provided by fixed charge. This is consistent with the observation that the density of surface states (containing mobile charge) is much lower than the 2DEG density. All these considerations also apply, *mutatis mutandis*, to hole gases at GaN/AlN [000-1] junctions.

Work performed in collaboration with Cyrus Dreyer, Haochen Wang, Sai Mu, Nicholas Adamski, Suhyun Yoo, Darshana Wickramaratne, Mira Todorova, Jörg Neugebauer, and Simon Fichtner, and supported by DOE, SRC, and ARO.

5:00pm **PCSI-SuA2-31 Subsurface Nitrogen in Diamond (001)-2×1-H Studied by Density Functional Theory**, *Shicai Wang*, Technion Israel Institute of Technology, China; *K. Huang*, Technion Israel Institute of Technology, Canada
To populate nitrogen centers in the near-surface region of diamond, there has been recent effort [1-3] of using activated dinitrogen to impact fully hydrogenated diamond surfaces as synthesized by chemical vapor deposition. There is implication [2-3] of nitrogen into the subsurface region (depth: 6 ± 5 Å) of the same diamond (001)-2x1-H by low energy N_2^+ ions. It

remains, however, unclear about the atomistic understanding into the configuration and bonding of the nitrogen species in the subsurface region of diamond (001)-2×1-H. Here, we present studies into subsurface nitrogen in diamond (001)-2x1-H by density functional theory simulations, revealing in each case information regarding structure, energy and vibration that depend on the atomistic coordination as detailed below.

We have studied 10 configurations of a single interstitial nitrogen in the topmost 3 layers of diamond (001)-2x1-H. In all configurations, the carbon network is strongly distorted by an interstitial nitrogen atom, in which 2 carbon-carbon bonds are cleaved. The interstitial nitrogen is bound to 3 neighboring carbon atoms, of which one carbon becomes sp^2 hybridized. The stability of the interstitial configuration depends on the location of nitrogen and the direction of the formed $C(sp^2)$-N bond, exhibiting formation energies of +4.83 to +11.04 eV. The most characteristic mode of vibration arises from the $C(sp^2)$-N bond, i. e., stretch (1530 to 1901 cm^{-1}/ 189.7 to 235.8 meV) and swing (1101 to 1389 cm^{-1}/ 136.6 to 172.2 meV). Migration of nitrogen interstitial is also evaluated, involving a series of steps and intermediates; the rate determining step is of a barrier of 6.02 eV.

We have also evaluated 3 configurations of a single substitutional nitrogen in the topmost 3 layers of diamond (001)-2x1-H. In all configurations, the carbon network is largely preserved, giving formation energy of +2.79 to +3.41 eV. The substitutional nitrogen is bound to four neighboring carbons, and the formed C-N bond is larger than a typical C-N single bond, giving the characteristic C-N swing vibration of 844 to 979 cm^{-1} (105 to 121 meV).

We have finally evaluated 6 configurations of a pair of nitrogen atoms in the topmost 3 layers of diamond (001)-2x1-H. Our computations were restricted to the N_{2i} species that mimics the encounter of an interstitial N_i and a substitutional N_s species. The formation energy depends on the location of N_{2i} and the direction of the formed N_i-N_s bond, ranging from +4.12 to +9.71 eV. The most characteristic motions of vibration arise from N-N stretch mode of 1419 cm^{-1} (176.0 meV), C-N swing mode of 968 cm^{-1} (120 meV) and N-N swing mode of 471 cm^{-1} (58.5 meV).

5:05pm **PCSI-SuA2-32 Decay Dynamics of a Monolayer Silver Film on Si(001)**, *Xiaohang Huang*, Guangdong Technion - Israel Institute of Technology, China; *K. Huang*, Guangdong Technion - Israel Institute of Technology, Canada
Under operando conditions, silicon-based semiconductor devices are subject to impulses from mechanical, thermal, electrical, and photonic excitations, leading inevitably to structural decay.[1–4]The dynamics associated with the decay process (e.g., rate, pathway and barrier) is of practical interest, because it is crucial for stability assessment, lifetime prediction, and performance optimization.

Here, we describe the decay dynamics of a monolayer silver film on Si(001). Extended in-situ monitors of the evolution of (2x2) Ag-film/Si(001), using ultra-high vacuum scanning tunneling microscopy between 245 K and 276 K, demonstrate the thermal decay of the silver film by successive detachment of silver tetramers at the edge of the film (shown in Figure S1a-b of the supplementary pages). Complementary measurements, using the "annealing/quenching" method, gave evidencethat the detached silver had transitioned into a mobile state, Ag(m), which is capable of migrating and aggregating into clusters on both bare and silver-covered silicon surfaces (as in Figure S1c of the supplementary pages). Based on these experimental findings, we propose a first-order kinetic model that centers on the reversible transition of silver between the (2x2) Ag-film and Ag(m). By applying this model to our experimental data, an excellent fit can be achieved, yielding an activation of 0.386 ± 0.010 eV for the (2x2) Ag-film to Ag(m) transition, and that of 0.332 ± 0.012 eV for the Ag(m) to the (2x2) Ag-film transition. The obtained pre-exponential factors are anomalouslylow, i.e. 2067 ± 877 s^{-1} for the (2x2) Ag-film to Ag(m) transition, and 90 ± 47 s^{-1} for the Ag(m) to the (2x2) Ag-film transition. Such low values of the pre-exponential factors are likely linked to an entropic effect, on which density functional theory simulations are underway to provide further insight.

5:10pm **PCSI-SuA2-33 Temperature-Dependent Recombination Rate Analysis of the Minority Carrier Lifetimes in Mid-Wave Infrared Antimonide based Materials**, *Haley B. Woolf*, New Mexico State University; *R. Carrasco, P. Weber, A. Newell, A. Duchane, C. Morath, D. Maestas*, Air Force Research Laboratory
Various mid-wave infrared III-V materials (lattice-matched InAsSb, GaInAsSbBi on GaSb, strain-balanced InAs/InAsSb and InGaAs/InAsSb superlattice on GaSb) are characterized by time-resolved photoluminescence over temperatures ranging from 4 to 295 K. The

samples are excited to low-excitation conditions, injections between 10^{15}-10^{16} electron-hole pairs/cm3 per pulse, which yields single exponential decay of the time-resolved photoluminescence where the minority carrier lifetime can be evaluated. The temperature dependent lifetime is analyzed using a recombination rate model to determine the temperature-dependent Shockley-Read-Hall (SRH), radiative, and Auger recombination rates. The SRH and Auger recombination rates effectively model the lifetime data above 100 K in all samples, and provide evaluations of the defect energy level, capture cross section defect concentration product, carrier concentration, and Bloch overlap parameter in each sample.

Below 100 K, the lifetime's temperature dependence is complicated by additional factors. Samples with lifetimes on the order of 1-2 μs or less exhibit an SRH-limited temperature dependence down to 4 K that is largely constant or slightly increasing with decreasing temperature due to the thermal velocity term in the SRH recombination rate. On the other hand, undoped lattice-matched InAsSb and strain-balanced InAs/InAsSb superlattice samples with longer lifetimes around 6-7 μs exhibit markedly different behavior. In the lattice-matched InAsSb sample, the lifetime begins to decrease with decreasing temperature, consistent with radiative recombination becoming increasingly dominant as temperature approaches zero. There is no indication of radiative recombination in the 6-7 μs lifetime strain-balanced InAs/InAsSb superlattice, however, which, remains constant with decreasing temperature. This may be a consequence of the non-unity wavefunction overlap in the superlattice that would increase the radiative lifetime. The GaInAsSbBi sample exhibits a rapidly increasing lifetime with decreasing temperature from ~0.3 μs at 100 K to 4 μs at 4 K, which may indicate that localization in this alloy is suppressing SRH at lower temperatures. These conclusions will be explored in the context of how well the recombination rate model predicts them and potential improvements to it.

PCSI

Room Keahou I - Session PCSI-SuE1

Organic and Hybrid Semiconductor Materials

Moderator: Ingmar Swart, University of Utrecht

7:30pm PCSI-SuE1-1 A Study of Stereochemical Recognition of Chiral Molecules Investigated by STM-Based Techniques, *Yuji Kuwahara,* Osaka University, Japan **INVITED**

The combination of a scanning probe microscope with a photon detector and a Raman spectrometer, referred to as a tunneling-electron-induced light emission (STM-LE) and a tip-enhanced Raman scattering spectroscopy (STM-TERS), is quite attractive and useful to explore the optical properties and chemical analysis of nanomaterials beyond the optical diffraction limit.

In this study, we performed the STM observation to elucidate structural configuration of chiral molecules adsorbed on the metal substrates accompanied with their optical and vibrational properties using our laboratory-built STM-LE and STM-TERS systems[1-4]. As for the chiral molecules, we usedracemic-mixture and enantiopure molecules of thechiral PTCDI*(N,N'*-Di-*n*-octyl-3,4,9,10-perylenetetracarboxylic Diimide) andthiaheterohelicene and their derivatives. We clearly observed the high resolution STM images for the chiral molecular assemblies, leading to the important perspective of stereochemical chiral recognition based on the formation of ordered molecular structures combined with their optical and vibrational characterizations. Theoretical calculation based on a density functional theory and a molecular dynamics simulation successfully identified the formation mechanism of the molecular self-assemblies in the chiral recognition schemes.[5] Moreover, we attempted to investigate the optical dissymmetry of chiral PTCDI molecules using STM-LE measurement, and that of helicene derivatives using the STM-TERS measurements for evaluating the optical activity and identifying the enantiomers of the chiral molecules at a molecular scale.

References

[1] P. Krukowski, Y. Kuwahara, *et al., J. Phys. Chem*. **C 120**, 3964–3977 (2016).

[2] S. Chaunchaiyakul, Y. Kuwahara *et al., J. Phys. Chem*. **C 121**, 18162–18168 (2017).

[3] P. Krukowski, Y. Kuwahara, *et al., Appl. Surf. Sci.*, **589**, 152860 (2022).

[4] S. Kimura, Y. Kuwahara, *et al., Phys. Chem. Chem. Phys.* **26**(43), 7658-7663 (2024).

[5] Changqing Ye, Y. Kuwahara et al., J Phys.Chem. C127(43), 21305-21312(2023)

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8:10pm PCSI-SuE1-9 N-Heterocyclic Carbene and Olefin Monolayers on Silicon, *Martin Franz,* Technische Universität Berlin, Germany*; M. Das,* Universität Münster, Germany*; C. Hogan,* Istituto di Struttura della Materia-CNR (ISM-CNR), Italy*; A. Das,* Universität Münster, Germany*; R. Zielinski, M. Kubicki,* Technische Universität Berlin, Germany*; M. Koy,* Universität Münster, Germany*; S. Chandola,* Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Germany*; M. Freitag,* Universität Münster, Germany*; U. Gerstmann,* Universität Paderborn, Germany*; C. Kosbab,* Technische Universität Berlin, Germany*; S. Brozzesi,* Università di Roma Tor Vergata, Italy*; M. Nehring, D. Liebig, V. Balfanz, J. Brühne,* Technische Universität Berlin, Germany*; W. Schmidt,* Universität Paderborn, Germany*; N. Esser, F. Glorius, M. Dähne,* Technische Universität Berlin, Germany

Organic overlayers have emerged into a promising surface modification or functionalization tool and N-Heterocyclic carbenes (NHCs) and their close relatives, the N-heterocyclic olefins (NHOs), were found to be particularly suitable in this regard forming highly ordered self-assembled monolayers (SAMs) on metal surfaces that exhibit superior properties to the widely used thiol-based SAMs. As silicon remains the material of choice in today's semiconductor technology a functionalization of its surfaces is of highest interest.

Here, a comprehensive scanning tunnelling microscopy (STM), density functional theory, and X-ray photoemission spectroscopy study of the growth of NHC and NHO monolayers on clean and modified silicon surfaces is presented [1-3]. We demonstrate the formation of highly ordered monolayers binding to the surface via a single Si–C bond (see Fig. 1). The monolayers exhibit high thermal stabilities and show large work function reductions. By systematically varying the sidegroups and the backbone of the molecules and investigating two different molecule classes (NHCs and NHOs), we obtain a profound understanding of the bonding, structure, and assembly of NHCs and NHOs on Si offering guiding rules for a targeted modification of Si surfaces.

[1] M. Franz et al., Nat. Chem. 13, 828-835 (2021).
[2] R. Zielinski et al., J. Mater. Chem. C 11, 7377 (2023).
[3] M. Das et al., Angew. Chem. Int. Ed. 62, e202314663 (2023).

8:15pm PCSI-SuE1-10 On Surface Synthesis of Graphite-N-Doped Molecular Graphene Nanostructures, *Dong Wang,* Institute of Chemistry, CAS, China

Graphene and its derivates have been widely investigated with the exotic electronic properties. Doping is one of the most important ways to tune the properties of graphene-based nanostructures and materials.

The π-conjugated di- and polyradicals is attractive as a designable platform to explore the molecules spin interaction and development of organic magnetic materials. The introduction of graphite-N is one of most promising way to realize the construction of the π-conjugated polyradicals platforms. here we present the construction of an NHC-derived 1,3,5-TMB (N-TMB). In the target N-TMB molecule, the TMB core is stabilized by three NHC modules, which are further fused by benzene rings to the backbone with the expectation of improving the stability and spin coupling of the triradical. The N-TMB exhibits threefold symmetry on Au(111) and is structurally verified by nc-AFM techniques. STS characterization combined with DFT calculations reveals the occurrence of strong charge transfer between N-TMB and the substrate, resulting in positively charged N-TMB3+ on Au(111) surface. We further design and synthesize other N-doped 0D and 1D molecular graphene nanostructures and exploit their electronic structures.

8:20pm PCSI-SuE1-11 Importance of Molecular Dipole Alignment and Surface Compensation in P-V Hysteresis of MAPbBr$_3$(001), *L. Freter,* Forschungszentrum Jülich GmbH, Germany*; H. Hsu,* National Taiwan University, Taiwan*; R. Sankar,* Academia Sinica, Taiwan*; C. Chen,* National Taiwan University, Taiwan*; R. Dunin-Borkowski, P. Ebert,* Forschungszentrum Jülich GmbH, Germany*; Y. Chiu,* National Taiwan University, Taiwan*; **Michael Schnedler,** Forschungszentrum Jülich GmbH, Germany

Metalorganic halide perovskites attracted extraordinary attention as low-cost photovoltaic materials, due to their rapid increase of the conversion efficiency within a few years only. However, it is unclear to what degree the reported conversion efficiencies extracted from current density versus voltage (*J-V*) curves are accurate, since *J-V* hystereses are known to make "bad cells look good". It is thus of paramount importance to unravel the physical mechanisms inducing hysteresis, but no consent has been achieved yet. We demonstrate the presence of a hysteresis in tunneling spectra acquired at 4.3 K on cleaved MA-Br terminated (001) surfaces of MAPbBr$_3$ single crystals. Simulations of the tunneling spectra reveal an underlying polarization-voltage (*P-V*) hysteresis, caused by an interplay of field-induced rotation and alignment of the MA molecules, stabilized by dipole-dipole interactions, and an ion-lattice relaxation. The field-induced, ferroelectric polarization in the bulk is compensated at the surface by an oppositely oriented, counteracting out-of-plane polarization component of the otherwise in-plane antiferroelectrically ordered surface dipole arrangement. This suggests that at low temperatures only ferroelectric effects govern the hysteresis in MAPbBr$_3$ and its related compounds, whereas at high temperatures thermally activated processes such as ion migration and charge trapping-detrapping dominate.

8:25pm PCSI-SuE1-12 A Rare Earth Modified Silicon Surface as a Template for Ordered Organic Growth, *M. Kubicki, **Martin Franz,** M. Dähne,* Technische Universität Berlin, Germany

The formation of self-assembled layers of organic molecules on solid surfaces is an important subject because of their possible application in advanced (opto)electronic devices.While the formation of self-assembled layers is well established on metal surfaces, the growth on silicon surfaces, which are still the material of choice in today's semiconductor technology, is much less studied. On pure silicon, the formation of ordered organic films is usually hindered by their high dangling bond density, so that an appropriate surface modification is required. Here we demonstrate the high potential of a rare earth modification for promoting an ordered growth.

Using scanning tunneling microscopy, we show that a terbium modified Si(111) surface enables the formation of highly ordered molecular monolayers, on the example of cobalt phthalocyanine (CoPc). CoPc belongs to the transition metal phthalocyanines being a class of organic semiconductors, which has been already employed e.g. in organic light emitting diodes, photovoltaic cells, and field-effect transistors.

Our data demonstrate that single CoPc molecules stay highly mobile at the TbSi$_2$/Si(111) surface at room temperature. By reaching a coverage of a full monolayer, a highly ordered film consisting of large domains of flat-lying CoPc molecules in an almost fourfold symmetry with different orientations is formed

[1] M. Kubicki, M. Franz, and M. Dähne, "A Rare Earth Modified Silicon Surface as a Template for Ordered Organic Growth", J. Phys. Chem. C **128**, 13347 (2024).

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PCSI
Room Keahou I - Session PCSI-SuE2

Wide Bandgap Materials I
Moderator: Alex Demkov, The University of Texas

8:30pm **PCSI-SuE2-13 Invited Paper**, *Debdeep Jena*, Cornell University
INVITED

9:10pm **PCSI-SuE2-21 "High Throughput" Exploration of Oxide MBE Growth Space through Cyclical in situ Growth and Etching**, S. Schaefer, D. Fébba, M. Smeaton, K. Egbo, G. Teeter, S. Hasan, W. Callahan, A. Zakutayev, *Brooks Tellekamp*, National Renewable Energy Laboratory
Beta phase gallium oxide (β-Ga$_2$O$_3$) is an emerging ultra-wide bandgap semiconductor that has attracted attention for its potential to outperform existing materials operating at high breakdown voltages and high temperature. Alloying of In and Al in β-Ga$_2$O$_3$ provides the ability to individually engineer the bandgap and lattice parameters of the material, providing a useful toolbox for heterostructure engineering. However, the tendency of (Al,In,Ga)$_2$O$_3$ alloys to form competing phases, along with the complex suboxide chemistry of Ga and In, results in a growth window that is difficult to map and an alloy which is difficult to control.

We report on a high-throughput molecular beam epitaxy (MBE) technique to screen the growth conditions for the ternary alloy (In$_y$Ga$_{1-y}$)$_2$O$_3$, and the application of these findings to the successful synthesis of monoclinic (Al$_x$Ga$_{1-x-y}$In$_y$)$_2$O$_3$. By leveraging the sub-oxide chemistry of Ga$_2$O$_3$ and *in-situ* monitoring by reflection high-energy electron diffraction (RHEED), a cyclical growth and etch-back method is developed to rapidly characterize the (In$_y$Ga$_{1-y}$)$_2$O$_3$ growth space. This cyclical method provides approximately 10x increase in experimental throughput and 46x improvement in Ga$_2$O$_3$ substrate utilization. Growth conditions for monoclinic (In$_y$Ga$_{1-y}$)$_2$O$_3$ are identified and targeted growths are characterized *ex-situ* to confirm improved In incorporation. These conditions are then used to grow quaternary (Al$_x$Ga$_{1-x-y}$In$_y$)$_2$O$_3$ with Al cation composition *x* ranging from 1% – 24% and In cation composition *y* ranging from 3% to 16%. The structural, chemical and optical properties of the alloys are investigated. An (Al$_{0.17}$Ga$_{0.76}$In$_{0.07}$)$_2$O$_3$ alloy lattice-matched to Ga$_2$O$_3$ is examined by high resolution microscopy, highlighting the correlation between surface facets and composition. Such lattice-matched material can be grown arbitrarily thick without elastic strain and relaxation, making it suitable for high voltage diodes, transistor barriers, and epitaxial dielectrics.

9:15pm **PCSI-SuE2-22 Stability of Interface Morphology and Thermal Boundary Conductance of Direct Wafer Bonded GaN|Si Heterojunction Interfaces Annealed at Growth and Annealing Temperatures**, K. Huynh, M. Liao, University of California Los Angeles; X. Yan, University of California Irvine; J. Tomko, T. Pfeifer, University of Virginia; V. Dragoi, N. Razek, EV Group, Austria; E. Guiot, R. Caulmilone, Soitec, France; X. Pan, University of Irvine; P. Hopkins, University of Virginia; *Mark Goorsky*, University of California Los Angeles
Evolution of the structural and thermal interfacial properties of direct wafer bonded (0001) GaN to (001) Si during annealing is investigated. Direct wafer bonding provides a pathway to fabricate and engineer heterointerfaces free of lattice mismatch restrictions. Here, an EVG° ComBond° wafer bonder was used to bond the GaN and Si under high vacuum at room temperature by first removing native oxide with an Ar$^+$ beam prior to bonding. We have demonstrated as-bonded GaN on Si with high thermal boundary conductance of 143 MW/(m^2·K) prior to annealing. High resolution transmission electron microscopy of the as-bonded structure revealed abrupt bonded interfaces with a ~1.3 nm amorphous interface due to the Ar$^+$ surface treatment. After annealing at 450 °C up to 7 hours, a 1 nm Ga-rich layer is observed across the interface near the surface of the Si in addition to SiN$_x$ formation at the original bonded interface. Further annealing at 700 °C up to 24 hours led to the formation of Ga-rich pyramidal features that form across the bonded interface in the Si along the (111) planes. While recrystallization was observed to have a beneficial impact in other bonded systems, the chemical and structural reconfiguration of these GaN-Si interfaces resulted in poorer interfacial thermal transport by a factor of two (71 MW/(m^2·K)). This reduction is attributed to the degradation of thermodynamically less stable phases as the GaN breaks down into SiNx and Ga in the presence of silicon.We show that high TBC can be achieved through wafer bonding of GaN and Si and that interfacial properties that are stable at typical device operating temperatures (250 °C), but higher temperature annealing processing steps are deleterious to thermal transport across GaN-Si interfaces.

9:20pm **PCSI-SuE2-23 Plasma Deposition of GaN Thin Films on Silicon Substrates at Low Temperature**, L. Hussey, J. Maurice, P. Roca I. Cabarrocas, *Karim Ouaras*, Ecole Polytechnique, France
Gallium nitride is attracting increasing attention in the semiconductor industry, especially for high-power and high frequency electronic applications, owing to its unique features, i.e. direct band gap of 3.4 eV, high electron mobility, good thermal stability, and elevated mechanical hardness. MOCVD and MBE are the most employed methods to produce high quality GaN layers, yet they have their own drawbacks. On the one hand, MOCVD uses toxic gases as precursors and operates at very high temperatures (~1000 °C) to enable the pyrolysis of precursors. On the other hand, MBE faces issues of (i) high cost associated with the use of ultra-high vacuum pumping, and (ii) scalability. Additionally, it also operates at high temperature. This latter point induces thermal mismatch strain due to large thermal expansion coefficient difference between GaN and Si that may produce interface defects, film cracking and wafer bowing upon cooling. A potential solution to avoid those issues is to resort to a lower temperature method such as low-pressure plasma deposition. In this work, we demonstrate the direct growth of GaN thin films on silicon substrate using reactive sputtering of a liquid Ga target by an Ar/N$_2$ plasma at room temperature [1]. The morphology, microstructure, and composition profile of the GaN thin films have been analyzed using a set of ex-situ solid-state characterization techniques while the plasma has been investigated using in-situ technics, including OES, MW interferometry and TALIF to measure electron density, gas temperature and N-atoms density, respectively. In the presentation, we will discuss the resulting properties of the films as a function of plasma characteristics.

[1] L. Srinivasan et al. J. Vac. Sci. Technol. A. Vol.41, Issue 5 (2023)

PCSI

Room Keahou I - Session PCSI-MoM2

High-k Dielectrics and Ferroelectrics

Moderator: **Peter Maurer**, University of Chicago

11:10am **PCSI-MoM2-33 Non-Volatile Optical Phase Shifters on Si Photonics Platform**, *Mitsuru Takenaka*, Y. Miyatake, R. Tang, K. Taki, N. Sekine, K. Watanabe, T. Akazawa, H. Sakumoto, D. Bhardwaj, M. Fujita, H. Tang, The University of Tokyo, Japan; K. Makino, J. Tominaga, N. Miyata, M. Okano, National Institute of Advanced Industrial Science and Technology (AIST), Japan; K. Toprasertpong, S. Takagi, The University of Tokyo, Japan
INVITED

A programmable Si photonic integrated circuit (PIC) [1] is emerging for various applications, including communication [2], computing [3, 4], and sensing [5]. To adjust its functionality, the optical phases of signals need to be controlled through multiple optical phase shifters integrated into the PIC. However, thermo-optic (TO) phase shifters, which are commonly used in silicon PICs, have high power consumption [6]. Moreover, their volatility leads to complex electrical wiring, especially when the number of phase shifters is large. As an alternative to TO phase shifters, we have investigated non-volatile optical phase shifters based on a III-V/Si MOS capacitor [7, 8], phase change materials [9], and ferroelectric HfZrO2 [10]. In this paper, we present our recent results of these non-volatile optical phase shifters.

[1]W. Bogaerts et al., Nature 586(7828), 207–216 (2020).[2]K. Tanizawa et al., Opt. Express 23(13), 17599 (2015). [3]Y. Shen et al., Nat. Photonics 11(7), 441–446 (2017). [4]X. Qiang et al., Nat. Photonics 12(9), 534–539 (2018). [5]X. Zhang et al., Nature 603(7900), 253–258 (2022).[6]M. Takenaka et al., J. Lightwave Technol. 37(5), 1474–1483 (2019).[7]J.-H. Han et al., Nat. Photonics 11(8), 486–490 (2017).[8]R. Tang et al., Laser Photon. Rev. 17(11), (2023).[9]Y. Miyatake et al., IEEE Trans. Electron Devices 70(4), 2106–2112 (2023). [10]K. Taki et al., Nat. Commun. 15(1), 3549 (2024)

11:50am **PCSI-MoM2-41 In-Situ Analytical Study on Atomic Layer Deposition of Metal Silicate Thin Films Using Hexachlorodisilane and Water**, *G. Kim, E. Lee, Yo-Sep Min*, Konkuk University, Republic of Korea
Atomic layer deposition (ALD) is a critical process in the fabrication of modern electronic devices due to its ability to precisely grow thin films through the chemical adsorption of precursors.[1] Various metal oxide films can be deposited at low temperatures using metal precursors such as alkoxides or halides, along with water as the oxygen precursor. However, when using hexachlorodisilane (HCDS) and H_2O for SiO_2 ALD, challenges arise at low temperatures or with limited precursor exposure, often necessitating higher deposition temperatures or the use of Lewis base catalysts like pyridine or ammonia.[2] Through in-situ analyses using Fourier transform infrared spectroscopy (FTIR) and quartz crystal microbalance (QCM), we propose that metal hydroxyl groups (M-OH, where M represents Al, Ti, or Zn) located near silanol (Si-OH) groups facilitate the chemisorption of HCDS and H_2O at low temperatures, eliminating the need for catalysts. To elucidate the role of these metal hydroxyl groups, we conducted in-situ analyses of the ALD processes for metal silicate using trimethylaluminum, $TiCl_4$, or diethylzinc with FTIR and QCM. The hydrogen bonding between M-OH (or M-O-Si) and silanol groups may enhance the nucleophilicity of the oxygen of silanol, thereby promoting SiO_2 ALD. Although the M-OH groups promote the growth of silica, they gradually become covered by silica layers as ALD cycles repeat, reducing their effectiveness as promoters. Since the basicity of M-OH affects the strength of hydrogen bonding with silanol, we investigated the basicity of these M-OH groups using acetylacetone (Hacac) as a probe molecule. Among the M-OH groups studied, Zn-OH exhibited the highest basicity, followed by Al-OH and Ti-OH. We also discuss the correlation between the basicity and the effectiveness of the M-OH promotor.

11:55am **PCSI-MoM2-42 Enhanced Dielectric Properties of HfO₂ Thin Films Produced via Novel Catalytic Atomic Layer Deposition Process**, *Sara Harris, M. Weimer, A. Dameron, D. Lindblad, A. Wang*, Forge Nano
Optimized high-κ dielectric materials are widely utilized as gate oxides and dielectric barriers in compound semiconductor devices such as GaN HEMT and MEMS [1].Monolithic high-κ dielectric materials have inherent performance tradeoffs demonstrated by hafnium oxide (HfO₂) which has a high dielectric constant but a low breakdown voltage and high leakage current limiting overall efficacy as a dielectric barrier[2]. Composite materials such as HfAlOx can improve dielectric performance by combining the high dielectric constant of HfO₂ with the wider band gap and higher breakdown voltage of aluminum oxide (Al₂O₃) unlocking capabilities for next generation dielectric materials [2]. Atomic layer deposition (ALD) exploits precise control over self-limiting surface chemistry allowing for discreet nanolayers that can be tailored to optimize bulk film dielectric performance with a level of control that is not possible via other deposition techniques (CVD and PVD). This work demonstrates HfO₂ thin films deposited via ALD with enhanced dielectric properties achieved through the addition of a novel catalytic conversion step known as a CRISP Process. HfO₂deposited via the CRISP process has 29% higher GPC, 7% higher density, more ideal stoichiometry, 44% less carbon impurity and larger crystal grains when compared to films growth with O₃ alone. In pursuit of high performing dielectric materials several compositions of ALD deposited nanolaminates were studied through the incorporation of small amounts of Al₂O₃ into bulk HfO₂. Discreet nanolayer formation is demonstrated via cross sectional scanning electron microscopy (SEM) shown in Figure 1. With varying amounts of Al₂O₃, dielectric constant, κ, can be increased from 16.2 to 19.2, the dielectric strength (breakdown voltage) can be increased from 6.9 to 7.8 MV/cm, and the leakage current density can be reduced from 3.3×10^{-9} to 8.1×10^{-12} J at 60Vm. Work is ongoing to tune layer composition for the best overall performance. In the future, full characterization in GaN HEMT devices is planned for both the HfO₂ – O₃ and HfO₂ – CRISP processes.

[1] S. Kol, et al., Acta Physica Polonica A 136, 6, (2019), pp. 873-881

[2]A.M. Mumlyakov et. al.,Journal of Alloys and Compounds V858 (2021), 157713

12:00pm **PCSI-MoM2-43 Improving Hot Electron-Induced Punchthrough (Heip) via Dual Sti Sidewall Process in Dram**, *Jaehyeon Jeon*, Sungkyunkwan University, Korea; B. Choi, Sungkyunkwan University (SKKU), Republic of Korea
As device scaling continues, higher electric fields develop in MOSFETs, leading to the generation of hot carriers in the channel and increased off-current due to hot-electron-induced punchthrough (HEIP) in pMOSFETs. In low-power DRAM, minimizing pMOSFET off-current is crucial to reducing standby power consumption, making HEIP immunity improvement essential for meeting standby current requirements. The primary factor behind HEIP degradation is electron trapping in the top region of the STI liner nitride. To enhance HEIP immunity, solutions such as increasing the gate length using a large tabbed-gate design or thickening the STI sidewall oxide to reduce electron trapping in the STI liner nitride have been proposed. However, while a large tabbed-gate design can improve HEIP immunity, it also increases chip size, making it impractical for low-power applications. A thicker STI sidewall oxide is a more viable solution, offering improved HEIP immunity without degrading DRAM performance. Nonetheless, in 10nm-scale DRAM products, increasing the core STI sidewall oxide thickness transforms the long-axis cell STI structure from an oxide-nitride configuration to a fully oxide-filled structure. This shift causes abnormal recess formation during cell gate fin patterning, resulting in VTS variability degradation. This paper presents and validates a process method that increases the core sidewall oxide thickness to improve HEIP immunity while maintaining the oxide-nitride structure in the cell STI region, which is critical for optimizing fin pattern formation.

PCSI

Room Keahou I - Session PCSI1-MoM1

Characterization of Interfaces and Devices (Transport, Optical, & Electronic)

Moderator: **Roman Engel-Herbert**, Paul-Drude Institute for Solid State Electronics

8:30am **PCSI1-MoM1-1 Atomic Scale Insights into Layered 2D Materials Epitaxy, Dopants and Defects**, *Jamie Warner*, The University of Texas at Austin
INVITED
Layered 2D Materials in the monolayer limit are primarily surfaces and interface with other materials through van der Waals interactions. However, the presence of defects creates dangling bonds that act as binding sites and disrupt the periodic van der Waals bonding. Understanding the interfacial coupling between different 2D monolayers and with other atoms, molecules and materials at the atomic scale is essential for building accurate models, and transmission electron

microscopy is a leading approach for studying atomic scale behavior. Here, aberration corrected scanning transmission electron microscopy, combined with electron energy loss spectroscopy is used to extract accurate insights into atoms and their local bonding in 2D materials and how epitaxy arises at the interfaces. This will include graphene, hBN and transition metal dichalcogenides of mixed form, including MoS_2, WS_2, SnS_2, $PtSe_2$, $PdSe_2$ and more. Insights into the epitaxy in twisted Moire systems of 2D will be shown, and how 4D-STEM, figure 1, can be used to see structural insights beyond conventional imaging such as electric field mapping around single dislocations [1], figure 2. The atomic structure of several dopant atoms at the interface and the role of surface carbon adsorbates on the adatom adsorption and migration will be presented. These results will provide detailed information about how individual atoms behave on 2D surfaces that are suspended and under in-situ heating up to 1000^oC.

9:10am PCSI1-MoM1-9 Beyond Chemical Composition: How Surface Science Can Measure Electronic Properties, *J. Johns, Sarah Zaccarine, J. Mann, K. Artyushkova,* Physical Electronics

X-ray photoelectron spectroscopy (XPS) is a widely used technique to analyze surface composition and chemistry. Often, scientists and engineers aiming to optimize material performance in a device require complementary information about the material's optical and electronic properties. This combined information is necessary in fields such as semiconductors, photovoltaics, (opto)electronics, batteries, and other chemical redox applications.

Fortunately, modern XPS spectrometers offer additional techniques to study the behavior of electrons in a system in addition to the chemical makeup of atoms and molecules in the surface. Reflection electron energy loss spectroscopy (REELS) can be used for optical band gap measurements as well as hydrogen content and carbon hybridization, additional chemical information beyond XPS. Ultraviolet photoelectron spectroscopy (UPS) is a similar method to XPS but with lower-energy UV photons instead of X-rays and higher spectral resolution, illuminating finer details of the valence band structure including work function and ionization potential. Inverse photoemission spectroscopy (IPES), as the name implies, uses the opposite process of XPS and UPS to probe the conduction band of metals and other conductive materials for insight into unoccupied band structure and measuring the electron affinity. Low-energy IPES (LEIPS) is uniquely suited to studying electronic structure of e-beam-sensitive organics that can be damaged by the traditional IPES method [1]. Combined, UPS and IPES/LEIPS can be used to calculate the electronic band gap for conductive materials, an invaluable property for studying charge transfer across an electrochemical interface.

This presentation will discuss the unique information that each of these techniques yields on electronic states in a surface. Guidance will also be shared on choosing an appropriate technique for a given analytical question, how to prepare and mount samples appropriately for the various analyses, and common pitfalls to avoid in data acquisition and interpretation.

[1] Yoshida, H. Chem. Phys. Lett. **539–540**, 180-185 (2012).

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9:15am PCSI1-MoM1-10 Enhancing Interface and Retention Characteristics in NAND Flash Memory by Increasing Poly-Si Thickness to Prevent Pin-Hole Formation, *Chansung PARK, B. Choi,* Sungkyunkwan University, Korea

In the fabrication of NAND Flash memory cells, the quality of the tunneling oxide (DTOX) layer is crucial for ensuring reliable operation and data retention. This study focuses on the impact of increasing the thickness of the polysilicon (Poly-Si) layer deposited on DTOX following channel hole etching. After tunneling oxide deposition, subsequent processing steps can introduce plasma damage and hydrofluoric acid (HF) damage, leading to the formation of pin-holes at the DTOX interface. These pin-holes adversely affect interface characteristics and compromise data retention. By optimizing the Poly-Si thickness, we aim to mitigate pin-hole formation, thereby enhancing the interface integrity. Our experimental results demonstrate that a thicker Poly-Si layer effectively protects the DTOX from plasma and HF damage, resulting in significant improvements in both the interface properties and data retention performance. This approach not only provides insights into the processing challenges faced in NAND Flash fabrication but also highlights the importance of interface engineering in advancing memory device reliability.

9:20am PCSI1-MoM1-11 Relation Ship between Defect Density and Photoreflectance Spectroscopy for $InAs_xP_{1-x}$ Metamorphic Buffer Layer, *J. Kim, Gyoung Du Park, G. Kim, T. Kang,* Yeungnam University, Republic of Korea*; S. Lee, D. Kim,* Korea Research Instutue of Standards and Science (KRISS), Republic of Korea

In recent decades, $InAs_xP_{1-x}$ metamorphic buffer layer have applicated in advancing infrared photodetectors, chemical gas sensors, and optical communication devices. To improve the devices performance utilizing metamorphic buffer layer, it is crucial to reduce defect density by growing with graded composition ratios. Therefore, we prepared three samples with different $InAs_xP_{1-x}$ (x=0.7, 0.55, 0.5) compositions to examine the differences in defect density based on composition. Afterward, we investigated how these density differences impacted the PR results, exploring the potential of using photoreflectance (PR) measurements to infer defect densities. First, to determine the dislocation density of each sample, X-ray diffraction (XRD) measurements were conducted, resulting in values of 1.32 $x10^7$, 5.37 $x10^6$, and 1.12 $x10^7$ for the x=0.7, 0.55, and 0.5 samples, respectively, confirming that the x=0.55 sample had the lowest defect density. Following that, the internal electric field (F) was calculated from the Franz-Keldysh oscillation (FKO) signals obtained through the PR signal. The calculated F at the main peaks were 162, 84, and 160 *kV/cm* for the x=0.7, 0.55, and 0.5 samples, respectively. For the x=0.55 sample, the F was approximately 80 *kV/cm* lower. While this result could be attributed to differences in the built-in potential caused by composition variations, the dramatic difference is not observed in the x=0.7 and x=0.5 samples. Therefore, the 80 *kV/cm* difference cannot be fully explained by composition-related built-in potential alone. In General, lower defect density in a semiconductor reduces the number of photo-generated carriers trapped by defect states, enhancing the field screening effect and resulting in a lower calculated F, as indicated by the FKO signal. Additionally, we performed PR measurement as a function of modulation frequency to determine the time constant to verify the process of photogenerated carriers being trapped at defect states. The results showed that the x=0.7, 0.55, and 0.5 samples exhibited time constants of 54.4, 43.9, and 51.5 *us*, respectively, with the x=0.55 sample having the lowest time constant. These results are due to the lower defect density in the x=0.55 sample, which reducing the probability of photo-generated carriers being trapped at defect states during transport. In conclusion, we proposed that PR spectroscopy, shows potential as a new method for investigating defect-related properties in metamorphic buffer layer structures.

9:25am PCSI1-MoM1-12 UPGRADED: Imaging Light-Matter Interactions using Low Kinetic Energy Photoelectrons, *A. Kim, A. Boehm, M. Berg, Taisuke Ohta, C. Doiron,* Sandia National Laboratories*; F. Vega,* Purdue University*; J. Yu, J. Klesko, S. Gennaro,* Sandia National Laboratories*; F. Liu,* los Alamos National Laboratory*; S. Smith, G. Copeland,* Sandia National Laboratories*; C. Chan,* University of Colorado at Boulder*; A. Mohite,* Rice University*; A. Cerjan,* Sandia National Laboratories*; T. Beechem,* Purdue University*; M. Sinclair, I. Brener, R. Sarma,* Sandia National Laboratories

In the photoemission process, the electromagnetic fields propagating within the material excite electrons above the vacuum level, with higher field intensity resulting in a greater number of photoemitted electrons. Photoelectron emission microscope (PEEM) directs the emitted photoelectrons onto an electron detector via electron optics that preserve their spatial origin. By extension, the spatial distribution of the electromagnetic field in engineered nanostructures, such as metasurfaces and photonic crystals, can be decoded from the photoelectron images.

In this talk, we will present results from three optical systems investigated using PEEM across a wide optical spectrum range. Using ultraviolet excitation, we examined Fabry-Perot resonances in thin film cavities of HfO_2 and SiO_2. The ultraviolet light is confined in oxides due to their higher refractive indices than that of the Si substrate. We use the cavity resonances to visualize the nanometer-scale inclusions embedded in the oxides using PEEM [1]. In the visible range, we examined dielectric metasurfaces of TiO_2 rods (i.e., meta-atoms) arranged in a square lattice. By comparing photoelectron images to finite-difference time-domain simulations, we determined the inelastic mean free path (IMFP) of the very low-energy (<1 eV) electrons to be ~35 nm. Because this IMFP is comparable to the height of the meta-atoms, the result highlights the sensitivity of photoelectron imaging to optical resonances supported within the meta-atom volume [2]. Extending to the near-infrared wavelength, we showed the polarization-dependent variation of the spectra of broken symmetry resonator metasurfaces. This work took advantage of potassium deposition on the surface to reduce work function, which enabled two-photon photoemission using near-infrared light [3]. In all three systems, we

show exemplars where the real-space near-field variations are intertwined with their spectroscopic signatures. These results demonstrate the applicability of photoelectron imaging with sub-optical wavelength resolution to examine light-matter interactions in volume-type photonic resonances supported by dielectric nanophotonic structures.

[1] M. Berg, F. Liu, S. Smith, R. G. Copeland, C. K. Chan, A. D. Mohite, T. E. Beechem, T. Ohta, Phys. Rev. Applied, **12**, 064064 (2019).

[2] A. R. Kim, C. F. Doiron, F. J. Vega, J. Yu, A. M. Boehm, J. P. Klesko, I. Brener, R. Sarma, A. Cerjan, T. Ohta, in preparation (2024).

[3] A. M. Boehm, S. D. Gennaro, C. F. Doiron, M. B. Sinclair, T. E. Beechem, R. Sarma, T. Ohta, Near-field Imaging of Optical Resonances in Silicon Metasurfaces Using Photoelectron Microscopy, APL Photonics, **9**, 066103 (2024).

9:45am PCSI1-MoM1-16 Examining Radiation Effects on the Electronic Structure and Defect Density of 1L WS2 through in-situ Photoemission Spectroscopy, *Christopher Smyth, A. Boehm,* Sandia National Laboratories*; K. Burns,* University of Virginia*; A. Kim, T. Ohta,* Sandia National Laboratories

Two-dimensional (2D) transition metal dichalcogenides (TMDs) exhibit a unique combination of high radiation tolerance and promising computing performance in an atomically thin profile. However, the relationship between ion irradiation, defect density, and electronic structure in TMDs has not been identified, and must be understood to characterize radiation resilience. Heavy ion fluences of $<10^{12}$ cm^{-2} degrade TMD device performance, but are currently untraceable by conventional TMD characterization techniques. Hence, the relationship between radiation-induced defect density and carrier concentration in monolayer (1L) transition metal sulfides (TMS) remains unresolved. Some reports indicate ion irradiation induces hole doping in TMS, whereas theory predicts electron doping by sulfur vacancies, which are the most abundant defect formed in TMS under ion irradiation.

In this talk, we irradiate suspended 1L WS_2 films with 5 MeV Fe^{2+} ions at fluences of 10^{11}-10^{13} cm^{-2} to controllably introduce defects, and examine the valence band density of states (DOS) using photoemission spectroscopy. Photoemission spectra (PES) show the highest occupied valence band DOS at the Γ-point in the Brillouin zone shift towards the vacuum level and Γ-point peak width increases up to an ion fluence of 10^{13} cm^{-2}. These spectral modifications substantiate a reduced band gap and excited photo-hole lifetime by enhanced screening with increased defect density. By calculating the defect density as a function of ion fluence using the Shockley-Read-Hall recombination model, we demonstrate that the PES exhibits an unprecedented sensitivity to defect concentrations on the order of 10^{12} cm^{-2} generated at an ion fluence of 10^{11} cm^{-2}. We further verify ion beam-induced defect densities using scanning transmission electron microscopy. Additional ion irradiations up to 10^{13} ions cm^{-2} cause electron doping as predicted by theory, but we detect hole doping after ion irradiation beyond the 10^{13} cm^{-2} fluence. This study highlights the high sensitivity of the Γ-point valence band PES to radiation-induced changes in defect density, band gap, and excited photo-hole state behavior in 1L WS_2 down to ion fluences of 10^{11} cm^{-2}.

9:50am PCSI1-MoM1-17 Scalable Synthesis of One-Dimensional Quantum Matter, *Ruhin Chowdhury, E. Renteria,* The University of New Mexico*; S. Addamane,* Sandia National Laboratories, USA*; D. Shima, D. Prakash, J. Neely,* University of New Mexico*; F. Cavallo,* The University of New Mexico

We present our recent efforts in the area of controlled synthesis of screw dislocations. Dislocations in semiconductors and other materials are generally considered detrimental in that they create scattering centers that lower carrier mobility, act as non-radiative carrier recombination centers, and induce growth instability of coherent thin films. Therefore, past research efforts have focused on hindering the formation of these line defects or annihilating them. Recent theoretical studies have demonstrated the prospect of repurposing screw dislocations as one-dimensional quantum matter [1,2], with potential applications in quantum computation and spintronics. These findings motivated our research on synthesis protocols of screw dislocations to achieve predictive control of their

spacing, arrangement, and width. Specifically, we investigated and established approaches to fabricate SDs in single-crystalline and widely used semiconductors, such as Si, GaAs, and SiC. The semiconductors are in nanomembrane (NM) form or sheets with nanoscale thickness and a lateral size-to-thickness ratio of at least 10^2. Our approach to controlled synthesis of SDs relies on overlaying two arrays of pixelated NMs of the same material at a non-zero twist angle or twisted bicrystals (TBiCs). Through this process, we create an array of disregistries at the interface that will serve as seeds for the growth of SDs. Pixelated NMs are obtained by top-down processing multilayered structures such as epitaxially grown GaAs thin films on AlGaAs sacrificial layers-coated GaAs substrates or SiC on insulator wafers. NMs provide more uniform interfacial bonding than their bulk counterpart and expand the palette of SDs hosts to include epitaxially grown ternary and quaternary alloys. High-temperature furnace annealing of TBiCs fosters the propagation of SDs from the interfacial seeds across the thickness of the NMs. We characterize the spatial distribution of SDs in NMs by plan-view transmission electron microscopy under a weak-beam condition. The spacing between SDs is correlated to theoretically calculated values using the measured twist angle between the NMs. The twist angle is obtained by selected area electron diffraction (SAED) patterns acquired from the TBiC.

[1] L. Hu, H. Huang, Z. Wang, W. Jiang, X. Ni, Y. Zhou, V. Zielasek, M. G. Lagally, B. Huang and F. Liu, "Ubiquitous Spin-Orbit Coupling in a Screw Dislocation with High Spin Coherency", Phys. Rev. Lett, 121, 066401 (2018).

[2] Y. Ran, Y. Zhang, and A. Vishwanath, "One-Dimensional Topologically Protected Modes in Topological Insulators with Lattice Dislocations", Nat. Phys. 5, 298 (2009).

9:55am PCSI1-MoM1-18 Structural Phase Transition and Electronic Structure of Epitaxial VO$_2$ Thin Films Prepared on a-Al$_2$O$_3$ Substrate, *Manish Kumar, S. Rani, H. Lee,* Pohang Accelerator Laboratory, POSTECH, Republic of Korea

Epitaxial thin films of thermochromic VO_2 were prepared on a-Al_2O_3 substrate using pulsed laser deposition (PLD) technique. Temperature dependent structural and electronic properties of the prepared epitaxial VO_2 thin films were studied by synchrotron X-ray diffraction (XRD) and X-ray absorption measurements. Temperature dependent synchrotron XRD measurements revealed the monoclinic to rutile structural phase transition (SPT) near 68°C in epitaxial VO_2 thin films of different thickness. A thermal hysteresis observed in the SPT during heating and cooling cycle signify the first order phase transition. Temperature dependent X-ray absorption linear dichroism (XLD) measurements at V L-edge and O K-edge; were carried out to examine the electronic structure of epitaxial VO_2 thin films. The modification in the electronic structure of epitaxial VO_2 thin films across the insulating monoclinic to metallic rutile phase transition were tracked.

10:00am PCSI1-MoM1-19 MBE-Grown Germanium Quantum Well Planar Josephson Junction, *Joshua Thompson, C. Gaspe, R. Card, J. Dong, K. Sardashti,* Laboratory for Physical Sciences*; S. Davari, H. Churchill,* University of Arkansas*; K. Serniak, T. Hazard,* MIT Lincoln Laboratory*; C. Richardson,* Laboratory for Physical Sciences

At the heart of a transmon qubit is the Josephson junction (JJ) which is engineered to create the anharmonic energy spacing needed to individually populate the two lowest energy levels in the system. Transmon qubits can incorporate two such JJs in a SQUID arrangement to achieve flux tunning of the qubit but require on-chip, current carrying flux lines. This presentation will discuss the characterization of undoped germanium quantum wells (Ge-QW) in a SiGe heterostructure and the fabrication of planar JJs for future integration into voltage tunable transmon qubits.

Strained Ge-QWs host heavy holes with high mobility and low effective mass. When combined with highly transparent superconducting contacts, they create a promising platform for combining voltage-controlled semiconductor materials with high fidelity superconductor qubit circuitry. The Ge-QW with SiGe spacer material is grown using Molecular Beam Epitaxy (MBE) and has a carrier mobility greater than 60,000 cm^2/Vs with a hole density less than 1×10^{12} cm^{-2}. Using a series of lithography and etching techniques, 100-nm to 500-nm long JJs are formed on a 2.5 μm tall SiGe mesa that is necessary to isolate the lossy SiGe from the rest of the superconducting circuit. Device design, fabrication challenges, and preliminary junction performance will be shown

10:05am PCSI1-MoM1-20 Neutron Reflectometry Studies of Interfacial Phenomena in Actinide and Actinide Related Thin Films, *I. Kruk, P. Wang,* Los Alamos National Laboratory*; D. Allred,* Brigham You*; K. Rector,* Los Alamos National Laboratory*; **Jaroslaw Majewski**,* Los Alamos National Laboratory, National Science Foundation

Studies of interfacial chemistry of actinides attract much attention due to interest in the power generation. In the power generation field, current research aims to reduce Pu and minor actinides in the spent light water reactor's fuel stockpiles. Therefore, considerable research efforts are underway to evaluate the suitability of Th as a nuclear fuel. Herein, in situ neutron reflectivity technology measures changes in the scattering length density (SLD) and thickness of a thorium, uranium, and cerium metal films in controlled environmental conditions: time-dependent exposition to oxygen and water vapors in various temperature regimes. Among other phenomena, our research uncovered non-stoichiometric thorium oxides, ThO_x, preferentially generated between the metal and its thermodynamically favored dioxide layers. The near perfect stoichiometric lattice and relative low O solubility of ThO_2 film limits the availability as well as diffusivity of O species interacting with ThO, and hence prevents or slows the successive further oxidation. These observations suggest that ThO has many advantages over ThO_2 as a potential nuclear fuel such as good breeding performance, high thermal conductivity and density with good chemical and temperature stability. Our studies of interaction the Cerium thin films with water vapors revealed homogenous penetration of physisorbed water into the layers of various oxygen stoichiometry and its complete removal upon decreasing of the relative humidity.

Key Words: Actinides, Chemistry of Thin Metal Layers, Neutron Reflectometry, Nuclear Fuel.

10:10am PCSI1-MoM1-21 Current Characteristics Depending on the Doping Concentration of the Barrier in the GaSb Based Unipolar Detector, *J. Kim, **Jong Hun Lee**, G. Kim, T. Kang,* Yeungnam University, Republic of Korea*; S. Lee, D. Kim,* Korea Research Instutue of Standards and Science (KRISS), Republic of Korea

The nBn detector consists of an n-type contact layer, a unipolar barrier that prevents electron transport, and an n-type absorber. Compared to the p-i-n structure, the nBn detector offers advantages such as low dark current and high-temperature operation. Due to these characteristic, nBn detector has been actively researched over the past years,particularly regarding the barrier doping concentration.

In the nBn detector, the dark current is known to decrease as the increase of the barrier donor doping concentration [1]. However, Zhuhas reported that Te doping in AlGaSb occur deep trap in 1988 [2]. These deep traps occur the leakage current such as trap assist tunneling (TAT) in the nBn detector. In addition, because the effect of barrier doping concentration on photocurrent has not been further investigated yet, to investigate the current characteristics of GaSb-based nBn detector depending on barrier doping concentration I-V measurements were performed. Dark current density at 80 K, 0.2 V were measured 0.009 A/cm^2 (undoped), 0.013 A/cm^2 ($2x10^{15}cm^{-3}$), 0.108 A/cm^2 ($2x10^{16}cm^{-3}$). Due to the negligible generation-recombination (G-R) current at low temperature,these results indicate the increase of TAT current due to rise of Te-related deep trap concentration. The exponent proportion of photocurrent to excitation light power at 300 K, 1 V were0.43 (undoped), 0.63 ($2x10^{15}cm^{-3}$), and 1.21 ($2x10^{16}cm^{-3}$).The exponent of lower than unity indicate that the carrier loss due to the recombination[3]. The reduce of carrier loss as the increase doping concentration was attributed that carrier injection due to the TAT and more efficiently carrier extraction due to higher carrier velocity. In conclusion, this study shows the importance of appropriate barrier doping concentration when the design of nBn detector through the rise of dark current and reduce of photocurrent loss as the increase of barrier doping concentration.

PCSI

Room Keahou I - Session PCSI-MoA1

Superconducting Qubits

Moderator: Chunhui (Rita) Du, Georgia Institute of Technology

2:00pm **PCSI-MoA1-1 Novel Josephson Effects in Superconductor-Semiconductor Systems**, *M. Gupta, G. Graziano, C. Riggert, L. Shani, G. Menning,* University of Minnesota, USA*; M. Pendharkar,* Stanford University*; C. Dempsey, J. Dong,* University of California at Santa Barbara*; P. Lueb, J. Jung,* Eindhoven University of Technology, The Netherlands*; R. Mélin,* Institut Néel, CNRS/UGA, Grenoble, France*; E. Bakkers,* Eindhoven University of Technology, The Netherlands*; C. Palmstrøm,* University of California at Santa Barbara*; **Vlad S. Pribiag**,* University of Minnesota, USA
INVITED

Superconducting nanostructures underpin the development of many promising quantum computing approaches and alternatives to conventional classical computing. Most work to date has focused on all-metallic Josephson junctions. Recent developments in materials synthesis and nanofabrication have enabled devices that combine superconducting and semiconducting properties. These provide new opportunities for science and technology that rely on the interplay between superconductivity, quantum confinement, ballistic transport and spin-orbit coupling, or which leverage gate-tuning of superconducting couplings. In this talk, I will present results from a few transport studies based on semiconducting nanowires and quantum wells coupled with superconductors. The talk will focus primarily on nanostructures with more than two superconducting terminals [1-4], which can be used to implement superconducting diodes and non-linear intermodulation with full electrostatic control or to realize unusual correlations between Cooper pairs, and could also serve as a platform for topological Josephson matter [5].

[1] M. Gupta *et al.,* arXiv:2312.17703 (2023).

[2] M. Gupta *et al.*, Nature Communications **14**, 3078 (2023).

[3] G. Graziano, M. Gupta *et al.*, Nature Communications **13**, 5933 (2022).

[4] G. Graziano *et al.*, Phys. Rev. B **101**, 054510 (2020).

[5] R. Riwar *et al.*, Nature Communications **7**, 11167 (2016).

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2:40pm **PCSI-MoA1-9 UPGRADED: First-Principles Studies of Schottky Barriers and Tunneling Properties at Al(111)/Si(111) and CoSi2(111)/Si(111) Interfaces**, *Johannes Kevin Nangoi, C. Palmstrøm, C. Van de Walle,* University of California, Santa Barbara
There has been recent interest in using Al(111)/Si(111) and CoSi$_2$(111)/Si(111) interfaces in novel merged-element transmons, which are proposed successors to the standard transmon qubits used in superconducting quantum computing. We present comprehensive first-principles studies of these interfaces, studying the relaxations of the atoms near the interface, calculating the formation energies and Schottky barrier heights, and providing estimates of the Josephson critical currents based on the Simmons/Tsu-Esaki tunneling model. We find that the formation energies and Schottky barrier heights are very similar for all Al(111)/Si(111) structures, yet vary significantly for the CoSi$_2$(111)/Si(111) structures. We attribute this to the more covalent character of bonding at CoSi$_2$/Si, which leads to configurations with distinct atomic and electronic structure. Our estimated Josephson critical currents, which govern the behavior of merged-element transmons, provide insight into the trends as a function of Schottky barrier height. We show that desirable qubit frequencies of 4–5 GHz can be obtained with a Si barrier thickness of 5–10 nm, and demonstrate that the critical current density as a function of Schottky barrier height can be modeled based on the tunneling probability for a rectangular barrier. We compare with experimental results where available, and discuss the implications of our results for actual devices.

3:00pm **PCSI-MoA1-13 Epitaxial Niobium Titanium Nitride Thin Films for Superconducting Quantum Circuits**, *Christopher Richardson, A. Thomas,* Laboratory for Physical Sciences*; E. Supple, B. Gorman,* Colorado School of Mines
Engineered superconducting thin film heterostructures are needed to create future generations of high-fidelity superconducting qubits. Through a structure-first approach, Plasma Assisted Molecular Beam Epitaxy is used to grow a niobium titanium nitride alloy superconductor directly on c-plane sapphire with an abrupt metamorphic interface. The ternary thin film, Nb$_{0.85}$Ti$_{0.15}$N, has an engineered lattice constant that is designed and synthesized to match the in-plane atomic spacing of aluminum nitride.

The best annealed films exhibit improved surface roughness to achieve a root-mean-square surface roughness less than 1 Å and improved superconducting critical temperature over 16 K. All films exhibit high quality factors at low powers, non-saturating superconducting microwave loss-behavior at high powers, and low kinetic inductance. These engineered superconducting thin films are ideal for the creation of an epitaxial Josephson junction and qubit devices that operate at higher temperatures.

In addition to exploring optimal growth parameters to produce thin ternary nitride superconductors, trilayers of NbTiN-AlN-NbTiN have been grown. Some of these samples have been measured using atomic probe tomography allowing crystallinity, homogeneity, and continuity of the AlN tunnel barrier to be quantitatively determined on the nanometer scale.[1]

[1] E. Supple, C. J. K. Richardson, & B. Gorman, J. Vac. Sci. Tech. A (2024).

3:05pm **PCSI-MoA1-14 Interface-Sensitive Microwave Loss in Tantalum Films Grown on C-Plane Sapphire for Quantum Information Applications**, *Anthony McFadden, T. Larson, S. Gill, A. Dixit,* NIST-Boulder*; J. Oh, L. Zhou,* Ames Laboratory*; F. Lecocq, R. Simmonds,* NIST-Boulder
Tantalum (Ta) has garnered much attention in the field of superconducting quantum computing recently because of multiple published reports showing a performance enhancement of Ta devices when compared to aluminum or niobium (Nb). Fabrication of high-performance Ta devices is thought to rely on the formation of the α-phase (body centered cubic) structure which typically requires heating the substrate during growth, while β-phase (tetragonal) Ta usually dominates the composition of films deposited at room temperature. Formation of two distinct elemental phases contrasts with niobium (Nb), which typically only forms α-phase thin films.

We systematically vary the growth temperature of sputtered Nb and Ta thin films deposited on c-plane sapphire (Al$_2$O$_3$(001)) resulting in thin films of β-Ta, mixed phase β- /α-Ta and α-Ta and Nb. The structural properties of the resulting thin films are measured with reflection high energy electron diffraction (RHEED), X-ray diffraction (XRD), atomic force microscopy (AFM), and transmission electron microscopy (TEM). Established lithography and dry etching processes are used to fabricate Hall bars for DC transport measurements and superconducting coplanar-waveguide resonators for microwave characterization in a dilution refrigerator.

Our measurements show that the structural and DC electrical properties of both Nb and Ta films are mostly consistent with prior reports, however, it was found that the microwave performance of superconducting resonators made from epitaxial Ta(111) films grown directly on Al$_2$O$_3$(001) was markedly poor. Considering these findings, the Ta/Al$_2$O$_3$(001) interface was tested by inserting either a thin, epitaxial Nb interlayer or by amorphizing the sapphire surface before Ta growth using an *in-situ* Ar plasma. Both of these approaches were found to enhance the internal quality factor (Q$_i$) of the superconducting resonators by nearly two orders of magnitude. This suggests that the epitaxial Ta(111)/Al$_2$O$_3$(001) interface is a significant source of microwave loss, which may be mitigated by modifying the sapphire surface before growth. Possible origins of this loss and methods to characterize and mitigate it will also be discussed.

3:10pm **PCSI-MoA1-15 Cryogenically Grown a-Ta on Inas for 2DEG-Based Josephson Junctions**, *Teun van Schijndel, J. Dong,* UC Santa Barbara*; Y. Gul,* University College London, UK*; D. Vera,* University of San Diego*; W. Yánez-Parreño, S. Chatterjee, C. Palmstrøm,* UC Santa Barbara
Josephson Junctions (JJs) are critical components in superconducting quantum circuits, including qubits, because of their nonlinear inductance [1]. Most commonly, JJ's in qubits consist of two aluminum superconductors separated by a thin aluminum oxide barrier. However, external control over the critical current and thus frequency of the qubit can only be achieved by applying magnetic flux through a superconducting quantum interference device. An alternative approach uses a semiconductor-superconductor heterostructure, allowing electric gate control of the JJ's critical current. In these systems, disorder, often introduced by superconductor/semiconductor interfacial reactions and during nanofabrication processes such as etching, can lead to heightened surface scattering [2], potentially leading to loss or decoherence.

Here, we are exploring the growth of Ta on InAs 2DEGs using a shadow mask technique in a low-temperature molecular beam epitaxy (MBE) system. This approach aims to eliminate nanofabrication-induced disorder near the junction. The 2DEGs are grown in an III-V MBE system, achieving mobilities exceeding 10^4 cm^2/V·s. After growth, the InAs samples were

capped with As. Before shadow mask deposition, the As cap was removed *in situ* by atomic hydrogen anneal. Reflective high energy electron diffraction (RHEED), scanning tunneling microscopy (STM), and X-ray photo spectroscopy (XPS) are used to investigate the semiconductor starting surface, the superconductor growth mode, and the extent of interfacial reactions. The Ta is grown at cryogenic temperatures (~7 K) to minimize interfacial reactions and to ensure the formation of the superconducting a-phase [3], allowing for the formation of highly transparent superconducting contacts. After optimization of the growth and resulting interface, JJ devices are fabricated using a shadow mask. Low-temperature electrical measurements (around 60 mK) are performed to determine the junction properties, including the critical current (I_c), the I_cR_n product, and the $I_{ex}R_n$ product. These values will allow us to evaluate the transparency of the superconducting contacts and determine if the junctions exhibit ballistic transport behavior. Comparisons will be made for Ta films grown at different substrate temperatures and we will report on correlations between interfacial reactions and Ta crystal structure with junction properties.

[1] P. Krantz, et al., Appl. Phys. Rev. 6, 021318 (2019)

[2] S. J. Pauka, et al., J. Appl. Phys. 128, 114301 (2020)

[3] T.A.J. van Schijndel, et al., arXiv preprint arXiv:2405.12417 (2024)

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3:15pm PCSI-MoA1-16 Low Temperature Deposition of Superconducting Aluminum Films for Quantum Information Applications, *Wilson J. Yánez-Parreño, T. van Schijndel,* University of California at Santa Barbara*; A. McFadden, R. Simmonds,* NIST-Boulder*; C. Palmstrom,* University of California at Santa Barbara

Aluminum is one of the most widely adopted superconductors for quantum information applications [1, 2]. It has well understood superconducting properties and a self-limiting oxide that is an ideal barrier in Josephson junction devices [1]. This together with the ability to grow it in a clean manner on low dielectric loss substrates like sapphire and silicon makes it the material of choice to make quantum information devices like transmon qubits [2], Nevertheless, a big disadvantage of superconducting aluminum is its low critical field of around Hc=100 Oe and critical temperature of Tc=1.2K which makes it non ideal in quantum applications that require higher temperatures or an applied magnetic field.

We explore the growth of superconducting aluminum films on c-plane sapphire and silicon (111) at room temperature and cryogenic temperatures of < 20 K during deposition. The films are synthesized in state of the art low-temperature molecular beam epitaxy equipment with in-situ reflection high energy electron diffraction (RHEED) characterization and a base pressure of < 5E-11 mbar. We characterize the structure and crystallinity of the films, the substrate and the interface using x-ray diffraction, RHEED, atomic force microscopy and X-ray photoelectron spectroscopy. We measure electrical transport in these films under perpendicular magnetic fields and temperatures as low as 70 mK and correlate the superconducting properties of aluminum with its structure. We find that low temperature deposition increases the degree of structural disorder which enhances the critical temperature and critical field of aluminum to Tc=1.5K and Hc = 690 Oe. We then fabricate superconducting microwave resonators on these films and study the loss in aluminum grown at cryogenic temperatures.

[1] C. R. H. McRae, et al. Review of Scientific Instruments 91 (2020).

[2] Aute, F., et al. Nature 574, 505-510 (2019).

3:20pm PCSI-MoA1-17 Strong Photon-Magnon Coupling Using a Lithographically Defined Organic Ferrimagnet, *Q. Xu, H. Cheung,* Cornell University*; D. Cormode,* The Ohio State University*; T. Puel,* University of Iowa*; S. Pal,* Cornell University*; H. Yusuf,* The Ohio State University*; M. Chilcote,* Cornell University*; M. Flatté,* University of Iowa*; Ezekiel Johnston-Halperin,* The Ohio State University*; G. Fuchs,* Cornell University

Hybrid quantum systems are attractive for emerging quantum technologies because they take advantage of the distinct properties of the constituent excitations. This is important because no single quantum system is ideal for every task, e.g., scalable quantum information processing, quantum sensing, long-lived quantum memory, and long-range quantum communication all have different requirements. In creating hybrid systems, it is advantageous to operate in the strong-coupling, low-loss regime, where the relaxation rates of the two distinct quantum systems are exceeded by the coupling rate between them. This allows the hybrid system to operate as a quantum interconnect, wherein quantum information can

be passed from one excitation to another. Thus, a central challenge is to couple distinct quantum systems strongly, with all elements maintaining long coherence times. An equally critical challenge is to fabricate the hybrid quantum devices using scalable and integrable approaches so that their engineered properties can be used in applications.

Here we demonstrate a cavity-magnonic system composed of a superconducting microwave resonator coupled to a magnon mode hosted by the organic-based ferrimagnet vanadium tetracyanoethylene (V[TCNE]x) [1]. This work is motivated by the challenge of scalably integrating a low-damping magnetic system with planar superconducting circuits. V[TCNE]x has ultra-low intrinsic damping, can be grown at low processing temperatures on arbitrary substrates, and can be patterned via electron beam lithography. The devices operate in the strong coupling regime, with a cooperativity exceeding 1000 for coupling between the Kittel mode and the resonator mode at T≈0.4 K, suitable for scalable quantum circuit integration. This is critically enabling for integration and scaling, permitting future designs in which magnonic waveguides can be tailored as couplers or can mediate interactions between different quantum excitations in a planar superconducting circuit. Focusing on the 3.6 GHz device, we present a detailed microwave transmission spectrum that reveals not only the expected avoided level crossing of the resonator mode and the uniform magnon mode (the Kittel mode, or simply magnon mode unless otherwise stated) but also the resonator mode is hybridized with a discrete spectrum of higher-order magnon modes that show a much narrower linewidth than the uniform mode (Fig. 1). This work paves the way for future hybrid magnonic quantum systems by establishing an integrated and scalable platform enabling arbitrary design of the magnonic elements.

[1] Q. Xu, *et al. Advanced Science*, 2310032 (2024); DOI: 10.1002/advs.202310032

PCSI
Room Keahou I - Session PCSI-MoA2

2D Materials and Graphene I
Moderator: Nitin Samarth, Penn State University

4:20pm PCSI-MoA2-29 Dielectric Tensor and Coupled Excitations in Layered (Magnetic) Semiconductors, *Ursula Wurstbauer,* University of Muenster, Germany **INVITED**

Two-dimensional materials exhibit unique properties due to their atomically thin structure and weak van der Waals (vdW) coupling between layers resulting in layer dependent properties. As in the case of the layered magnetic semiconductor CrSBr, individual layers are ferromagnetically ordered below the Neel temperature (T_N≈132K), while adjacent layers are coupled antiferromagnetically. Due to the highly anisotropic electronic bands in CrSBr, electronic and excitonic states at the fundamental band-gap behave quasi-one-dimensional [1]. Moreover, the resulting excitonic transitions are highly sensitive to the collective spin order. Below the critical temperature, an external magnetic field applied along the magnetic hard directions drives the system from the antiferromagnetic into a ferromagnetically ordered state causing a quadratic red-shift of the exciton energies theoretically explained by spin-allowed charge transfer changing the composition and nature of excitons [2]. By resonant inelastic light scattering (RILS) experiments in resonance with those excitons, we reveal and study strong coupling between charge, lattice and spin degrees of freedom.

Moreover, thin CrSBr film host self-hybridized polaritons [3]. To develop a better understanding of the extraordinary light-matter interaction in CrSBr, we access the materials dielectric tensor in the paramagnetic phase by spectroscopic imaging ellipsometry that is hard to access by alternative approaches such as reflectance measurements due to the strong anisotropy. In agreement with theory, we extract highly anisotropic dielectric functions along the crystallographic main axes with strong excitonic resonances particularly in the plane [4].

We gratefully acknowledge the fruitful collaboration with Florian Dirnberger, Julian Klein, Zdeněk Sofer, Marie-Christin Heißenbüttel, Thorsten Deilmann and Michael Rohlfing.

[1] J. Klein et al. ACS Nano, 17, 6, 5316–5328 (2023).

[2] M.-C. Heißenbüttel et al. arXiv:2403.20174.

[3] F. Dirnberger et al. Nature 620, 533–537 (2023).

[4] P.M. Piel, S. Schaper et al (2024).

5:00pm PCSI-MoA2-37 Above Room Temperature Ferromagnetism in Epitaxially Grown Films of the 2D Magnets Fe₅GeTe₂ and Fe₃GaTe₂, *H. Lv, T. Shinwari, K. I. A. Khan, M. Hanke, A. Trampert, J. Herfort, R. Engel-Herbert, Joao Marcelo J. Lopes,* Paul-Drude-Institute for Solid State Electronics, 10117 Berlin, Germany

2D magnetic materials and van der Waals (vdW) heterostructures are promising building blocks for the realization of novel devices with integrated electronic, optical, and magnetic functionalities [1]. However, most of the studies on these materials have so far been performed using bulk crystals and flakes, both not suitable for integration in device processing. Hence, it is crucial to develop their scalable growth in order to realize highly uniform films and heterostructures with well-defined interfaces. It also requires that each material component of the heterostructure remains functional, which ideally includes magnetic order above room temperature for the 2D magnets. Among different candidates, the 2D ferromagnetic metals Fe_5GeTe_2 (FGeT) and Fe_3GaTe_2 (FGaT) show a great potential due to their relatively high Curie temperature and perpendicular magnetic anisotropy [2,3]. In this contribution, we will report on scalable growth of FGeT and FGaT films on epigraphene/SiC(0001) via molecular beam epitaxy. Structural characterization using different methods reveals the formation of continuous and crystalline FGeT and FGaT films (e.g., Fig 1a). Moreover, magneto-transport and magnetometry measurements reveal ferromagnetic order persisting above 350 K with an out-of-plane anisotropy (see Fig. 1b,c). We will discuss in detail the correlation between structure and magnetism, showing the effects of thickness, Fe composition, and the formation of metastable phases on the magneto-transport properties of the materials. These results represent an important advance beyond non-scalable bulk crystals and flakes, thus marking a crucial step towards future applications.

[1] J. F. Sierra *et al.*, Nat Nanotech. **16**, 856 (2021).

[2] S.N. Kajale *et al.,* Nat Commun. **15**, 1485 (2024).

[3] H. Lv et al., Small **19**, 2302387 (2023); IEEE Trans. Magnetics **60**, 4100505 (2024).

5:05pm PCSI-MoA2-38 Electrical Side-Gate Control of Magnetic Anisotropy in a Composite Multiferroic, *Katherine Johnson,* Ohio State University*; K. Collins, M. Newburger, M. Page,* Air Force Research Laboratory*; R. Kawakami,* Ohio State University

Composite multiferroics consisting of a ferroelectric material interfaced with a ferromagnetic material can function above room temperature and exhibit improved magnetoelectric (ME) coupling compared to single-phase multiferroic materials, making them desirable for applications in energy-efficient electronic devices. This work studies the coupling between molecular beam epitaxy grown ferromagnets in a multiferroic heterostructure. The electrical control of magnetoresistance and magnetic anisotropy of single-crystalline $Fe_{0.75}Co_{0.25}$ on PMN-PT(001) is investigated using a side-gate geometry. Angle-dependent magnetoresistance scans reveal that the origin of this effect is strain-mediated magnetoelectric coupling. This electrical control of magnetic properties could serve as a building block for future magnetoelectronic and magnonic devices.

PCSI
Room Keahou I - Session PCSI-MoA3

Magnetic Materials (2D, Monolayers, & Heterostructures
Moderator: Debdeep Jena, Cornell University

5:20pm PCSI-MoA3-41 UPGRADED: Molecular Beam Epitaxy Growth and Stoichiometry-Induced Ferromagnetism in Altermagnetic Candidate MnTe, *Matthew Brahlek,* Oak Ridge National Laboratory, USA

The field of spintronics has seen much excitement around predictions of altermagnetism due to potential applications related to the associated novel spin-moment textures. MnTe stands out as a prominent altermagnetic candidate because of its layered A-type antiferromagnetic structure, high Néel temperature (approximately 310 K), and semiconducting properties. However, critical challenges remain regarding (1) how to synthesize high-quality, well-controlled samples and (2) understanding the fundamental properties of this material.

Our study presents two key findings. The first is that on lattice-matched InP(111), slight differences in the InP surface can be used to effectively select different polymorphs of MnTe when grown by molecular beam epitaxy (MBE). More specifically, the termination of the InP (111) substrate seems to be critical factor. In termination ((111)A)) triggers the nucleation of the NiAs structure, the candidate altermagnetic structure, whereas termination with P ((111)B) stabilizes the ZnS structure, which is also antiferromagnetic and has a relatively large bandgap of ~2 eV.

Regarding the properties of MnTe in the NiAs structure, we reveal that the electronic and magnetic properties are influenced by the natural stoichiometry of MnTe [1]. Electronic transport measurements and in situ angle-resolved photoemission spectroscopy reveal that the films are inherently metallic, with the Fermi level situated in the valence band. The band structure aligns well with first-principles calculations for altermagnetic spin-splitting. Neutron diffraction confirms the antiferromagnetic nature of the film with planar anisotropy, while polarized neutron reflectometry indicates weak ferromagnetism, attributed to a slight Mn-richness inherent to the MBE-grown samples. Combined with the anomalous Hall effect, this work demonstrates that the electronic properties are significantly impacted by the weak ferromagnetism.

Overall, this research highlights potential mechanisms for investigating and ultimately controlling altermagnetic properties, thus paving the way for diverse spintronic applications.

[1] Michael Chilcote, Alessandro R Mazza, Qiangsheng Lu, Isaiah Gray, Qi Tian, Qinwen Deng, Duncan Moseley, An-Hsi Chen, Jason Lapano, Jason S Gardner, Gyula Eres, T Zac Ward, Erxi Feng, Huibo Cao, Valeria Lauter, Michael A McGuire, Raphael Hermann, David Parker, Myung-Geun Han, Asghar Kayani, Gaurab Rimal, Liang Wu, Timothy R Charlton, Robert G Moore, Matthew Brahlek, Advanced Functional Materials 2405829 (2024) 10.1002/adfm.202405829 [https://doi.org/10.1002/adfm.202405829]

5:40pm PCSI-MoA3-45 Imaging and Writing Chiral Antiferromagnetic Domains in the 2D Triangular Antiferromagnet Co₁/₃NbS₂, *Scott Crooker,* Los Alamos National Laboratory

The family of intercalated niobium and tantalum dichalcogenides, $M_{1/3}NbS_2$ and $M_{1/3}TaS_2$ (where the *3d* magnetic atom M= V, Cr, Mn, Fe, Co, Ni), are van der Waals materials that host a wide range of fascinating magnetic properties. $Co_{1/3}NbS_2$ is an antiferromagnet (AFM) that features layers of Co spins on a 2D triangular lattice (see Fig.1) -- an archetypal frustrated network that can lead to complex magnetic topologies. Despite its vanishing net magnetization, $Co_{1/3}NbS_2$ was recently shown to exhibit a giant anomalous Hall effect [1], suggesting a nontrivial AFM order and potential for AFM electronic and spintronic devices. Recent neutron diffraction studies point to a non-coplanar 3Q AFM order with scalar spin chirality [2]. In contrast to conventional collinear AFM order, this (and certain other) complex AFM spin configurations <u>can</u> allow for off-diagonal elements the conductivity, σ_{xy}, which in turn generates anomalous and topological Hall effects in transport studies.

Crucially, $\sigma_{xy}(w)$ are frequency-dependent, and at optical frequencies they generate Kerr rotation and magnetic circular dichroism (MCD). Thus, the full power of optical methods, including spectroscopy and spatially-resolved imaging, can now be applied to investigate the complex AFM order in $Co_{1/3}NbS_2$. Here we show [3], using light spanning infrared to ultraviolet (1-3 eV), that MCD is a powerful and incisive probe of chiral 3Q AFM order in these van der Waals magnets. Measurements at different photon energies are compared with DFT calculations. Scanning MCD microscopy is used to directly image chiral AFM domains, and also, to demonstrate optical writing of chiral 3Q domains. These studies suggest routes to AFM spintronic devices based on $Co_{1/3}NbS_2$ and related 2D magnets.

Fig. 1 a) Structure of $Co_{1/3}NbS_2$, with 2D triangular lattices of Co spins. b) MCD vs. *B, T* shows onset of giant MCD and hysteretic AFM switching below the AFM ordering temperature T_{Neel} ≈28.5 K.c) Direct optical imaging of chiral AFM domains. d) Optical writing of chiral AFM domains.

[1] N.J. Ghimire *et al*, Nat. Comm. **9**, 3280 (2018); G. Tenasini *et al*, Phys. Rev. Res. **2**, 023051 (2020).

[2] H. Takagi *et al*, Nat. Phys. **19**, 961 (2023).

[3] E. Kirstein *et al*, submitted.

5:45pm PCSI-MoA3-46 Electrostatic Extension of Magnetic Proximity Effect in La₀.₇₅r₀.₄MnO₃, *Q. Lan, M. Schnedler, L. Freter,* Forschungszentrum Jülich GmbH, Germany*; C. Wang,* Southern University of Science and Technology, China*; K. Fischer,* National Institute of Technology, Japan*; R. Dunin-Borkowski, Philipp Ebert,* Forschungszentrum Jülich GmbH, Germany

Many fascinating magnetic effects emerge at interfaces between layers with different magnetic orders. Interface confinement is intimately related to the magnetic proximity effect, which typically has a spatial extent of only a few atomic layers. This short extent is due to the underlying physical coupling

mechanisms, such as the exchange interaction, the Dzyaloshinsky-Moriya interaction, interface states, rehybridization, and reconstruction, all of which are highly localized. We use off-axis electron holography to reveal an exceptionally long-range magnetic proximity effect reaching ~40 nm at a ferromagnetic (FM)/ paramagnetic (PM) interface in $La_{0.7}Sr_{0.3}MnO_3$ (LSMO). This wide extent arises from carrier diffusion and drift across the interface, which changes the Mn^{3+}/Mn^{4+} ratio and thereby the density of magnetic moments and local Curie temperature. We determine the carrier concentration dependence of the Curie temperature and unravel the physical mechanism of the electrostatic extension of magnetic proximity effects, fundamentally reshaping our understanding of micromagnetism in perovskites.

5:50pm PCSI-MoA3-47 Toward a First-Principles Theory of Rare-Earth Ions in Crystals, *Y. Lee, Z. Ning,* Ames National Laboratory*; R. Flint,* Ames Laboratory*; R. McQueeney,* Ames National Laboratory & Iowa State University*; I. Mazin,* George Mason University*; **Liqin Ke**,* Ames National Laboratory

Density functional theory (DFT), including its extensions designed to treat strongly correlated localized electron systems such as DFT+U and DFT+dynamical mean field theory, has proven exceedingly useful in studying the magnetic properties of solids. However, materials with rare earths (R) have remained a notable exception. The most vital rare-earth magnetic properties, such as magnetocrystalline anisotropy (MA), have been notoriously elusive due to the ubiquitous self-interaction error present in nearly all available DFT flavors. In this work [1], we show explicitly how the orbital dependence of self-interaction error may contradict Hund's rules and plague MA calculations, and how analyzing DFT metastable states that respect Hund's rules can alleviate the problem. We systematically investigate and discuss several rare-earth-containing families, RCo_5, $R_2Fe_{14}B$, RFe_{12}, and RMn_6Sn_6, to benchmark the MA calculations in DFT+U. For all compounds we investigated, we found that our methodology reproduces the magnetic easy-axis, easy-plane, and non-trivial easy-cone anisotropies in full agreement with low-temperature experimental measurements. Besides the fully-numerical ab initio approach, we further illustrate an efficient semi-analytical perturbation method that treats the crystal field as a perturbation in the limit of large spin-orbit coupling. This approach evaluates the rare-earth anisotropy by assessing the dependence of crystal-field energy on spin-quantization axis rotation using 4f crystal-field levels obtained from non-spin-orbit calculations. Our analytical method provides a quantitative microscopic understanding of the factors that control MA and can be used for predicting new high-MA materials. Finally, in addition to bulk materials, we explore the potential of utilizing rare-earth MA in 2D materials.

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5:55pm PCSI-MoA3-48 Defect Mediated Helical Phase Reorientation by Uniaxial Stress, *T. Kim, H. Zhao, L. Ke,* Ames National Laboratory*; **Lin Zhou**,* Iowa State University

Chiral magnetism has attracted extensive research attention due to its fundamental science and technological importance. In chiral magnet domains, the competition between exchange and Dzyaloshinskii–Moriya interaction (DMI) causes the spins to wind periodically on a plane either perpendicularly (helix) or with a canting angle (cone) along a specific direction, defined as a propagation vector (Q) [1]. Strain engineering enables precise control of nanoscale magnetism while minimizing energy consumption [2]. However, the spatial evolution of strain-induced spin rearrangement, critical for deterministic control of chiral magnetic structures, remains unclear.

In this study, we utilize in-situ Lorentz transmission electron microscopy to manipulate and monitor the reorientation of the helical phase under quantitatively applied uniaxial tensile stress. Our results demonstrate that the Q vector direction of the helical phase can be tuned using external stress. The underlying mechanisms that govern the spin reorientation are magnetic defect mediated, which involve either "break-and-reconnect" events, or dislocation gliding and annihilation within the helices. Simulations prove that the strain-induced anisotropic DMI plays a significant role in driving the reorientation of the helical phase. Our findings provide valuable insights into energy-efficient manipulation of magnetic nanophase for information technology.

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PCSI

Room Keahou I - Session PCSI-MoE

STM Controlled Surface "Lego" and Panel Discussion

Moderator: Paul M. Koenraad, Eindhoven University of Technology, Netherlands

7:45pm **PCSI-MoE-1 Engineering Qubits in Silicon with Atomic Precision**, *Michelle Simmons*, UNSW, Australia   **INVITED**

The realisation of a large-scale error corrected quantum computer relies on our ability to reproducibly manufacture qubits that are fast, highly coherent, controllable and stable. The promise of achieving this in a highly manufacturable platform such as silicon requires a deep understanding of the materials issues that impact device operation. In this talk I will demonstrate our progress to engineer every aspect of device behaviour in atomic qubits in silicon for fast, controllable exchange coupling [1], fast, high fidelity qubit initialisation and read-out [2]; low noise all epitaxial gates allowing for highly stable qubits [3]; and qubit control [4,5] that provide a deep understanding of the impact of the solid-state environment [6] on qubit designs and operation. I will also discuss our latest results in quantum machine learning [7], analogue simulation [8,9] and demonstration of the highest efficiency Grover's algorithm to date [10].

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8:25pm **PCSI-MoE-9 Local Probe Investigations of Topological States of Matter**, *Ingmar Swart*, University of Utrecht, Netherlands   **INVITED**

Topological insulators are renowned for their robust edge modes, which offer the prospect of dissipationless transport of electrons. The boundary state manifests in one dimension lower than the material itself, e.g., 0D end states for 1D chains. However, boundary modes do not necessarily have a topological origin. For example, the well-known surface state of crystals of noble metals with (111) termination is topologically trivial. To establish the nature of a boundary mode, topological invariants such as the Chern number, the winding number, or the Zak phase can be computed directly from

the phase of the wavefunction. For solid-state materials, the phase of the electronic wave function is not experimentally accessible. Instead, topological invariants can be extracted from transport experiments via the quantization of conductance at values proportional to the Chern number. However, transport measurements do not provide local information, essential to study the influence of defects. In addition, it can be difficult to contact the edge (end) mode of 2D materials.

In my talk, I will present recent results of our investigations of various topological insulators using scanning tunneling microscopy and spectroscopy. In particular, using artificial lattices assembled atom-by-atom, I will introduce Wannier center spectroscopy, a tool to distinguish the phases of boundary-obstructed topological insulators beyond 'just' the observation of an edge mode. Furthermore, I will discuss experiments and simulations on finite-sized Bi2Se3 crystals, where we studied the transition from a 3D to a 2D topological insulator, as well as the influence of various types of defects on the electronic structure.

9:05pm **PCSI-MoE-17 Panel Discussion**,

PCSI

Room Keahou I - Session PCSI-TuM1

Oxide Semiconductor Materials I

Moderator: Bharat Jalan, University of Minnesota

8:30am PCSI-TuM1-1 Atomistic Simulations for Understanding the Behavior of Dopants and Impurities in Ga2O3 and Related Alloys, *Joel Varley,* Lawrence Livermore National Laboratory **INVITED**
Gallium oxide (Ga_2O_3) is rapidly developing as one of the most promising ultra-wide bandgap platforms for next-generation power electronics owing to properties like a high breakdown field, controllable (*n*-type) electrical conductivity, and commercially-available single-crystal substrates that can be grown via a number of industrially-scalable processes. Beyond exhibiting a number of polymorphs with similarly attractive properties, alloying with Al into Ga_2O_3 to form ($Al_xGa_{1-x})_2O_3$ (AGO) alloys can lead to a significant increase of the band gap to potentially access higher power device figures of merit, analogous to the AlGaN system but spanning a much larger rage of ~4.8 eV-8.6 eV. Despite the progress with Ga_2O_3 and related alloys, a number of open questions remain on the nature of fundamental defects and the role of impurities and dopants in determining the observed optical and electrical properties of these materials. This is even more of an open question in the lesser studied alloys like AGO, particularly regarding the effectiveness of donor doping and how to overcome the possibility of compensation in the limit high Al-contents. In this work we survey the current understanding of point defects in Ga_2O_3, focusing on their potential optical and electrical consequences from insights gained through first-principles-based calculations employing hybrid functionals. We discuss what is known about donor and acceptor dopants, as well as their interactions with native defects and impurities incorporated through growth and processing steps. These results provide guidance for controlling defect populations and the electrical conductivity in Ga_2O_3 and related alloys and for facilitating next-generation power electronics based on this ultra-wide bandgap semiconductor family.

9:10am PCSI-TuM1-9 UPGRADED: What Happens When a Dopant Doesn'T Go Where You Expect It to Go? The Case of MBE-Grown Yb-Doped SrTiO3 on Si(001), *Scott Chambers,* Pacific Northwest National Laboratory; *E. Ramerez, D. Guragain, J. Ngai,* University of Texas at Arlington; *P. Sushko, K. Koirala, Y. Du, N. Govind, M. Bowden,* Pacific Northwest National Laboratory; *D. Biswas, T. Lee,* Diamond Light Source, UK; *C. Weiland,* National Institute of Standards and Technology (NIST); *J. Woicik,* National Institute for Science and Technology (NIST)
We present the structural and electronic properties of Yb-doped $SrTiO_3$/Si(001) grown by molecular beam epitaxy. Other rare-earth dopants that result in *n*-type conductivity in the ABO_3 perovskite lattice typically substitute for Sr at the *A*-sites. In contrast, Yb is shown to substitute predominantly for Ti at the perovskite *B*-sites based on data from atomically resolved scanning transmission electron microscopy and energy dispersive spectroscopy, as well as extended x-ray absorption fine structure measurements. An atom beam flux (f) mismatch was present during film deposition because it was *assumed* that Yb would occupy *A*-sites. As a result, the fluxes were set such that $f_{Yb} + f_{Sr} = f_{Ti}$. The formation of Yb_{Ti} rather than Yb_{Sr} results in Sr vacancies and extraneous (i.e. non-lattice) Ti atoms in the films. Yb exhibits two distinct charge states as determined by x-ray absorption spectroscopy and associated theoretical modeling, +2.7 and +2.1. These aliovalent dopants are compensated by donor electrons from oxygen vacancies that form during epitaxial film growth. The defect complexes resulting from the flux mismatch, together with oxygen vacancies, lead to deep-level electron traps that were detected by resonant photoemission and predicted to be stable by *ab initio* theory, as well as much higher sheet resistance than that associated with, for instance, La-doped $SrTiO_3$ films. *Ab initio* calculations show that the preference for *B*-site occupancy is driven by low oxygen chemical potential at the growth front as required to successfully deposit epitaxial STO on Si without amorphous SiO_2 formation at the interface.

9:30am PCSI-TuM1-13 Thickness-Dependent Optical Constants of SnO2 Thin Films on Si Grown by Atomic Layer Deposition, *Yoshitha Hettige, S. Zollner,* New Mexico State University; *A. Pratap Singh, B. Dutta, S. Chattopadhyay,* Indian Institute of Technology Indore, India
Zinc oxide (ZnO) and strontium titanate ($SrTiO_3$) have tunable optical constants that can be useful for optoelectronic applications. We study a third oxide, tin oxide (SnO_2), and investigate if its optical constants are also tunable. SnO_2 is a wide band gap semiconductor with attractive electrical, optical, *etc* properties. It is commonly used in gas sensors, solar cells, batteries, and energy-saving coatings. SnO_2 thin films were grown on a Si substrate using atomic layer deposition.

X-ray reflectivity (XRR) was performed for each SnO_2 thin film on Si. It was found that the SnO_2 thin film thicknesses are around 10-60 nm with an approximately 2 nm thick SiO_2 interfacial layer due to the wet cleaning before the deposition. We measured the ellipsometric angles ψ and Δ of SnO_2 thin films on Si at room temperature on a J. A. Woollam UV ellipsometer at 65° to 75° angles of incidence from 0.5 to 6.5 eV. We used a Tauc Lorentz oscillator to model the data for SnO_2 thin films. After obtaining a reasonable fit for SnO_2, we also performed a uniqueness fit for the film thickness. We compared the film thickness from all three techniques; XRR, Tauc Lorentz fit, and uniqueness fit. Finally, we extracted the dielectric function (ε) of the SnO_2 thin film from the obtained Tauc-Lorentz fit and compared it with all samples. The results show that the dielectric function (real ε_1 and imaginary ε_2 part) varies with thickness by no more than 15%. This observation is probably because of the weaker excitonic effects in SnO_2 or because the excitonic effects are not screened as for ZnO or $SrTiO_3$.

9:35am PCSI-TuM1-14 Regulating the Phase Transition of Vanadium Dioxide Thin Films, *Manish Kumar, S. Rani, H. Lee,* Pohang Accelerator Laboratory, POSTECH, Republic of Korea
Vanadium dioxide (VO_2) is a popular thermochromic material owing to its potential applications in intelligent windows, sensors, and diverse electronic devices. VO_2 displays a distinctive metal-insulator transition (MIT) that occurs around 68°C temperature, which is accompanied by a structural transition and a dramatic change in the optical properties [1]. During this transition, the material shifts between its low-temperature insulating (transparent to near infrared rays) monoclinic phase (M1) and its high-temperature metallic (opaque to near infrared rays) rutile phase (R). From application perspective, it is highly imperative to stabilize VO_2 thin films with control on the phase transition properties. Ion-implantation is one of the effective route to tune the properties of VO_2 thin films [2, 3]. In the present work, we have studied B+ ion implanted VO_2 thin films.

Thin films of VO_2 were prepared by radio frequency (RF) magnetron sputtering technique. Apart from the pristine sample, three samples were implanted by B+ ions at different fluence ranging 5×10^{13} ions/cm^2 to 5×10^{14} ions/cm^2. B+ ions implanted VO_2 thin films revealed modified structural, electrical and optical properties. Structural phase transition and MIT temperatures were found to decrease with increasing implantation dose. Moreover, for ion-implanted VO_2 thin films, temperature dependent transmittance measurements depicted the shift in optical transition towards room temperature side. Such control of phase transition in VO_2 thin films is very crucial for device applications.

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9:40am PCSI-TuM1-15 Formation of Transparent and Conductive SWCNT/SiO2 Composite Thin-Films on Pet Substrates Using Molecular Precursor Method, *Hiroki Nagai, K. Igarashi, M. Sato,* Kogakuin University, Japan
Transparent conductive films (TCF) are essential for optoelectronic devices, such as transparent electrodes for light-emitting diodes and solar cells. Transparent thin films of indium tin oxide (ITO) and fluorine tin oxide (FTO) on glass substrates are the most widely used for these purposes [1]. These typical TCO thin films provide an electrical resistivity of 10^{-3} Ω·cm and a high transmittance of over 80% in the visible-light region. Carbon nanotubes (CNTs)/inorganic composites have received much attention due to their optical, mechanical, electrical, and thermal properties. However, the poor adhesion of CNTs onto the substrate becomes a problem during the usage. SiO_2 is a highly transparent insulating material in the UV, visible,

and infrared regions. Therefore, if conductivity can be added to SiO₂, it will become a new transparent conductive film with high adhesion. The single-walled carbon nanotube (SWCNT)-silica composite thin film on a quartz glass was formed by ultraviolet irradiation (20–40 °C) onto a spin-coated precursor film. With 7.4 mass% SWCNTs, the electrical resistivity reached 7.7×10^{-3} Ω·cm after UV irradiation. The transmittance was >80% at 178–2600 nm and 79%–73% at 220–352 nm. Heat treatment increased the transparency and pencil hardness without affecting the low electrical resistivity. Raman spectroscopy and microscopic analyses revealed excellent film morphology with good SWCNT dispersal. The low refractive index (1.49) and haze value (<1.5%) are invaluable for transparent windows for novel optoelectronic devices. Herein, we also report a promising composite thin film as a transparent and conductive material on PET (polyethylene terephthalate) substrates for flexible transparent conductive films.

9:45am **PCSI-TuM1-16 Phototransistor Array Based on Plasma-Engineered Amorphous Metal Oxide Semiconductors with Ferroelectric Dielectrics**, *Uisik Jeong, S. Kim,* Sungkyunkwan University (SKKU), Republic of Korea

The potential for next-generation electronic applications has expanded significantly with the development of energy-efficient, high-performance broadband photodetectors utilizing cost-effective amorphous metal oxide semiconductors. Current commercially available photodetectors use various semiconductors to detect light across different wavelengths, from ultraviolet (UV) to near-infrared (NIR). However, their versatility is limited by the need for specific materials to target different wavelengths. This study explores the use of indium gallium zinc oxide (IGZO) as a metal oxide semiconductor, eliminating the need for additional external photo absorption layers. To enhance charge carrier generation and create subgap states in the IGZO film, hydrogen (H2) plasma treatment was applied, enabling wide-spectrum detection from UV to NIR without extra layers. Furthermore, a ferroelectric and high-k dielectric was introduced as the gate dielectric to induce a strong electric field in the channel, resulting in low-power operation. The H2 plasma-treated IGZO phototransistors demonstrated ultra-high photoresponsivity and detectivity over a broad range of wavelengths (400 to 1000 nm), making them a promising candidate for next-generation optoelectronic devices. This study presents a favorable approach for advancing energy-efficient, cost-effective, and high-performance broadband photodetectors.

9:50am **PCSI-TuM1-17 Improvement of Electrical Properties and Low-Temperature Development of Sol-gel Processed In-Ga-Zn-O Thin-Film Transistors Using UV-DI**, *Giyoong Chung, y. kim,* Sungkyunkwan University (SKKU), Republic of Korea

The vulnerability of solution-processed metal-oxide semiconductors is significantly influenced by organic chemical-induced defects such as voids, holes, and organic residues. Moreover, solution-processed Oxide TFTs require a high temperature process to vaporize various organic compounds. Hydroxyl radicals (OH•), known as strong oxidants, are effective in eliminating and decomposing organic compounds.

In this study, we introduced UV-DI with hydroxyl radicals into the IGZO Sol-Gel mixture to produce lower boiling points components and deposit IGZO active layers with fewer defects. Hydroxyl radicals were generated in deionized (DI) water through an O₃/UV process, confirmed via potassium iodide (KI) and ultraviolet-visible (UV-vis) spectroscopy analysis. The intensity of the absorbance peaks at wavelengths of 290 nm and 350 nm increased with longer UV irradiation times. Additionally, we found that the density of hydroxyl radicals in DI water could be modified by adjusting the initial volume of DI water while maintaining the same UV irradiation duration. A DI water volume of 4.5 ml resulted in a higher concentration of hydroxyl radicals compared to 1.5 ml of DI water. Thermogravimetric and differential scanning calorimetry (TG-DSC) analysis revealed that the organic materials in the IGZO solution mixture with UV-DI treatment began to decompose at a lower temperature (121.6℃) than those in the pristine IGZO mixture (144.5℃). An abrupt weight loss was also observed in the IGZO solution with UV-DI compared to the pristine IGZO solution.The field-effect mobility and sub-threshold slope of the a-IGZO TFTs made with ozonated water were improved compared to the conventional process, increasing from 1.37 to 1.44 cm^2/V·s and decreasing from 0.24 to 0.20 V/dec, respectively. In addition, threshold voltage shifts over 7000 seconds under negative-bias stress conditions (NBS) were -7.25 V and -5.67 V for pristine IGZO and IGZO with UV-DI, respectively.

These results suggest that the addition of ozonated water to the sol-gel mixture is a simple method to achieve high-performance TFTs by reducing organic chemical-induced defects through low-temperature processing.

9:55am **PCSI-TuM1-18 A Study on the Impact of Thin Metal Films on Contact Resistance in IGZO FET**, *Juseong Min,* Sungkyunkwan University, Samsung Electronics, Republic of Korea

Indium gallium zinc oxide (IGZO) is regarded as a highly promising material in semiconductor applications such as thin-film transistors (TFTs) and memory devices, due to its excellent properties, including low leakage current and high electron mobility [1,2]. However, there are still unresolved issues with IGZO, one of which is the high contact resistance between IGZO and source/drain electrodes, which significantly affects the performance of miniaturized transistor devices. Therefore, understanding and improving the contact resistance of IGZO is essential [3]. Various factors influence the contact resistance between IGZO and metals, but the metal's work function and the interaction between the metal and IGZO are particularly critical [4,5].

In this study, various thin metal films with a thickness of less than 5 nm were inserted between the electrodes and IGZO in transmission line model (TLM) devices to investigate the effect of metal oxide formation on contact resistance (fig.1). Based on these results, we analyzed how the metal's work function, oxidation tendency, and the band structure of metal oxides influence the contact properties with IGZO, and proposed strategies to effectively reduce contact resistance. These findings are expected to serve as valuable foundational data for improving the performance of various IGZO-based semiconductor devices.

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10:00am **PCSI-TuM1-19 Exploration of VO₂ Thin Films with Oxygen Deficiency**, *SUNITA RANI, M. KUMAR, H. LEE,* Pohang Accelerator Laboratory, POSTECH, Republic of Korea

VO₂ has captured the attention of researchers due to its thermochromic properties and rapid semiconductor-to-metal transition. The semiconductor-to-metal shift occurs within the monoclinic M1 phase around 343K, coupled with a transformation from monoclinic to rutile crystal structure. The transparency of the monoclinic phase to near-infrared (NIR) radiation stands in contrast to the NIR opaqueness of the rutile phase. Maintaining precise stoichiometry in VO₂ is crucial, as even slight adjustments in oxygen levels can lead to the stabilization of different VO₂ polymorphs. Additionally, fine-tuning the stoichiometry offers a means of controlling the characteristics of VO₂. With this motivation, we have prepared stoichiometric and oxygen deficient VO₂ thin films on differently oriented sapphire substrates by radio frequency (RF) sputtering technique. The stoichiometric VO₂ thin films depicted characteristic semiconductor to metal transition around 343K. We noticed a complete suppression of semiconductor to metal transition in oxygen deficient VO₂ thin films and a metallic behavior was seen throughout the studied temperature range i.e. 273K to 373K. Oxygen deficiency led to significant modifications in the structural, electronic and optical properties of VO₂ thin films.

PCSI
Room Keahou I - Session PCSI-TuM2

Wide Bandgap Materials II
Moderator: Joel Varley, Lawrence Livermore National Laboratory,

11:00am **PCSI-TuM2-31 Diamond High Power and Voltage MOSFETs: Inch-Sized Wafer Growth, Doping, Static and Dynamic Characteristics**, *MAKOTO KASU, N. Saha,* Saga University, Japan INVITED

Diamond possesses an ultrawide bandgap energy of 5.47 eV, a breakdown field of >10 MV/cm), higher thermal conductivity (22 W/cmK), and higher electron and hole mobilities (4500 and 3800 cm²/Vs, respectively) than GaN and SiC. Therefore, diamond is considered to be the most capable candidate for the power semiconductor device application. Diamond single-crystal substrates have been limited to sizes of 4 mm. Diamond heteroepitaxial growth has not been achieved because of a large difference in coefficients of thermal expansion between diamond and foreign substrate materials. Recently, we have demonstrated a two-inch-diameter diamond wafer grown on Ir/sapphire (a-Al₂O₃) (11-20) substrate [1]. Diamond heteroepitaxial layer exhibited the highest crystal quality, such as

TDD of 1.4×10^7 cm^{-2}, and XRCFWHM of 98 arcsec [2]. We clarified diamond's nucleation process on Ir/sapphire surface by AFM, TEM, and EDS [3]. For diamond p-channel MOSFETs, so far impurity doping into diamond has not been successful because of extremely high activation energy. But we haveestablished p-type doping on the H-terminated diamond using NO$_2$ gas [4], and thermal stabilization and gate insulation withALD Al$_2$O$_3$ layer [4]. We have fabricated diamond MOSFET (Fig. 1) demonstrating high drain current density (I$_D$)of 0.68 A/mm, a low ON-state resistance of 50 Ω·mm, andextremely high OFF-state breakdown voltage (V$_{BR}$) of −2568 V. The specific on-state resistance, (R$_{ON,spec}$) was determined to be 7.54 mΩ·cm^2, and the maximum available power, i.e., BFOM (= V$_{BR}^2$/R$_{ON,spec}$) has been obtained to be 874.6 MW/cm^2 (Fig. 2), the highest ever in diamond, ~40% of GaN's top value [5]. Further, we demonstrated fast turn-on (t$_{on}$) and turn-off (t$_{off}$) switching times of 9.97 ns and 9.63 ns, respectively [6]. The first stress measurement was performed, showing 190 h of stable operation under a DC gate bias and drain bias stress [7]. No evident degradation in I$_D$ was observed throughout the stress period; the gate current (I$_G$) increased after 83 h of stress due to the charge injection into the Al$_2$O$_3$ layer, although it did not influence the I$_D$.

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11:40am **PCSI-TuM2-39 Adsorption and Thermal Evolution of Nitrogen Species on Diamond Surfaces**, *Kai Huang*, Guangdong Technion-Israel Institute of Technology, China

Layer-by-layer construction of diamond devices for spin-sensing calls for atomistic understanding of the nitrogen species on diamond surfaces.[1] As motivated by recent spectroscopic measurements (e.g., X-ray photoelectron spectroscopy, high-resolution electron energy loss spectroscopy and temperature-programmed desorption) on diamond surfaces impacted by N$_2$ plasma,[2] we conducted density functional theory simulations to gain atomistic details into the adsorption and thermal evolution of the resulted nitrogen species, as below.

1. **Diamond(001).** We find that nitrogen plasma attacks the C=C dimers on the pristine diamond(001), forming nitrogen-dimers in a horizontal configuration, h-N$_2$(ad).[3] The formation of h-N$_2$(ad) is capable of resolving some discrepancy in the literature. the desorption of N$_2$(ad) on pristine diamond(001) follows a concerted process with a barrier of 0.91 eV. By contrast, there emerges a new state of nitrogen-dimers in a vertical configuration, v-N$_2$(ad), in addition to h-N$_2$(ad). [4] Consequently, the desorption of N$_2$(ad) is altered into a stepwise fashion, giving an overall barrier of 2.36 eV.

2. **Diamond(111).** On bare domains of diamond, as represented by the models of C(111)-2x1 and graphite-like C(111), N$_2$(ad) is identified as major surface species; the desorption of N$_2$(ad) proceeds on both models via a concerted process of breaking two C-N bonds.[5] By contrast, there is evidence of formation of (NH)$_2$(ad) via the insertion reaction of N2 plasma on hydrogenated domains of diamond, as represented by the models of C(111)-2x1-H and C(111)-1x1-H. Interestingly, contrasting dynamics of desorption of (NH)$_2$(ad) are presented on these two models; that is, via sequential breaking of two C-N bonds on C(111)-2x1-H, and via concerted breaking of both C-N bonds on C(111)-1x1-H.[6]

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11:45am **PCSI-TuM2-40 Atomic and Electronic Structure Prediction for Heterostructural Interfaces with Ultra-Wide Gap Materials** , *Stephan Lany, S. Mahatara,* 15013 Denver West Pkwy

First-principles calculations can be an invaluable tool for modeling of interface properties. However, such calculations require detailed knowledge of the atomic structure, which is often not known experimentally. This is especially true for heterostructural interfaces between materials with different bulk crystal structures. Thus, interface atomic structures are often constructed by making plausible assumptions but without confirmation that the structure actually represents a free energy minimum. Atomic force relaxation alone is generally insufficient, because it only yields a local total energy minimum. A more rigorous approach requires the sampling of the configuration space. In general, we distinguish commensurate and incommensurate interfaces, where the former display a 1:1 matching of the in-plane primitive cell lattice vectors whereas the latter require construction of a coincidence site lattice for the matching of two 2D supercells. As an example of a commensurate heterostructural interface, we consider the case of wurtzite AlGaN alloys on rocksalt TaC (111) substrates, where the lattice matching of the hexagonal interface primitive cell occurs at high Al compositions for ultra-widegap applications. Using an algorithm for systematic enumeration of the stacking sequences promoting the transition from the rocksalt to the wurtzite structure, we perform high-throughput density functional theory calculations for energy minimization. Subsequent electronic structure calculations for the most favorable structures reveal the band alignment, Schottky barrier, and electronic interface density of states. We will further discuss the outlook for other substrate/film combinations and the case of incommensurate interfaces.

11:50am **PCSI-TuM2-41 Si Diffusion Into Self-Organized GaN Nanocolumns Grown on Si(111) by RF-MBE**, *Tohru HONDA*, N. GOTO, Y. HOSOYA, T. ONUMA, T. YAMAGUCHI, Kogakuin University, Japan

The small-size micro-LED displays requests micrometer-scale pixels. The monolithic fabrication of GaN-based LEDs (monolithic integration) is also interesting for high-dense integration. In a view of the optical isolation of integrated LEDs, GaN nanocolumns grown on Si is interesting for the monolithic integration, because threading dislocations in them can be reduced (filtering effect) [1]. However, Si atoms will be diffused into the GaN nanocolumns. In this study, these carrier concentrations as a function of the amount of a Mg dope (compensation of electron carrier) are estimated using Raman spectra.

GaN nanocolumns (NCs) was grown on the substrate using plasma-assisted molecular beam epitaxy (RF-MBE). The growth time was 60 min., the growth temperature was 1020 °C, the Ga flux was 9.0×10^{-7} Torr, the N$_2$ flow rate was 2.0 ccm, and the RF power was 400 W. In a case of a Mg dope, its beam equivalent flux of 5.7×10^{-9}Torr was adopted. Raman spectra of GaN nanocolumns were observed using a 532-nm-line of YAG: Nd. The modes of E2 and LO-phonon-plasmon coupled (LOPC) modes [2] are shown in Figs. 1 and 2. The peak shift of E2 modes means the amount of strain in the layers. The strain in GaN NCs grown on Si is free compared with that in GaN layers grown on sapphire by MOVPE. It means that the NCs have the low dislocation densities due to "filtering effect" [1]. On the other hand, a very weak peak of the LOPC mode was observed form the GaN NCs. This means to the high electron carrier concentration in GaN NCs. The LOPC mode in carrier compensated GaN NCs using a Mg dope (Mg concentration was estimated using a local vibration mode) is also observed. A clear LOPC peak was observed. These peak positions indicate that the Si concentration in GaN NCs is approximately 100 ppm.

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11:55am **PCSI-TuM2-42 Realization of Smooth Surface and Interface in Mist CVD Growth of Rocksalt structured-MgZnO/MgO MQWs**, *Hiroyuki Aichi, T. Onuma,* Kogakuin University, Japan

Rocksalt (RS) structured-Mg$_x$Zn$_{1-x}$O alloys have bandgap energies ranging from 2.45 to 7.78 eV [1,2]. They are candidate materials for deep and vacuum ultraviolet light emitters. Our group has grown atomically flat single-crystalline RS-Mg$_x$Zn$_{1-x}$O films on (100) MgO substrates using the mist chemical vapor deposition (mist CVD) method [3]. The CL spectra at 300 K exhibited the shortest near-band-edge emission peak at 187 nm. The RS-Mg$_x$Zn$_{1-x}$O/MgO for $x \gtrsim 0.6$ was confirmed to have type-I band alignment by the X-ray photoelectron spectroscopy measurements [4]. This study reports

on growths of RS-Mg_xZn_{1-x}O/MgO multiple quantum well (MQW) structures by the mist CVD method.

RS-Mg_xZn_{1-x}O/MgO MQW structures were grown on (100) MgO substrates at 725°C. Magnesium acetate tetrahydrate and zincacetate dihydrate were used as source precursors. The x in the well layer was controlled by molar ratio of magnesium($[Mg]^L$ = [Mg]/([Mg]+[Zn])) in the sourcesolution. The structure consisted of a 30-nm thickMgO cap layer, 10 periods of MQW composed of 3-nm-thick RS-$Mg_{0.73}Zn_{0.27}$O well and 10-nm-thick MgO barrier, and a 200-nm-thick MgO buffer layer.

As shown in Fig. 1, the structure exhibited atomically-flat smooth surface morphology with root mean square (RMS) roughness of 0.30 nm. Thevalue is comparable to those obtained for the RS-Mg_xZn_{1-x}O single layers [3]. As shown in Fig. 2, distinct observationof the +1st, 0th, -1st, and -2nd order satellite peaks impliesrealization of excellent interface flatness and periodicity. Furthermore, cross-sectional STEM image showed a well-defined layered structure with abrupt interfaces.

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12:00pm PCSI-TuM2-43 Si-Integrated Epitaxial BaTiO₃ for Ultra-Low Loss, Efficient Modulators in Silicon Photonics, *Alex A. Demkov, A. Posadas, A. Raju, D. Wasserman,* The University of Texas at Austin

The integration of optical components with traditional silicon technology, known as integrated silicon photonics (SiPh), is experiencing explosive growth. It offers many advantages such as lower power consumption, higher speed, and higher bandwidth when compared to the traditional CMOS-based information technology [1,2]. Electro-optic (EO) modulators are among the key active photonic components of SiPh, they can modulate either the amplitude or the phase of light. The operation of some of the most promising high frequency EO modulators is based on the linear EO effect, commonly referred to as the Pockels effect [2]. The linear EO effect constitutes the change in the refractive index of a material in response to an external electric field. Silicon is transparent below 1.1 eV and demonstrates extremely low optical loss, around 0.1 dB/m that is ideal for integrated photonic devices with applications in optical communications, optical neuromorphic and quantum computing, however, Si doesn't exhibit linear EO effect [3]. Barium titanate BaTiO3 (BTO) is an emerging material in SiPh with one of the largest known linear electro-optic coefficients. However, in BTO-based devices, high optical losses are consistently observed, typically an order of magnitude larger than those observed in lithium niobate. I will show that the origin of optical loss in BTO waveguides is non�absorptive and is caused by internal interfaces, aka planar defects such as e.g., ferroelectric domain walls. I will then discuss monolithic barium titanate photonic structures fabricated from BTO grown epitaxially by RF-sputtering on silicon-on-insulator substrates. Three types of test structures will be discussed: simple cut-back structures, high-Q ring resonators, and high-Q racetrack resonators. The record low loss of our monolithic barium titanate waveguide structures enables the demonstration of high-Q resonators with quality factors of Q > 100, 000. The low loss of the barium titanate photonic structures, coupled with barium titanate's large non-linear optical response offers a path to compact and high efficiency barium titanate photonic devices and structures for high-speed modulation, optical computing, and non-linear applications. This research is supported by a Multidisciplinary University Research Initiative from the Air Force Office of Scientific Research (AFOSR MURI Award No. FA9550-22-1-0307).

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Room Keahou I - Session PCSI-TuE

Rump Session: Quantum Computation Materials and Devices and Panel Discussion

Moderator: Christopher Palmstrøm, University of California, Santa Barbara

7:00pm **PCSI-TuE-1 Challenges & Opportunities for Developing Superconducting Quantum Information Systems**, *Raymond Simmonds*, National Institute of Standards and Technology, Boulder

Developing large-scale quantum information processors has become a major industrial goal over the last few years. Of the many quantum systems available to tackle this difficult task, superconducting circuits have shown impressive results thus far and appear to be posed to scale up rapidly. In fact, systems with over 1,000 superconducting qubits have already been built and operated. [1] Although scaling the number of qubits as well as the infrastructure to control and measure them is an outstanding challenge, it seems that individual qubit coherence still must improve in order to lower the overhead required to successfully perform quantum error correction, vital for quantum computations. About 20 years ago [2], two-level system defects were found to reside in qubit Josephson junctions: "We report spectroscopic data that show a level splitting characteristic of coupling between a two-state qubit and a two-level system. ...Although two-level systems are known to exist in amorphous materials, the sensitivity of our Josephson qubit at the quantum level has allowed us to uncover individual two-level microwave resonators hidden within a 40-yearold technology. ...We predict that improvements in the coherence of all Josephson qubits will require materials research directed at redistributing, reducing, or removing these resonator states." Since that time, coherence has improved tremendously, but two-level system defects not only in the tunnel junction but residing at all material interfaces continue to pose a significant challenge.

In this presentation, I will provide a basic introduction to superconducting qubits, their fabrication, measurement, and coupled operations. Then, I will focus on some of the difficulties associated with developing superconducting circuits for large scale quantum information processors. Specifically, I will provide a historical overview of early measurements that showed the influence of individual two-level system point defects on qubit operations. In addition, distributions of these defects on surfaces can also work collectively to degrade the coherence of quantum circuits. Even with these defects present, enormous progress has been made thus far in developing quantum information processors. Tackling the remaining materials science challenges associated with fabricating superconducting quantum circuits could lead to a new understanding of creating clean material systems or finding ways to engineer microwave two-level defects as coherent qubits.

7:30pm **PCSI-TuE-7 Spin-Orbit Qubits with Holes in Silicon and Germanium**, *Dominik Zumbuhl,* University of Basel, Switzerland   **INVITED**

8:00pm **PCSI-TuE-13 The Critical Role of Interfaces in Si/SiGe Quantum Dot Qubits: Valley Splitting and Radiation Impacts**, *Mark Eriksson,* University of Wisconsin-Madison   **INVITED**

Interfaces and other atomic-scale materials features are critical to the operation, properties, and robustness of Si/SiGe quantum dot qubits. In this talk I discuss two important examples.First, the atomic-scale structure of the quantum well in Si/SiGe heterostructures plays the dominant role in determining the valley splitting.This splitting, which arises from a coupling between the two z-valleys in the silicon band structure, determines the energy gap that protects spin-up and spin-down qubit states.If the valley splitting is small, the qubits fail.While the interface between the quantum well and the upper quantum well barrier by itself does cause some valley splitting, recent results demonstrate a new method: silicon quantum wells containing short wavelength oscillations in the concentration of added germanium atoms can significantly increase the valley splitting.Second, there are deeper, buried defect layers that in principle can trap charges induced by external radiation.I will discuss recent experiments that imitate such radiation impacts in Si/SiGe quantum devices using fiber optic illumination on the back of the wafer to deposit energy and induce bursts of electron-hole pairs deep in the bulk of the wafer. We find that some of the generated charge – mostly negative charge (electrons) – migrates to the top region of the wafer and shifts the offset charge of quantum dot qubits. We are able to identify abrupt jumps in the offset charge that appear to arise from trapping of individual electrons. Based on the magnitude of the jumps in the offset charge, the charge trapping occurs within a few hundred nanometers of the qubit. Importantly, the device can be very stable both before and right after the single-charge trapping, as we demonstrate by turning off the optical illumination as soon as a charge jump is observed.

8:30pm **PCSI-TuE-19 Panel Discussion**,

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Room Keahou I - Session PCSI-WeM1

Point Defects (for Quantum Information Applications) I

Moderator: Kai-Mei Fu, University of Washington

8:30am **PCSI-WeM1-1 Room Temperature Optically Detected Magnetic Resonance of Single Spins in GaN**, *Gregory Fuchs,* Cornell University

INVITED

High contrast optically detected magnetic resonance (ODMR) is a valuable property for reading out the spin of isolated defect color centers at room temperature. Spin-active single defect centers have been studied in wide bandgap materials including diamond, SiC, and hBN; each with associated advantages for applications. We report the discovery of ODMR in two distinct species of bright, isolated defect centers hosted in GaN [1]. In one group, we find negative ODMR of a few percent associated with a metastable electronic state, whereas in the other, we find positive ODMR of up to 30% associated with the ground and optically excited electronic states. We examine the spin symmetry axis of each defect species and we establish coherent control over a single defect's ground-state spin. Given the maturity of the semiconductor host, these results are promising for scalable and integrated quantum sensing applications.

[1] J. Luo, Y. Geng, F. Rana, and G. D. Fuchs, "Room temperature optically detected magnetic resonance of single spins in GaN," *Nat. Maters* **23**, 512 (2024).

9:10am **PCSI-WeM1-9 UPGRADED: Er Sites in Si for Quantum Information Processing**, *Sven Rogge,* UNSW, Australia

Rare-earth ions in a solid-state host exhibit low homogeneous broadening and long spin coherence at cryogenic temperatures, making them promising for a range of quantum applications, such as optical quantum memories and optical-microwave transductions. Emitters with long electron spin and optical coherence in Si, a leading material platform for electronic and photonic technologies, are especially attractive for quantum applications. Here, we report on the observation of eight Er sites in Si that have both long optical coherence and electron spin lifetime. We measured 1 ms spin coherence for two sites in a nuclear spin-free silicon crystal (<0.01% ^{29}Si), which appeared to be instrumentally limited. Using Alternating-Phase CPMG sequence, we extended the spin coherence of one of the sites to 40 ms. Measurements with naturally abundant Si revealed that the Er electron spin coherence was limited by coupling to ^{29}Si nuclear spins. The measured homogeneous linewidths of all 8 sites are below 100 kHz, and inhomogeneous broadening approaches 100 MHz [1, 2]. These results were achieved for Er implanted from 200 and 700 nm from ^{28}Si surface at 10^{16} cm^{-3} level. The Er homogeneous linewidth and spin coherence were addressed using optical comb-based spectral hole burning and optically detected magnetic resonance techniques. To enhance Er emission collection efficiency, samples were directly positioned atop specially fabricated superconducting single photon detectors and resonantly excited via fibre optics. The demonstration of a long spin coherence time and narrow optical linewidth in multiple sites show that Er in ^{28}Si is an exceptional candidate for future quantum information and communication applications and can be used for single photon frequency multiplexing schemes. Finally, integration into silicon on insulator nanophonic devices is discussed.

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9:30am **PCSI-WeM1-13 Simulating X-STM Images of Iso-Electronic Dopants in Semiconductors Using DFT**, *Thomas Verstijnen, D. Tjeertes, E. Banfi, P. Koenraad,* Eindhoven University of Technology, Netherlands

The sizes of devices and active regions in semiconductor devices are reaching the atomic scale. This requires us to have an understanding and control over defects at this level as well. A technique that is very well suited to investigate semiconductors at this scale is Cross-Sectional Scanning Tunneling Microscopy (X-STM). We employ this technique to study iso-electronic dopants in III-V semiconductors. We study these dopants since they can locally modify band gaps and other electronic characteristics of a semiconductor which makes them interesting for device fabrication. These X-STM images that we generate can be difficult to interpret however, since the Local Density of States (LDOS) of a material is probed rather than the topology of the material surface alone.

For this reason we combine this experimental technique with Density Functional Theory (DFT). We have developed a method to simulate LDOS planes above a surface supercell which can be more directly compared to the X-STM images we generate. This can help us understand the underlying topology of the X-STM images as well as helping us understand what it is that we are seeing when starting X-STM measurements on unknown materials or dopants.

This combination of techniques is applied to three different doped materials: N doped InAs, B doped GaAs and Tl doped GaAs. The N doped InAs and B doped GaAs were used to test the technique since a lot of data about both of those systems studied with X-STM is available. [1] The Tl doped GaAs however, is a material which is not measured before with X-STM and therefore the DFT simulations have helped with the interpretation of the X-STM data. In all three cases we find a strong correspondence between the X-STM and DFT results as seen in Figure 1.

9:35am **PCSI-WeM1-14 GaAsGe Ternary Alloys Studied by Cross-sectional Scanning Tunneling Microscopy**, *Aurelia Trevisan, W. van Lierop,* Eindhoven University of Technology, Netherlands*; J. Ripalda,* Spanish National Research Council (CSIC), Instituto de Microelectrónica de Madrid, Spain*; Y. González,* Spanish National Research Council (CSIC) · Instituto de Microelectrónica de Madrid, Spain*; P. Caño, E. Navarro,* Spanish National Research Council (CSIC), Instituto de Microelectrónica de Madrid, Spain*; R. Juluri, A. Sanchez,* University of Warwick, UK*; P. Koenraad,* Eindhoven University of Technology, Netherlands

Similarly to Si, Ge exhibit an amphoteric behavior when used as dopant in GaAs, i.e. it can substitute both Ga and As atoms [1]. In molecular-beam-epitaxy-(MBE)-grown GaAsGe, at low doping concentration, Ge preferentially substitute either Ga or As atoms depending on the growth condition, i.e. the As2 to Ga ratio in the molecular beams [2]. However, at high doping concentration, Ge is expected to substitute Ga and As atom to the same extent [1],[3]. A GaAs/GaAs:Ge structure comprising of seven 50 nm-thick GaAs:Ge layers with decreasing Ge concentration (5% - 0.01% Ge) grown by MBE was analyzed by cross-sectional scanning tunneling microscopy (X-STM). All the layers aside the 5% Ge one were imaged by X-STM. In filled-states X-STM images, the Ge atoms appear as bright features with different shapes depending on where they are located in the GaAs lattice, i.e. whether they are sitting on a Ga or As site and at what depth below the cleaved surface (0th layer). Several features are identified in the layer at lower Ge concentration (0.01% Ge, L7). Of these features we assume that some correspond to a Ge atom sitting on a Ga-site located at different depth below the cleaved surface. Similarly, some other features are related Ge atoms on As-sites located at different depth below the surface. These different features have been classified and related to the Ge position below the cleaved surface through symmetry considerations taking into account the contribution of the different surface states to the X-STM images, namely the A4 and A5 state located in the valence band and the C3 and C4 located in the conduction band [4], [5]. Other observed features are given by Ge located deeper below the cleaved surface (5th layer or lower), interstitial atoms and vacancies that can be either intrinsic or caused by the cleave of the sample. Additionally, we calculated the Ge concentration in the measured layers and we compared it to the nominal concentration. We found that for most the layers, the experimental concentration is comparable to the nominal one. With this study, we aim to gain further insight into the preferential incorporation of Ge in GaAs, which is difficult to determine with other techniques.

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[5] D. Tjeertes *et al., Phys. Rev. B.* 104, 125433 (2021)

9:40am **PCSI-WeM1-15 Imaging Rare-Earth Dopant Clusters in SiC in 3D Using Multislice Electron Ptychography**, *Shake Karapetyan, M. Thomas,* Cornell University*; U. Kaiser, J. Biskupek,* Ulm University, Germany*; D. Muller,* Cornell University

There has been a long-standing interest in exploring rare-earth dopants and clusters within wide-bandgap materials as a platform for quantum computing [1]. Atomic-scale characterization of these dopants is crucial for understanding activation mechanisms and optimizing doping strategies. Multislice electron ptychography (MEP) is a new approach capable of imaging the atomic distribution of dopants inside a material, offering sub-Ångstrom lateral resolution and a few nanometers depth resolution, making it possible to visualize atomic-scale vibration envelopes and single

dopants [2, 3]. Here, we use MEP to image the effects of implanting Sm and Co atoms in SiC, a prototypical host whose rare-earth-doped defect centers display promising photonic and spintronic functionality [4].

Figure 1 presents a region of SiC containing Sm dopant clusters, comparing MEP with conventional Annular Dark Field (ADF) imaging. The MEP reconstruction reveals depth dependent features showing that the Sm atoms occupy Si positions inside the sample and displace nearby C and Si atoms, even whole columns (yellow arrow) – details that ADF fails to capture. This new capability to study atomic defects in 3D not only deepens our understanding of defect behavior in complex materials but also allows us to tackle such problems in the actual device structures needed for optoelectronic and quantum computing.

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9:45am **PCSI-WeM1-16 Controlling with External Fields the Quantum-Mechanical Core-Hole Manganese Spin in III-V Semiconductors**, *Julian Zanon,* Eindhoven University of Technology, Netherlands*; M. E. Flatté,* University of Iowa

For applications in quantum devices the control of spin-degree of freedom has been one the major goals in semiconductor physics in the past few years. In III-V semiconductors (e.g., in GaAs or InSb) this could be achieved with manganese impurities. Manganese forms a complex, where a $J = 3/2$ hole from the host aligns antiferromagnetically with the 5/2 spin of the 3d5 manganese core [1]. STM images with theoretical calculations showed the potential to characterize the spatial structure of a single manganese [2] and the exchange interaction between manganese pairs [3]. Classically treating the manganese core spin, its orientation would affect the spatial structure of the manganese complex [2]. In our work, based on previous ESR measurements [1], we show a new pathway to treat the manganese core fully quantum-mechanically and, using an analytical treatment to treat the hole part of the wavefunction, we suggest a coherent manipulation of spatial structure of a single manganese in bulk III-V semiconductors. We also investigate how a surface affects the spatial structure.

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PCSI
Room Keahou I - Session PCSI-WeM2

Point Defects (for Quantum Information Applications) II
Moderator: Gregory Fuchs, Cornell University

11:00am **PCSI-WeM2-31 Quantum Point Defects in Wide Band Gap Semiconductors: Donor Properties in ZnO and Charge States of Diamond**, *X. Wang, E. Hansen, V. Niaouris, C. Pederson, N. Yama,* University of Washington*; L. Vines,* University of Oslo, Norway*; **Kai-Mei Fu**,* University of Washington **INVITED**

Quantum point defects which exhibit both spin and optically active states are attractive qubit candidates for quantum sensing and network technologies. Here we present progress on two qubit systems: shallow donors in ZnO and deep vacancy-related defects in diamond.

In direct band-gap semiconductors, the bound-electron spin states of shallow donors forming the qubit states can be optically accessed via the donor-bound exciton (D^0X) with high radiative efficiency. We have recently measured the optical and coherence properties of In defects in ZnO, *in situ* doped and formed by implantation and annealing. We observe an inhomogeneous linewidth of several GHz [1], longitudinal spin lifetimes up to 0.5 s [2] and coherence times up to 50 μs which are limited by substrate purity [3]. Two-laser spectroscopy also reveals the large, 100 MHz hyperfine coupling of the In electron spin-1/2 to the In nuclear spin- 9/2 [4]. Thus,

there is a path toward deterministic formation of In donors with access to a nuclear spin memory. Further, we have demonstrated isolation of single In donors by probing only a small sample volume [5]. We further investigate the role of substrate purity by studying In donors fabricated in high-purity ZnO grown by molecular beam epitaxy. Finally, we discuss the outlook for new defect centers in an ultra-pure ZnO host.

A fundamental property that must be controlled in any defect-based technology is the charge state. We demonstrate the use of deep-ultraviolet (DUV) radiation to dynamically neutralize nitrogen- (NV) and silicon-vacancy (SiV) centers in diamond [6]. We first examine the conversion between the neutral and negatively charged NV states by correlating the variation of their respective spectra, indicating that more than 99% of the population of NV centers can be initialized into the neutral charge state. We then examine the time dynamics of bleaching and recharging of negatively charged SiV[-] centers and observe an 80% reduction in SiV[-] photoluminescence within a single 100-μs DUV pulse. Finally, we demonstrate that the bleaching of SiV[−] induced by the DUV is accompanied by a dramatic increase in the neutral SiV^0population; SiV^0 remains robust to extended periods of near-infrared excitation despite being a non-equilibrium state. Our results on two separate color centers at technologically relevant temperatures indicate a potential for above-band-gap excitation as a universal means of generating the neutral charge states of quantum point defects on demand.

PCSI
Room Keahou I - Session PCSI-WeM3

Photoemission Spectroscopy
Moderator: Gregory Fuchs, Cornell University

11:40am **PCSI-WeM3-39 Surface and Interface Effects on the Electronic and Magnetic Properties of NiCo$_2$O$_4$ Thin Films**, *Arjun Subedi, B. Giri, D. Yang,* University of Nebraska–Lincoln*; A. N'Diaye,* Advanced Light Source, Lawrence Berkeley National Laboratory*; T. Komesu, X. Xu, P. Dowben,* University of Nebraska–Lincoln

The surfaces of epitaxial complex oxide thin films could differ chemically from its bulk. The distinctly different surface can lead to different surface electronic and magnetic properties compared to the bulk properties of the thin films. Using angle-resolved x-ray photoelectron spectroscopy (ARXPS) of the NiCo$_2$O$_4$ (NCO) thin films, NCO thin film surfaces are found to be Ni-rich and there exist surface-to-bulk core level shifts in binding energies of the Ni $2p_{3/2}$ and Co $2p_{3/2}$ core levels [1, 2]. While the Ni-rich conducting NCO thin film surface undergoes irreversible metallic to non-metallic (dielectric) phase transition, the highly reduced surface of the NCO thin film undergoes reversible phase transition from highly dielectric to much diminished dielectric (or highly enhanced metallic) character with temperature [2]. We have proposed a modified Arrhenius-type model for the core level binding energy change with temperature in x-ray photoelectron spectroscopy (XPS) of dielectric oxide thin films, and activation energies for thermal stimulations of the carriers are thus estimated [2]. Spin-polarized inverse photoemission spectroscopy (SPIPES) and angle-resolved x-ray magnetic circular dichroism (XMCD) of Ni-rich NCO thin film show that the surface spin moments of the film are canted, although the same film in the bulk is known to possess perpendicular magnetic anisotropy (PMA). When a thin platinum (Pt) layer was deposited on the NCO film, the spin moment canting at the interface of Pt/NCO increased dramatically, leading to significantly different spin ordering at the interface compared to the bulk spin ordering (PMA) of the NCO thin film. The reversibility in electronic phase transition can ultimately lead to two controlled, programmable and non-volatile electronic phase states, whereas spin-canting surfaces and interfaces make NCO thin films interesting for spintronics.

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11:45am **PCSI-WeM3-40 Spectroscopic Calculations for Trivalent Lanthanide Ions**, *Tharnier O. Puel,* University of Iowa*; J. Lizarazo-Ferro, R. Zia,* Brown University*; M. E. Flatté,* University of Iowa

It is known that spin of optically addressable solid-state defects can be coherently manipulated using electric fields, enabling precise control over the photoluminescence spectra of spin defects when integrated into electrical junctions. Additionally, spin defects are also sensitive to electric

and magnetic field noise, for example, electric field noise from surface charge fluctuations can be a significant source of spin decoherence. In this study, we examine trivalent lanthanide ion defects in crystals using a semi-empirical Hamiltonian, where parameters are empirically fitted to experimental data. By diagonalizing the Hamiltonian, we are able to predict key spectroscopic properties of these defects, including optical transition rates, oscillator strengths, magnetic dipole transitions, parity-forbidden electric dipole transitions, AC Stark shifts, and g-tensors for low-energy excitations. We have compared our results against the well-established calculations from Carnall et al. The Journal of Chemical Physics 90, 3443 (1989), for the lanthanide ions in LaF$_3$ and make available the *qlanth* software for easy reproducibility of the results. These findings are essential for advancing the control of rare-earth-based quantum devices and for understanding the mechanisms underlying their decoherence.

11:50am PCSI-WeM3-41 Brillouin-Zone-Selection Effects in Angle-Resolved Photoemission Spectroscopy of Silicon, *Niels van Venrooij,* University of Iowa, Netherlands*; P. Constantinou, T. Stock,* University College London, UK*; V. Strocov,* Paul Scherrer Institut, Switzerland*; G. Aeppli,* ETH Zurich, Switzerland*; N. Curson, S. Schofield,* University College London, UK*; M. Flatté,* University of Iowa

The advancement of semiconductor-based atomic-scale quantum electronics hinges on a deep understanding of the electronic properties of subsurface δ-layers[1]. In this rapidly evolving field, soft X-ray angle-resolved photoemission spectroscopy (SX-ARPES) has emerged as a pivotal, non-destructive probing tool[2]. The large energy range of SX-ARPES allows for measurements across a broad momentum space, covering multiple Brillouin zones. During these measurements, interference effects from photoemission across different atoms in a unit cell can lead to pronounced intensity fluctuations between adjacent Brillouin zones, even causing some bands to vanish. In this study, we present the first detailed observations of such photoemission structure factor effects from a cubic semiconductor, revealing periodic fluctuations in both the valence and conduction band states of δ-doped silicon. By applying a simple tight binding calculation to Fermi's golden rule we are able to calculate the structure factor of Silicon and reproduce our experimental findings with a minimal number of approximations. Our findings pave the way for investigations at higher photon energies in the hard X-ray domain, crucial for exploring deeper δ-layers (~10 nm) typical in silicon quantum electronic devices.

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11:55am PCSI-WeM3-42 A Topological Superconductor Tuned by Electronic Correlations, *Haoran Lin,* University of Chicago*; C. Jacobs,* West Virginia University*; C. Yan,* University of Chicago*; G. Nolan,* University of Illinois at Urbana-Champaign*; P. Singleton, Y. Bai, Q. Gao, G. Berruto, D. Nguyen,* University of Chicago*; X. Wu,* Chinese Academy of Sciences, China*; C. Liu,* Penn State University*; N. Guisinger,* Argonne National Laboratory*; P. Huang,* University of Illinois at Urbana-Champaign*; S. Mandal,* West Virginia University*; S. Yang,* University of Chicago

A topological superconductor, characterized by either a chiral order parameter [1] or a chiral topological surface state in proximity to bulk superconductivity [2], is foundational to topological quantum computing. Similar to other topological phases of matter, it can be profoundly tuned by electronic correlations through the modification of low-energy Fermiology, but not elucidated so far.

We present the study of a unique topological superconducting phase emerging in 10-unit-cell-thick FeTe$_x$Se$_{1-x}$ films grown on SrTiO$_3$ substrates [3]. By combining molecular beam epitaxy (MBE) growth with *in-situ* angle-resolved photoemission spectroscopy (ARPES) (Fig. 1), we investigate the electronic band structures of these thin films. When the Te content x exceeds 0.7, we observe a rapid increase of the effective mass for the Fe d$_{xy}$

band, with the emergence of a topological surface state and superconductivity; however, near the FeTe limit, the system enters an incoherent regime where the topological surface state becomes unidentifiable, and superconductivity is suppressed. Theory [4] suggests that the electron-electron interactions in the odd-parity xy$^-$ band with a strong d$_{xy}$ character lead to an orbital-selective correlated phase. Our work establishes FeTe$_x$Se$_{1-x}$ thin films as a unique platform where electronic correlations sensitively modulate topological superconductivity, suggesting opportunities to use tunable electron-electron interactions to engineer new topological phases in a broad class of materials.

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PCSI

Room Keahou I - Session PCSI-WeA1

Semiconductor Heterostructures: Growth, Nanostructures, & Interfaces II

Moderator: Karen Kavanagh, Simon Fraser University

1:30pm PCSI-WeA1-1 Atomic Layer Deposition: Surface Processes Unlocking Advanced Materials in the Semiconductor Industry, *Erwin Kessels, A. Mackus, B. Macco,* Eindhoven University of Technology, Netherlands **INVITED**

Atomic Layer Deposition (ALD) has emerged as a critical technique in the precise fabrication of materials employed in advanced semiconductor devices. ALD offers unparalleled control over film thickness, uniformity, and composition at the atomic scale, also on complex 3D structured surfaces that have become commonplace in the semiconductor industry. Understanding of the surface processes that govern ALD, including the intricate interplay of surface reactions, is fundamental to achieving high-performance materials for next-generation semiconductor devices in the so-called Ångstrom era. This presentation will delve into the fundamental aspects of the physics and chemistry at the surface during ALD and explore how surface processes dictate film growth and material properties. Focus will be given to emerging materials under ALD investigation, such as ferroelectric oxides, 2D transition metal dichalcogenides (TMDs), and amorphous oxide semiconductors, along with how advances in surface process understanding can address challenges in controlling the material properties and their scaling behavior.

2:10pm PCSI-WeA1-9 Characteristics of Electrochemically Deposited Lightly-doped Co(P) Film on a Self-Assembled Monolayer-Sealed NiSi Substrate as an Interconnect Material for Nanoscale Device, *Jau-Shiung Fang,* National Formosa University, Taiwan

As semiconductor devices continue to shrink in size, the average free path of electrons causes a notable rise in resistivity and a decline in the performance of traditional copper interconnects. A strategy to improve the electromigration resistance of a copper line involves alloying it with a lightly-doped element without significantly suffering its electrical conductivity. A comprehensive review of the literature reveals that phosphorous-incorporated Co films are frequently investigated, primarily because these alloyed films demonstrate both low resistivity and outstanding barrier/self-strengthening performance. [1-3] However, the incorporation of phosphorous into cobalt has been rarely explored for interconnecting materials. In this study, Co(P) films were fabricated through electrochemical deposition on self-assembled monolayers-sealed NiSi substrates. The proposed schemes present a promising interconnect material, offering an alternative to the conventionally used copper in contemporary nanoscale devices, especially as a plug material in direct contact with a nickel silicide (NiSi) gate and source/drain material.

Co(P) alloy films were fabricated on self-assembled monolayers-sealed NiSi substrates through electrochemical deposition. The charge and nucleation mechanism of the Co(P) film were assessed through current density-time curves, while the diffusivity of ions in the electrolyte was also analyzed. Additionally, EIS impedance and Tafel curves (supplementary Fig. 1) were employed to validate the diffusion coefficients and corrosion rate of the resulting Co(P) films. The experimental findings indicate that the Co film possesses a resistivity of 11.1 $\mu\Omega$ cm. Cottrell curves (supplementary Fig. 2) were utilized to evaluate the diffusivity of Co ions during electrochemical deposition, revealing diffusivity values ranging from approximately 8.02 to 56.2×10^{-8} m^{2}s^{-1}. Analysis of the crystal structure through XPS and XRD reveals the incorporation of phosphorous into the Co lattice, suggesting that the Co(P) film exhibits high thermal stability and corrosion resistance. The outcomes of this study have practical implications for the electrochemical deposition of Co(P) as a contact material on NiSi substrate, particularly for applications in future nanoscale devices.

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[+] Author for correspondence: jsfang@nfu.edu.tw

2:15pm PCSI-WeA1-10 Low Temperature Ge/Si Heterojunction by DC Sputtering, *Yi-Jhen Wang, H. Huang, Y. Lai, C. Lin,* Tatung University, Taiwan
This study investigates the fabrication and optimization of germanium (Ge) films on silicon (Si) substrates for high-sensitivity optical sensing applications. Ge with its small bandgap of 0.67 eV [1], effectively absorbs long-wavelength red light, making it suitable for photodetectors. This research used DC magnetron sputtering, rapid thermal annealing, and filament evaporation.

This research examined the influence of various process parameters, including deposition time, power, and substrate type on the properties of the Ge thin films. The results revealed that Ge thin films with an illuminated area of 113 mm2 deposited on n-type Si substrates at 13.26 W/cm2 showed good performance. After RTA treatment, there is a 180% increase in carrier mobility and a 50% reduction in resistivity compared with the pre-annealed condition. X-ray diffraction (XRD) analysis confirmed a preferential (400) similar to orientation [2]. The experiment further investigated the impact of various light sources on the illumination current-voltage (I-V) characteristics. As the illumination power and light absorption increased, the base temperature of the Ge/Si substrate also increased. The illumination gain is defined as $|Ilight|/ |Idark|$ at $v=-1.45$ V.The illumination Gain was stable even illumination the power reached a maximum of 1.2W. The Gain was 300% under the illumination of 800 nm wavelength and 250% for 700 nm wavelength. To conclude, the study provides insights into the optimal fabrication processes and the impact of rapid thermal annealing on the performance of Ge thin films.

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2:20pm PCSI-WeA1-11 Optical and Structural Properties of Group-IV Oxides Produced by Rapid Thermal Oxidation, *D. Ortega, Danissa Ortega, H. Woolf, A. Moses, C. Armenta, J. Love, S. Yadav, S. Zollner,* New Mexico State University; *M. Mircovich,* Arizona State University

There is great interest in germanium and germanium-tin alloys as optical sensors, especially short-wave infrared detectors, but little is known about thermal oxidation of thin Ge-Sn alloy layers on a bulk semiconductor substrate. We report a comparative study of the rapid thermal oxidation of bulk Ge, thick relaxed epitaxial Ge on Si, and Ge-Sn alloys on Si produced by chemical vapor deposition. Layer thickness, roughness, composition and strain, optical constants, and infrared-active molecular vibrations were characterized using spectroscopic ellipsometry, high-resolution x-ray diffraction, atomic force microscopy, and Fourier-transform infrared spectroscopy.

Before oxidation, the surfaces were ultrasonically cleaned in deionized water at room temperature and dried with nitrogen to achieve a low native oxide layer with less than 1 nm thickness. The ellipsometric angles ψ and Δ were acquired on a J.A. Woollam vertical angle spectroscopic ellipsometer (VASE) from 0.5 to 6.5 eV and on a J.A. Woollam Fourier-transform infrared spectroscopic ellipsometer (FTIR-VASE) from 0.03 to 0.6 eV at incidence angles ranging from 60-80°. The ellipsometric angles were then modeled with a three-layer model: Si substrate, pure Ge (or Ge-Sn) layer, and GeO$_2$, to obtain initial conditions. The initial strain was determined using high-resolution x-ray diffraction (HRXRD), including symmetric (004) and asymmetric (224) reciprocal space maps and rocking curves.

The samples were then rapidly thermally annealed in pure oxygen at temperatures ranging from 525-575°C in 40 psi pressure for up to 2 hours to create a range of thermal oxide layers on different types of surfaces. After oxidation, HRXRD and ellipsometric angles are measured again and compared to pre-oxidation results.

2:25pm PCSI-WeA1-12 Growth Evaluation and Electrochemical Properties of Lab6 Thin Films Deposited by HiPIMS, *César D. Rivera Tello, J. Pérez Alvarez, M. Flores, L. Huerta,* Universidad de Guadalajara, Mexico
Lanthanum hexaboride (LaB$_6$) thin films are widely used due to their exceptional electron emission, thermionic and interesting mechanical properties. The LaB$_6$ has a crystal structure, increasing the hardness and improving the mechanical properties. Besides, the LaB6 films can promote a scavenger effect, that decreases surface impurities that could contribute to the corrosion increments, and the high reactivity with oxygen also helps to increase the corrosion resistance. However, the obtention of these properties can also present challenges in thin films' physical vapor deposition processes. In this sense, the High Impulse Magnetron Sputtering

(HiPIMS) deposition parameters such as the pulse width can influence the morphology, and density of the films. In the present study, we analyze the influence of duty cycle of the deposition processes on the ionization, bonding, structural, and electrochemical properties of the films. Two films were deposited on silicon 001 and 52100 metallic alloy, varying the pulse width (50 and 60 μs). The ion energy distribution function (IEDF) of the LaB_6 species in the plasma deposition was evaluated by the IEDF curves obtained by a quadrupole mass spectrometer detector. The morphology and thickness of the LaB_6 thin films were analyzed from cross-sectional images using a field-emission scattering electronic microscope (FESEM). Electrochemical Impedance Spectroscopy (EIS) was made of the two films deposited on the metallic alloy. Raman spectroscopy and X-ray diffraction revealed higher crystallinity in the 50-film. Furthermore, this film showed better corrosion resistance. These results demonstrated how the pulse width and duty cycle in the HiPIMS process can significantly influence the crystallinity and overall quality of LaB_6 thin films.

2:30pm PCSI-WeA1-13 Facile and Inexpensive Development of Nano-Structured Polymer Layers for Surface Enhanced Raman Spectroscopy Applications, *L. Jiang,* Tuskegee University*; N. Korivi,* Oregon Institute of Technology

Surface-enhanced Raman scattering (SERS) is a spectroscopic method for label-free detection of trace analytes, providing insights into the chemical bonds of molecules on nano-structured metal surfaces known as SERS substrates. Since its discovery with pyridine on silver, advancements in nanotechnology have led to various substrate fabrication methods, primarily using colloidal metal nanoparticles or electron beam lithography for nanostructured surfaces [1,2]. However, colloidal substrates can be unstable and prone to contamination, while electron beam lithography is costly and yields small active areas. This limits the mass production of large-area SERS substrates, hindering their widespread use [3]. Recent efforts have focused on low-cost, thin-film substrates, such as metal nanoparticle layers on flower petals or eggshell membranes [4, 5]. We report the development of low-cost nano-structured polymer surfaces for use as SERS substrates. This method involves molding a silicone elastomer (PDMS) over treated chicken eggshells. The eggshells are cleaned and etched in hydrochloric acid to create a nano-scale texture. A PDMS pre-polymer mixed with toluene is poured over the eggshell, which is then cured at room temperature for 24 hours. After dissolving the eggshell in hydrochloric acid, a PDMS layer with complementary nano-features remains. This layer is coated with a thin gold layer, which is expected to enhance Raman signals through localized surface plasmon resonance. Current efforts are focused on evaluating the nanostructured surface for SERS applications, with the thinning of the pre-polymer improving the interface by filling gaps in the eggshell mold.

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PCSI
Room Keahou I - Session PCSI-WeA2

Materials for Catalysis, Energy Storage, and Energy Harvesting
Moderator: Mitsuru Takenaka, The University of Tokyo

2:35pm PCSI-WeA2-14 Scalable Si-Based Metal-Insulator-Semiconductor Photoanodes for Water Oxidation Fabricated Using Nanosphere Lithography and Thin Film Reaction, *E. Yu, Yunho Choi, S. Wu, J. Risberg, S. Kim,* University of Texas at Austin

Photoelectrochemical (PEC) water splitting is a promising approach for converting solar energy into storable hydrogen, offering a sustainable alternative to fossil-based hydrogen production. PEC cells rely on semiconductor materials to absorb sunlight and generate mobile charge carriers that drive the hydrogen and oxygen evolution reactions. Si-based photoelectrodes are especially attractive due to their optimal bandgap, high charge mobility, long diffusion lengths, and cost-effective, scalable manufacturing process. To improve the stability of Si-based PEC cells, metal-insulator-semiconductor (MIS) structures have emerged as a promising approach [1]. MIS photoanodes integrate ultrathin insulating layers that protect the Si surface while maintaining charge transfer efficiency. The thickness of the insulator is critical:ultrathin layers facilitate effective charge tunneling, whereas thicker layers enhance long-term stability in corrosive environments.

In our previous work, we demonstrated that localized conduction paths formed via an Al/SiO_2 thin-film reaction enable low-resistance charge extraction through thick insulating layers, while also providing excellent stability and scalability to full-wafer photoanodes [2]. However, the performance of such photoelectrodes can be limited by nonuniformity in thin-film reaction behavior. We have now demonstrated a method for creating more controllable and uniform localized conduction paths on the photoanode by employing nanosphere lithography (NSL), a low-cost and highly scalable patterning technique. NSL is used to create a patterned mask for Al deposition that enables the density and locations of Al/SiO_2 thin-film reactions and consequently metal catalysts to be precisely controlled, leading to improvements in both photocurrent density and onset voltage. Moreover, a technique we have recently developed for extremely rapid large-area nanosphere monolayer formation [3] makes this patterning approach easily scalable to fabrication of full-wafer photoanodes and therefore, highly promising for large-scale PEC applications.

2:40pm PCSI-WeA2-15 Development of Bi_2Te_3-based Thermoelectric Thin Films Using Advanced Pulsed Laser Deposition System, *Yakubu Sani Wudil,* King Fahd University, Saudi Arabia

This study presents the pulsed laser deposition of n-type selenium (Se)-doped bismuth telluride ($Bi_2Te_{2.7}Se_{0.3}$) and n-type bismuth telluride (Bi_2Te_3) nanostructures at varying substrate temperatures. The effects of substrate temperature on the structural, morphological, and thermoelectric properties of these nanostructures were systematically explored. Density functional theory (DFT) simulations were conducted to examine the electronic structures, partial, and total densities of states of the unit cells of the compounds. Surface and structural characterization revealed highly crystalline nanostructures with pronounced grain boundaries. A comparative analysis underscores the impact of Se inclusion on the thermoelectric performance of the Bi_2Te_3 matrix. The study also highlights the substrate temperature-dependent variations in the thermoelectric figure of merit (ZT). Notably, the room temperature thermoelectric power factors (PF) of 2765 $\mu W/mK^2$ for pure Bi_2Te_3 and 3179 $\mu W/mK^2$ for Se-doped Bi_2Te_3 demonstrate their promise for cooling and power generation applications. The Se-doped Bi_2Te_3 exhibited a room temperature ZT value of 0.92, representing a 30% improvement over the pure phase. This enhancement is attributed to the reduction in thermal conductivity due to increased phonon scattering at the interfaces in the doped material.

2:45pm PCSI-WeA2-16 Molecularly Engineered Siloxane Binders: Elevating Lfp Cathode Efficiency Under High Active Mass Loading, *Asuman Celik-Kucuk, T. Abe,* Kyoto University, Japan

Previously, we demonstrated that siloxane structures (Sx@04 and Sx#O@06) mitigate the corrosive effects of LiTFSI by forming a protective layer on aluminum current collectors, enhancing lithium stability and battery performance *(Journal of Power Sources 556 (2023) 232520).* Our recent research revealed that siloxane-based polymers (Sx@04) used as binders in LiFePO4 (LFP) cathodes significantly improve rate capability and cycling stability compared to traditional binders like PVDF and PEO *(Journal of Power Sources 581 (2023) 233478).* Building on these findings, we focused on modifying siloxane-based binders (Sx#O@32) to further improve their performance in LFP cathode applications. Testing at 60°C showed that LFP cathodes with Sx#O@32 had superior cyclic stability at 0.5 C, outperforming both Sx@04 and PVDF. Even at high mass loadings, Sx#O@32 maintained better cycling stability than PVDF. Additionally, the Sx#O@32 binder reduced ionic diffusion resistance (Rp) and charge transfer resistance (Rct), facilitating smoother lithiation and delithiation during battery operation. This enhanced performance is attributed to the low internal resistance of the composite electrodes using Sx#O@32. The stronger adhesion observed in these electrodes is likely due to increased cohesion from network formation via anion solvation of low molecular weight siloxane oligomers, enhancing performance over Sx@04 and PVDF binders.

Biography: I hold dual PhDs in applied chemistry from Tohoku University (MEXT scholarship) and polymer chemistry from Gebze Technical University. With a strong background in organic and inorganic polymeric materials, I specialize in the design and application of advanced hybrid materials for electrochemical devices, including rechargeable batteries and fuel cells. My career includes work as an assistant professor at Marmara University and a

visiting researcher at Kyoto University, contributing to significant projects like NEDO's RISING-2. I have authored 37 journal articles, hold two patents, and received prestigious awards such as the L'Oréal–UNESCO National Fellowship and a Hirose Foundation fellowship.

2:50pm PCSI-WeA2-17 Minimizing Ion/Electron Pathways Through Ultrathin Conformal Holey Graphene Encapsulation in Li- and Mn-Rich Layered Oxide Cathodes for High-Performance Lithium-Ion Batteries, *Heejoon Ahn,* 222 Wangsimni-ro, Seongdong-gu, Republic of Korea*; S. Kim,* Hanyang University, Korea

Lithium-ion batteries (LIBs) are increasingly favored due to their attractive features. The design of the cathode in LIBs plays a critical role in determining cell capacity, operating voltage, and overall cost. Lithium- and manganese-rich (LMR) cathode materials stand out as promising candidates for the next generation of cathode materials due to their ability to operate at high voltages and provide capacity exceeding 250 mAh g^{-1}. However, despite these appealing characteristics, LMR faces challenges in commercialization due to factors such as poor rate capability and rapid capacity and voltage decay during cycling. These are closely associated with the fundamental structural issues arising from the two distinct phases of LMR materials, slow reaction kinetics and structural degradation occurring through side reactions between the electrode and electrolyte. In this study, we introduce a carbon encapsulation technique that integrates polyethylenimine (PEI) and holey graphene onto the LMR surface, aiming not only to augment electrical conductivity but also to facilitate ionic conductivity. Despite its low carbon content of 0.1 wt%, the suggested PEI/holey graphene-encapsulated LMR demonstrates enhanced cycle stability and rate performance for the LMR electrode. Moreover, the thin and uniform PEI/holey graphene encapsulation layer serves a dual purpose by easing the movement of Li^+/e^- on the LMR surface and providing a protective barrier against physical and chemical aggressions. Throughout cycling assessments, the PEI/holey graphene-encapsulated LMR mitigates the leaching of transition metals, mitigating microcrack formation and irreversible structural alterations compared to bare LMR. Consequently, the proposed PEI/holey graphene encapsulation emerges as an attractive technology for high-performance LIB design, concurrently elevating the cycle stability and rate performance of LMR electrodes.

2:55pm PCSI-WeA2-18 The Interplay between Gaseous Water and Surface Hydroxyl on Diamond(001) via Hydrogen Bonding, *Huiqun Xiao, K. Huang,* Guangdong Technion Israel Institute of Technology, China

Hydrogen bonding plays a pivotal role in water sciences, governing dynamics such as proton transfer,[1-3] phase transition,[4] solvation,[5] and dissociation.[6] For example, Kumagai et al.[1] have demonstrated a relay reaction of proton-transfer of a chain of $H_2O(OH)n$ (n≤4) on Cu(110) via hydrogen bonding by inelastic electrons. For thermal reaction, Huang et al.[6] reported on the enhanced dissociation of $(H_2O)_2$ on Si(001) by intermolecular hydrogen bonding; the dissociation barrier of $(H_2O)_2$ was computed as 73-87 meV as against that of a single H_2O of 273-307 meV. Here, we describe the interplay between a surface hydroxyl on diamond(001) and a gaseous water via hydrogen bonding, as revealed by density functional theory simulations given in parts.

1. *Migration of hydroxyl on C(001) catalyzed by water.* It is found that surface hydroxyl on diamond(001) is capable of interacting with a gaseous water via hydrogen-bonding, forming a complex, OH(surf)...H_2O(ad), which exhibits enhanced adsorption energies of 0.47 eV. By a series of cooperative motions of this complex and the underlying substrate atoms, the adsorbed water molecule is dissociated; the resulting fragment of hydrogen recombines with the prior OH(surf) to form water, whereas the other fragment of hydroxyl is deposited to the adjacent carbon-dimer site. Effectively, this process represents the water-catalyzed migration of surface hydroxyl on C(001), exhibiting an isotropic barrier of 0.33 eV. These findings are in contrast to anisotropic migration of hydroxyl on diamond(001) in the absence of water; the barriers vary from 1.96 eV along [10] to 2.24 eV along [110].

2. *Self-catalyzed dissociation of water on C(001).* It has been established that the water physisorbs on C(001), from which there is a competition that strongly favors desorption (adsorption energy computed as 0.24 eV) over dissociation (barrier computed as 0.39 eV). The dissociation products are fragments of hydrogen (H) and hydroxyl (OH) at a surface dimer of C(001), at which the dynamics of a new incoming water molecule is altered. We find that this new incoming water is

molecularly adsorbed over the surface hydroxyl via hydrogen bonding, leading to an enhanced adsorption energy of 0.52 eV. Subsequent dissociation proceeds in two steps, in which the adsorbed water first overcomes a barrier of 0.25 eV to a metastable state, and thereafter dissociates to form surface hydroxyl and hydrogen atoms at the neighboring dimer site (dissociation barrier computed as 0.39 eV). It follows that the dissociation of water proceeds in a self-catalyzed fashion, in which one product fragment (surface hydroxyl) enhances the dissociation significantly.

3:00pm PCSI-WeA2-19 Development of High-Performance Hydrogen Generation Catalyst Based on Fluorine-Doped Tin Oxide Aerogel, *Hyung-Ho Park,* Yonsei University, Korea

The electrochemical hydrogen evolution reaction (HER) and oxygen evolution reaction (OER) are efficient methods for generating clean, sustainable, and dense energy sources. Nørskov's theoretical study states that Pt is the most effective catalyst for HER due to its low Gibbs free energy (ΔG ~0) or moderate M-H bonding toward H* adsorption. Unfortunately, its scarcity and high cost limit its practical use. To overcome these drawbacks, high surface area carbon in the form of core-shell, wrapped, or dispersed structures has been used as a metal catalyst support, forming complexes with the metal and providing impressive resistance against corrosion.

In this presentation, an "aerogel" system is introduced to fabricate an ultra-low-density and highly porous metal support of SnO_2.[1] The aim is to meet the fundamental criteria for an ideal metal support structure, including resistance to corrosion, high conductivity, high porosity, large specific surface area, and strong metal-support interaction. SnO_2 aerogel was synthesized using a sol-gel method, leveraging the benefits of an aerogel system to impart three significant advantages to SnO_2: ultra-low density, which reduces the electrode's weight; a large surface area to achieve optimal metal catalyst dispersion; and high porosity, facilitating ion insertion and mass transfer. Additionally, anion doping of SnO_2 with fluorine at the atomic level during synthesis was conducted to improve conductivity. This doping resulted in an observable bandgap expansion, and the one-step synthesized F-doped SnO_2 (F-SnO_2) exhibited higher conductivity, significantly reducing the electrochemical charge transfer resistance compared to undoped SnO_2. Subsequently, a sputtering technique was used to deposit nanometer-scale Pt on the colloidal F-SnO_2 surface. The resulting hybrid structure (F-SnO_2@Pt) demonstrated enhanced HER activity and impressive catalytic stability even after prolonged oxidation activity.[2]

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3:05pm PCSI-WeA2-20 In Situ X-Ray Absorption Spectroscopy (XAS) Study of CeO₂-Based Catalysts for CO₂ to Methane Conversion, *Irene Barba-Nieto, Y. Wang, J. Moncada, J. Jimenez,* Brookhaven National Laboratory*; M. Fernández-García,* Instituto de Catálisis y Petroleoquímica (CSIC), Spain*; J. Rodriguez,* Brookhaven National Laboratory

Carbon dioxide (CO_2) is the primary gas responsible for the greenhouse effect in Earth's atmosphere, leading to higher global temperatures and climate change. In order to limit global warming to 1.5 °C and achieve net zero carbon dioxide emissions by 2050, it is essential to advance industrial processes that facilitate the generation of clean fuels from CO_2; one of the most promising strategies in this regard is the utilization of CO_2 and its transformation into valuable chemicals.

This study examines the effectiveness of two catalyst types, Ru-CeO_2 and Ru-CeO_2-TiO_2 systems, for the conversion of CO_2 into methane. The results demonstrate that, despite a lower Ru content, TiO_2-containing systems exhibit significantly enhanced catalytic activity for CO_2 conversion to methane. To understand this fact, in situ X-ray absorption measurements have been carried out on the Ru K-edge and Ce L_3-edge analyzing their behavior under H_2, CO_2 and H_2+CO_2.

The XAS findings indicate that the presence of TiO_2 in the catalysts stabilizes the metallic state of Ru, which remains in this state during the methanation reaction. Moreover, TiO_2 promotes the formation of Ce^{3+}, enhancing the catalysts' reactivity. This effect is attributed to TiO_2 facilitating an electronic transfer at the interface and perturbing the regular fluorite geometry of ceria, thus promoting the presence of Ce^{3+}. The presence of Ce^{3+} significantly impacts the catalytic properties of the sample, aiding in the

oxidation-reduction of Ce and stabilizing Ru. Consequently, the presence of reduced cerium plays a crucial role in determining the surface chemistry of the catalyst, crucial for efficiently converting CO_2 into methane.

3:10pm PCSI-WeA2-21 Properties of Spongy Structured BaTiO₃ Prepared by R.F. Magnetron Sputtering for Energy Harvester, *S. Kim,* Department of Energy Materials & Chemical Engineering, Kyungpook National University, Republic of Korea*; Sang-Shik Park,* 1Department of Energy Materials & Chemical Engineering, Kyungpook National University, Republic of Korea

A sustainable energy-harvesting technique, which can transfer various forms of energy from the surrounding environment into electricity, could be an alternative to remedy the shortcomings of traditional battery technology [1-3]. New piezoelectric and triboelectric materials for energy harvesting are being widely researched to reduce their processing cost and complexity and to improve their energy conversion efficiency. In this study, $BaTiO_3$ films of various thickness were deposited on Ni foams by R.F. magnetron sputtering to study the piezoelectric and triboelectric properties of the porous spongy structure materials. Then piezoelectric nanogenerators (PENGs) were prepared with spongy structured $BaTiO_3$ and PDMS composite. The output performance exhibited a positive dependence on the thickness of the $BaTiO_3$ film, pushing load, and poling. The PENG output voltage and current were 4.4 V and 0.453 μA at an applied stress of 120 N when poled with a 300 kV/cm electric field. The electrical properties of the fabricated PENG were stable even after 5,000 cycles of durability testing. The triboelectric nanogenerators (TENGs) were fabricated using spongy structured $BaTiO_3$ and various polymer films as dielectrics and operated in a vertical contact separation mode. The maximum peak to peak voltage and current of the composite film-based triboelectric nanogenerator were 63.2 V and 6 μA, respectively. This study offers new insights into the design and fabrication of high output nanogenerators using spongy structured materials.

PCSI
Room Keahou I - Session PCSI-WeA3

Spin Transport and Spintronics
Moderator: Michael Flatté, University of Iowa

4:00pm PCSI-WeA3-31 Quantum Sensing of Moiré Magnetism, *Chunhui (Rita) Du,* Georgia Institute of Technology, USA   **INVITED**

Moiré magnetism featured by stacking engineered atomic registry and lattice interactions has recently emerged as an appealing quantum state of matter at the forefront of condensed matter physics research [1]. Nanoscale imaging of moiré magnets is highly desirable and serves as a prerequisite to investigate a broad range of intriguing physics underlying the interplay between topology, electronic correlations, and unconventional magnetism. In this talk, I will present our recent work on using nitrogen-vacancy (NV) centers to perform nanoscale quantum sensing and imaging of magnetic domains and spin fluctuations in twisted double trilayer (tDT) chromium triiodide CrI_3. We show that intrinsic moiré domains of opposite magnetizations appear over arrays of moiré supercells in low-twist-angle tDT CrI_3 [2]. In addition, spin fluctuations measured in tDT CrI_3 reveal two distinct magnetic phase transitions with separate critical temperatures within a moiré supercell [3]. Our results enrich the current understanding of exotic magnetic phases sustained by moiré magnetism and highlight the opportunities provided by quantum spin sensors in probing microscopic spin related phenomena on two-dimensional flatland.

[1] T. Song et al., Science **374**, 1140 (2021).

[2] M. Huang et al., Nat. Commun. **14**, 5259 (2023).

[3] S. Li et al., Nat. Commun. **15**, 5712 (2024).

4:40pm PCSI-WeA3-39 Strong on-Chip Microwave Photon-Magnon Coupling Using Ultralow-Damping Epitaxial Y₃Fe₅O₁₂ Films, *S. Guo, D. Russell, J. Lanier, H. Da, C. Hammel, Fengyuan Yang,* The Ohio State University

Yttrium iron garnet ($Y_3Fe_5O_{12}$, YIG) is one of the best magnetic materials for magnon-based quantum information science (QIS) because of its extremely low damping loss. For scalable on-chip QIS devices, ultralow-damping YIG films at mK temperatures are desired. However, almost all epitaxial YIG films are grown on rare-earth-containing garnet substrates which cause very large damping at low temperatures, hindering the use of YIG films for QIS studies. We report ultralow damping at 2 K in epitaxial $Y_3Fe_5O_{12}$ thin films grown on a diamagnetic $Y_3Sc_2Ga_3O_{12}$ (YSGG) substrate that contains no rare-earth elements (Figs. 1a-1b). The extremely low damping of the YIG epitaxial

films on diamagnetic YSGG substrates at very low temperatures is highly promising for QIS studies. As an initial step in this regard, we integrate the YIG/YSGG films with superconducting resonators for the study of coupling between magnons in a YIG film and microwave photons emitted by a superconducting coplanar waveguide resonator (Fig. 1c). We observe strong coupling between magnons in patterned YIG thin films and microwave photons in a superconducting Nb resonator at 2 K (Fig. 1d). This is the first demonstration that ultralow-damping YIG epitaxial films on YSGG can be integrated with superconductor resonators to achieve strong microwave photon-magnon coupling at few Kelvin temperatures. Such ultralow-damping YIG films offer advantages over metallic ferromagnets for on-chip hybrid quantum systems that incorporate magnonic conduits, microwave superconductor resonators, and superconductor qubits for QIS applications that operate in the mK regime.

[1] S. D. Guo, D. Russell, J. Lanier, H. T. Da, P. C. Hammel, and F. Y. Yang, Nano Lett. **23**, 5055 (2023).

4:45pm PCSI-WeA3-40 Device Architectures for Characterizing Spin Transport Through Chiral Defects in Semiconductors, *Jordan Neely, F. Haines, E. Renteria, R. Chowdhury, D. Prakash, D. Shima, F. Cavallo,* University of New Mexico

Recent theoretical studies have shown that screw dislocations (SDs) support the interplay of Rashba and Dresselhaus spin-orbit coupling (SOC). Such a phenomenon makes these line defects suitable hosts of coherent spin transport. Specifically, spin polarization arising from SD-induced coupling lies in a much narrower range of angles (0 to 90°) than that resulting from the Rashba or Dresselhaus effects. Furthermore, this spin polarization is protected from changes in electron momentum caused by scattering, potentially leading to a relatively long coherence time. In this work, we demonstrate the fabrication of device architectures for characterizing spin transport due to the unique interplay of Rashba and Dresselhaus SOC in SDs. We fabricated a vertical spin valve (VSV) based on single-crystalline semiconductor nano-membranes (NMs) engineered with 2D arrays of screw dislocations (SDs) throughout their thickness. The device includes a bottom soft ferromagnetic contact (e.g., NiFe), the NMs, and a top hard ferromagnetic contact (e.g., Co). The constitutive material of the NM may be Si, Ge, III-V compounds, or SiC. The first step in the fabrication of the VSV is patterning the NM into a 2D array of pixels with lateral sizes of a few hundred micrometers. At this stage of the process, the NM is bonded to a sacrificial-layer-coated substrate. The pixels are released in place by selective etching of the sacrificial layer. An adhesive stamp removes the pixels from the original substrate and transfers them onto a second array of patterned pixels at a controlled twist angle. Pixelation of NMs reduces the release time and increases the yield of the transfer process. The twisted NM pairs or twisted bicrystals (TBiCs) are then annealed at high temperature in an inert atmosphere to foster the propagation of the SDs. Annealed TBiCs are transferred to a bulk substrate coated with a soft ferromagnet. A dielectric barrier and a hard ferromagnet contact are fabricated using conventional top-down processes. The TBiCs top and bottom surfaces are left to oxidize in air at or above room temperature before the ferromagnets-NMs contacts are fabricated. We anticipate the interfacial oxides will facilitate spin injection from the ferromagnetic layers into SDs by direct tunneling. Structural characterization of the fabricated devices includes cross-sectional and plan-view transmission electron microscopy (TEM) to analyze the chemical and physical structure of the inter-faces and verify the occurrence of the SDs, respectively.

4:50pm PCSI-WeA3-41 Orbital Hall Effect and Orbitronics in Magnetic Multilayers, *I. Lyalin, Y. Zhu, Roland Kawakami,* The Ohio State University

Orbitronics is an emerging field based on orbital currents, or the flow of orbital angular momentum, just as spintronics is based on spin currents. Analogous to the spin Hall effect (SHE) where a charge current produces a transverse spin current, an orbital Hall effect (OHE) can generate a transverse orbital current. Recently, magneto-optical measurements detected orbital accumulation at the surfaces of Ti [1] and Cr [2], providing the most direct evidence for the OHE. Currently, many of the basic properties of orbital currents are being established. Here, we report results on (1) the generation of torques on a magnetic layer from orbital currents and (2) the transparency of interfaces to orbital currents.

In the first study, we utilize magneto-optic Kerr effect (MOKE) to measure the orbital torque generated by an in-plane charge current in Cr/Fe bilayers. In the Cr layer, the charge current is converted to a transverse orbital current via OHE. After the orbital current enters the Fe layer, it is converted to a spin current by spin-orbit coupling, which in turn imparts a torque on the Fe magnetization through the exchange interaction. We call this the

"orbital torque." Interestingly, the orbital torque increases with the Fe thickness, which suggests that the orbital current is able to penetrate deeply into the Fe layer. Repeating the study on Pt/Fe bilayers where both spin currents and orbital currents are present, the Fe thickness dependence suggests that the torque from spin current is more interfacial in nature while the orbital torque is more bulk-like within the Fe layer.

In the second study [3], we utilize MOKE to investigate the transparency of orbital currents across interfaces. In Cr/X/Ni trilayers, where layer X is varied across the periodic table, we quantify the effect that the X layer has on the orbital torque on the Ni layer. Figure 1 shows the orbital torque efficiency in Cr/X/Ni. Comparing to the value without the X layer gives the transmission of orbital current across the X layer. Similar experiments on Pt/X/Ni investigate the transmission of spin current across the X layer. Comparing the results for Cr/X/Ni and Pt/X/Ni indicates that the transparency of orbital currents is similar to or greater than the transparency of spin currents for several X layers.

[1] Y. -G. Choi et al., Nature 619, 52 (2023).

[2] I. Lyalin et al., Phys. Rev. Lett. 131, 156702 (2023).

[3] I. Lyalin and R. K. Kawakami, Phys. Rev. B 110, 104418 (2024).

PCSI
Room Keahou I - Session PCSI-WeA4

2D Materials and Graphene II
Moderator: Scott Crooker, Los Alamos National Laboratory

4:55pm **PCSI-WeA4-42 UPGRADED: Topotaxy in 2D Materials: Towards Synthesis of Novel 2D Materials by Surface Reactions**, *Matthias Batzill*, University of South Florida
Topotaxy is a surface reaction of deposited elements with a substrate, during which the substrate retains some structural characteristics. Such newly formed materials thus have a crystallographic relationship with the original substrate. For 2D materials, surface reactions with single molecular layers may enable their transformation into new 2D crystals. Here the potential for making new 2D materials by topotactical reactions of transition metal dichalcogenides (TMDs) with transition metals are investigated. Three distinct examples are discussed: (i) the transformation of $PtTe_2$ into Pt_2Te_2 by reaction with Pt atoms; (ii) the reaction of Cr or Mn with bilayer VSe_2 to form $VSe_2/Mn(Cr)/VSe_2$, and (iii) reaction of $MoTe_2$ with Mo to create mirror twin grain boundaries that may self-organize in periodic lattice networks (Figure (c)). The common concept in these surface reactions is that the reacted metals occupy ad- or ab-sorption sites which maintain a low energy van der Waals termination and thus enables the creation of new (meta) stable 2D materials. The three examples discussed here, illustrate the diversity of possible reaction products and the potential for synthesizing novel 2D materials by topotaxy.

5:15pm **PCSI-WeA4-46 Thickness Calculation of HBN and Graphene Using RGB Colors**, *Gabriel Ruiz*, New Mexico State University; *B. Xie*, University of California Santa Barbara
The main objective of our research is primarily due to the required scientific exploration in the properties of a two-dimensional material called graphene. In order to achieve our goals, we want to induce a flat band graphene in order to maintain a nice platform that allows study of correlating physics. When graphene is combined with other materials in van der Waals heterostructures, we can electronically tune its band flatness. When achieved, electron kinetic energy decreases. This allows us to observe and study various correlation phenomena. Using Van der Waals heterostructures as a methodology for the measurement and alteration of graphene requires atomically homogeneous material to build it. The homogeneity of these materials plays an important role when using them to build our heterostructures.

We normally obtain them through mechanical exfoliation then search for them under a microscope. However, it is complicated to characterize the exact thickness of these materials optically. With this problem we looked for a solution by creating a program code. We seek to indicate through saturation comparisons between the different layers of hexagonal boron nitride (HBN) which serves as a dielectric material required for the composition of the heterostructure and Graphene. The code has been polished and altered to generate more efficiency towards the search for homogenous 2D materials. This project will significantly improve the efficiency for us to search for better flakes. Eventually leading to a higher device quality and potential observation of novel physics phenomena.

5:20pm **PCSI-WeA4-47 Optoelectronic Properties of MoS2/Graphene Heterostructures Prepared by Dry Transfer Method for Light-induced Energy Harvesting Applications**, *Sanju Gupta*, Penn State University and Gdansk University of technology
Optoelectronic properties of atomic thin van der Waals heterostructures (vdWHs) comprising transition metal dichalcogenides that harvest light energy are of paramount interest. In this work, the effects of underlying single and bi-layer graphene (Gr) layers on structural and physical properties of MoS_2/Gr vertical heterostructures *i.e.,* (1-2L) MoS_2/(1-2L) Gr, besides additional interfaces including MoS_2 folds/edges [$MoS_2(1L+1L)$)/Gr(1L)] and $MoS_2(1-2L)$/Au, are investigated to unravel the excitonic properties. By employing correlative scanning probe microscopy combined with micro-spectroscopy, we observed multiple effects related to excitons (*i.e.,* redshifted neutral exciton, ratio of charged exciton or trion to neutral exciton population, and long-tailed trions) and surface electronic properties (*i.e.,* reduced work function suggesting electron transfer) in addition to significantly enhanced near-field Raman spectra, apparent n-p type current rectification behavior and increase in photo-generated carriers. These experimental findings are attributed to interlayer electronic interactions while minimizing Fermi level pinning at MoS_2/Au interface, commonly observed in 2D semiconductor-3D metal junction, and corroborated with theoretical DFT calculations, which deepened our understanding of dissimilar 2D materials junctions. Integrating MoS_2 with optimal number of graphene layers as 'nanospacer' signified substrate engineering that are versatile for key optoelectronic and photovoltaic applications [1, 2, 3, 4].

[1] Gupta S., Johnston A., Khondaker, A., Optoelectronic properties of MoS_2/graphene heterostructures prepared by dry transfer method for light-induced energy applications, *J. Electron. Mater.* 51 (2022) 4257.

[2] Gupta, S., Johnston, A., Khondaker, S., Correlated KPFM and TERS imaging to elucidate defect-induced inhomogeneities in oxygen plasma treated 2D MoS_2 nanosheets, *J. Appl. Phys.* 131 (2022) 164303.

[3] Gupta S., Dimakis N., First-Principles Calculations Integrated with Experimental Optical and Electronic Properties for MoS_2/Au and MoS_2/Graphene/Au Heterostructures, Appl. Surf. Sci. 623 (2023) 156948.

[2] Gupta *et al.,* Appl. Surf. Sci. **623**, 156948 (2023).

5:25pm **PCSI-WeA4-48 The Case of the Missing Sulfur**, *M. Fawzy,* Dept. of Physics, Simon Fraser University, Canada*; M. Mohammadzadehb, A. Abnavi, T. de Silva, R. Ahmadi, H. Ghanbari, F. Kabir, A. Hasani, M. Adachi,* School of Engineering Science, Simon Fraser University, Canada*; Karen Kavanagh,* Dept. of Physics, Simon Fraser University, Canada

M. Fawzy[a], M. Reza Mohammadzadeh[b], A. Abnavi[b], T. de Silva[b], R. Ahmadi,[b], H. Ghanbari,[b], F. Kabir[b], A. Hasani[b], M. M. Adachi[b] and K. L. Kavanagh[a]

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A common strategy for obtaining an ohmic contact to any semiconductor is to form a tunnel junction using a heavily doped surface layer. Independent of the magnitude of the interfacial barrier, the narrow width of the depletion layer allows for efficient tunneling and a linear current-voltage transport. This has worked well for classical bulk devices where transport is through a thick crystal. The low resistance ohmic contact can be a large area, placed for example at the bottom of a wafer. For two-dimensional semiconductors, such as MoS_2, the transport of interest is typically parallel to the surface meaning lateral contacts are required. However, if the semiconductor is an exfoliated triangular flake, parallel contacts become naturally asymmetric in area once the metal is evaporated and patterned on top. It was also soon noticed by a few groups that different area contacts resulted in rectification (10^5 decades), even when the same metal was used, with the *smaller* area contact having the lower resistance ohmic transport. In particular, the application of different area reactive Cr/Au contacts on (20-60) nm thick exfoliated MoS_2 flakes has been an effective method to fabricate a two terminal diode that has been applied towards optoelectronics and biosensing applications [1-2].

The latest example from our collaboration is the sensing of volatile gases using a UV optically powered asymmetric MoS_2 diode [3]. Shown in the figure is a schematic diagram of the device (55 nm thick MoS_2) with a set of I-V characteristics as a function of UV power. This presentation will discuss the likely mechanisms as a function of metal thickness, contact edge lengths, and MoS_2 source and thickness. Topics such as Fermi level pinning, sulfur reaction and diffusion, and buried depletion regions might be discussed.

Corresponding author: kavanagh@sfu.ca

[1] Flexible High-Performance Photovoltaic Devices based on 2D MoS_2 Diodes with Geometrically Asymmetric Contact Areas, Amin Abnavi, Michael M. Adachi, et al. *Adv. Funct. Mater.* **33** (2022) 2210619.

[2] Ultrasensitive rapid cytokine sensors based on asymmetric geometry two-dimensional MoS_2 diodes, Thushani de Silva, Mirette Fawzy, et al., *Nature Comm.* **13**, 7593 (2022).

[3] A Photovoltaic Self-Powered Volatile Organic Compounds Sensor Based on Asymmetric Geometry 2D MoS_2 Diodes, Mirette Fawzy, MR Mohammadzadeh, et al. *ECS Sensors Plus,* in press (2024).

5:30pm PCSI-WeA4-49 Formation of Twin-Free Single Phase β-in$_2$Se$_3$ Layers via Selenium Diffusion Into InP(111)B Substrate, *Kaushini Wickramasinghe, C. Forrester,* City College of New York, City University of New York*; M. McCartney, D. Smith,* Arizona State University*; M. Tamargo,* City College of New York, City University of New York

Indium selenide, In_2Se_3, has recently attracted growing interest due to its remarkable properties, including room temperature ferroelectricity, outstanding photoresponsivity, and exotic in-plane ferroelectricity, which open up new regimes for next generation electronics [1, 2]. In_2Se_3 also provides the important advantage of tuning the electrical properties of ultra-thin layers with an external electrical and magnetic field, making it a potential platform to study novel two-dimensional physics [3]. Yet, In_2Se_3 has many different polymorphs [4], and it has been challenging to synthesize single-phase material, especially using scalable growth methods, as needed for technological applications. We recently reported the growth of twin-free ultra-thin layers of In_2Se_3 prepared by a diffusion driven molecular beam epitaxy approach, and twin-free Bi_2Se_3 layers grown on these unique virtual substrates [5].

In this study, we use aberration-corrected scanning transmission electron microscopy (STEM) to characterize the microstructure of these materials. We emphasize features of the In_2Se_3 layer and In_2Se_3/InPinterface which provide evidence for understanding the growth mechanism that leads to the twin-free and single-phase In_2Se_3. Here we show that high quality In_2Se_3 and Bi_2Se_3 crystalline layers that are fully twin-free and largely free of defects, can be achieved using InP(111)B substrates. STEM observations also show that the sample consists primarily of single phase β-In_2Se_3. Close observation of the InP/In_2Se_3 interface provides evidence for a mechanism in which Se first displaces P in the zinc blende InP, followed by a crystal structure transformation to the rhombohedral In_2Se_3 structure. This result implies that In atoms are not mobile during the transformation, thus resulting in twin-free In_2Se_3. This mechanism for the In_2Se_3 formation also explains the resulting pure β-phase In_2Se_3. Understanding and controlling the mechanism of single-phase In_2Se_3 formation enables application of this approach to other heteroepitaxial structures involving layered, vdW materials on 3D crystalline substrates.

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[2] C. Xie, C. Mak, X. Tao, F. Yan, Adv. Func. Mater. **27**, 1603886(2017)

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[4] N. Balakrishnan, E. D. Steer, E. F. Smith, Z. R. Kudrynskyi, Z. D. Kovalyuk, L. Eaves, A. Patanè, P. H. Beton, 2D Mater. **5**, 035026(2018)

[5] K. S. Wickramasinghe, C. Forrester, M. C. Tamargo. Crystals. **13**, 677(2023)

5:35pm PCSI-WeA4-50 Interface-Induced and Tunable Electron-Phonon Scattering in Hexagonal Boron Nitride, *Håkon Røst,* University of Bergen, Norway*; A. Skarpeid, S. Cooil,* University of Oslo, Norway*; A. Åsland,* Norwegian University of Science and Technology (NTNU), Norway*; A. Generalov, A. Preobrajenski, C. Polley, T. Balasubramanian,* MAX IV Laboratory, Sweden*; J. Wells,* University of Oslo, Norway

Over the last decade, the layered compound hexagonal boron nitride (hBN) has received significant attention due to its compatibility with most low-dimensional van der Waals (vdW) materials [1]. It resembles graphene both in lateral size, crystalline structure, and Debye frequency, but due to its dissimilar sub-lattices, it hosts a wide energy band gap separating the valence and conduction bands [2]. Recently, hBN was predicted to host strong electron-phonon coupling (EPC) in its electronic π- and σ-bands [3], reminiscent of the interactions that have been reported (and debated) from the σ-bands of graphene [4]. More recently [5], we verified this EPC from energy renormalizations – or "kinks", in the hBN bandstructure.

We will discuss the observable EPC in mono- and multilayer hBN, showcasing how the coupling changes with the substrate interaction, the number of stacked hBN layers, and the intercalation of adatoms (see Figure 1). We will also discuss the generality of EPC at large binding energies and its potential presence in other materials with finite electronic band gaps.

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[2] J. Robertson, *Phys. Rev. B* **29**, p. 2131 (1984).

[3] E. Thingstad et al., *Phys. Rev. B* **101**, p. 214513 (2020).

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[5] H. I. Røst et al., *Nano Lett.* **23**, pp. 7539-7545 (2023).

5:40pm PCSI-WeA4-51 Investigating Modulation of Coulomb Interaction in Graphene on a High-k Dielectric, *Rubi Km,* Los Alamos National Laboratory*; J. Hu,* National University of Singapore*; M. Bal,* Radboud University Nijmegen, Netherlands*; M. Chan,* Los Alamos National Laboratory*; A. Ariando,* National University of Singapore*; U. Zeitler,* Radboud University Nijmegen, Netherlands*; N. Harrison,* Los Alamos National Laboratory

Graphene on $SrTiO_3$ (STO) exhibits interesting quantum phenomena, such as quantum Hall ferromagnetism [1] and charge-density-wave order [2]. These effects are believed to stem from the large dielectric permittivity of STO [1,2,3,4], which is expected to significantly screen Coulomb interactions in graphene. However, angle-resolved photoemission spectroscopy (ARPES) measurements reveal that the Fermi velocity of carriers in graphene on STO is comparable to that of graphene on conventional substrates SiO_2 and hBN [5], suggesting minimal screening of Coulomb interactions.

To further investigate the electronic band properties and resolve the question of interaction screening in graphene on STO, we conducted electrical transport measurements in high magnetic fields up to 60 T, across a broad temperature range of 1.5–300 K. In this talk, we will present findings inferred from the quantum Hall effect and quantum oscillations results on graphene/STO devices (Fig 1). Our detailed analysis of the back-gate and temperature dependence of these phenomena indicates a strong effect of the STO substrate on the Fermi energy of graphene, but not on its Fermi velocity.

5:45pm PCSI-WeA4-52 MBE Growth of Transition Metal Dichalcogenides, *Matthew Swann, Z. Li,* The Ohio State University*; C. Helton,* Columbus State Community College*; R. Kawakami,* The Ohio State University

3D materials such as silicon have been the workhorse of the semiconductor industry for decades. However, as transistor technology approaches nanoscale, the performance of these materials is seriously impacted by short-channel effects. In contrast, 2D van der Waals materials hold several distinct advantages, including relative immunity from short-channel effects and a lack of dangling bonds. Monolayer transition metal dichalcogenides (TMDs) have been shown to exhibit modest and direct bandgaps, making them ideal semiconductors. Field effect transistors (FETs) fabricated utilizing exfoliated TMDs have already exhibited high On/Off ratio, small hysteresis and small subthreshold swing, and high mobilities. Exfoliated materials are typically of high quality but aren't scalable. While methods like chemical vapor deposition (CVD) can grow these materials to scale more economically, molecular beam epitaxy (MBE) can deposit large-area films with atomically precise thickness, as well as precisely control the composition of deposited films, making it ideal for studying the transport properties of TMDs. While the growth of TMDs on c-sapphire is common in CVD, its use in MBE growth is uncommon due to the large lattice mismatch between TMDs and c-sapphire. Growth on c-sapphire requires temperatures 900°C and higher in ultra-high vacuum in order to make oriented films [1], without which, a randomly oriented polycrystalline film is obtained. [2,3] Our films are grown with precise thickness control, are highly crystalline, and uniform. The aggressive heating that is required to obtain oriented films causes chalcogenide vacancies to accumulate in the film, which has been demonstrated with annealing temperatures as low as 600°C. The accumulation of these vacancies lead to increased scattering of charge carriers and shorter exciton lifetimes. We will discuss the optical and transport properties of the films.

[1] M. Nakano, Y. Wang, Y. Kashiwabara, H. Matsuoka, and Y. Iwasa, Layer-by-Layer Epitaxial Growth of Scalable WSe2 on Sapphire by Molecular Beam Epitaxy, Nano Lett. **17**, 5595 (2017).

[2] M. T. Dau et al., Millimeter-scale layered MoSe2 grown on sapphire and evidence for negative magnetoresistance, Applied Physics Letters **110**, 011909 (2017).

[3] A. Roy, H. C. P. Movva, B. Satpati, K. Kim, R. Dey, A. Rai, T. Pramanik, S. Guchhait, E. Tutuc, and S. K. Banerjee, Structural and Electrical Properties of MoTe2 and MoSe2 Grown by Molecular Beam Epitaxy, ACS Appl. Mater. Interfaces **8**, 7396 (2016).

5:50pm **PCSI-WeA4-53 Improvement of HfO₂ on TMDCs using Thermal Expansion Coefficient difference with Substrate**, *Sukheyon Eom, J. Park,* Sungkyunkwan University (SKKU), Republic of Korea

Recently, two-dimensional Transition Metal Dichalcogenide (TMDCs), such as MoS_2, have gained attention as next-generation semiconductor materials. However, due to the nature of these 2D materials, which lack dangling bonds that form interlayer bonds, it is challenging to form gate oxide materials like high-k materials. To address this, methods such as plasma or functional group treatment for surface modification of 2D materials and the use of interlayer materials like h-BN have been attempted. However, surface treatment methods can cause damage to the MoS_2 surface, leading to performance degradation, and interlayer materials like h-BN are mostly low-k, requiring very thin EOT formation, which introduces other side effects.

In order to overcome these challenges, methods for directly forming high-k materials via Atomic Layer Deposition (ALD) have been explored. The representative method is the CVD-ALD Mode approach using physical adsorption as a seed due to the low binding energy of 2D materials. While materials like HZO and Al_2O_3 have been successfully deposited using this method, bulkier materials like HfO_2 tend to form islands and pinholes, resulting in non-uniform growth.

To achieve uniform HfO_2 on MoS_2, PMMA is used as substrate material which induce strain by thermal expansion coefficient differences. The thermal expansion coefficients of MoS_2 and SiO_2 are generally known to be 7.0×10^{-6} /K and 0.5×10^{-6} /K, respectively. The difference in the thermal expansion coefficients between these two materials is 6.5×10^{-6} /K. In contrast, the thermal expansion coefficient of PMMA is around 7.5×10^{-5} /K, indicating a difference of 6.8×10^{-5} /K with MoS_2, which is more than 10 times higher. Therefore, it is expected that the strain induced by the difference in the thermal expansion coefficient with PMMA will be higher compared to that with a Si substrate. As we expected, uniform HfO_2 is formed on MoS_2 (Fig 1). This method is expected to be utilized in next-generation semiconductor devices structure as it does not damage the channel.

PCSI

Room Keahou I - Session PCSI-ThM1

Topological Materials

Moderator: Sven Rogge, University of New South Wales, Australia

8:30am **PCSI-ThM1-1 Chirality, Spin and Orbital in Dna-Type Chiral Materials**, *Binghai Yan,* Pennsylvania State University   **INVITED**
In chemistry and biochemistry, chirality represents the structural asymmetry characterized by non-superimposable mirror images for a material like DNA. In physics, however, chirality commonly refers to the spin-momentum locking of a particle or quasiparticle in the momentum space. While seemingly unrelated characters in different fields, the structural chirality leads to the electronic chirality featured by the orbital-momentum locking encoded in the wavefunction of chiral molecules or solids, i.e. the chirality information transfers from the atomic geometry to the electronic orbital. The electronic chirality provides deep insights into the chirality-induced spin selectivity (CISS), in which electrons exhibit salient spin polarization after going through a chiral material. I will introduce the most recent experimental progress and understanding on chirality-driven spintronics, optoelectronics, and their implications in biochemistry.

9:10am **PCSI-ThM1-9 Distinguishing Surface and Bulk Electromagnetism via Their Dynamics in an Intrinsic Magnetic Topological Insulator**, *Khanh Duy Nguyen,* W. Lee, University of Chicago; *J. Dang, T. Woo,* University of Florida; *G. Berruto, C. Yan, C. Ip, H. Lin, Q. Gao,* University of Chicago; *S. Lee,* Penn State University; *B. Yan,* Weizmann Institute of Science, Israel; *C. Liu, Z. Mao,* Penn State University; *X. Zhang,* University of Florida; *S. Yang,* University of Chicago
Bringing magnetism to the itinerant electronic states on the surface of three-dimensional (3D) topological insulators (TIs) is foundational to a variety of low-dimensional topological orders [1, 2]. The magnetism in 3D TIs can be established via various mechanisms. However, the unconventional Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction on the material surface is required for the time-reversal (T) symmetry breaking on the topological surface states (TSSs) in magnetic TIs (MTIs)[3]. This mechanism has been predicted to enhance the surface magnetism of 3D MTIs, where the itinerant Dirac fermions with vanishing Fermi momenta strongly favor ferromagnetic coupling [4]. Thus, the 2D RKKY interaction fundamentally determines the size of the T-symmetry–broken energy gap, and, consequently, the operating temperatures of low-dimensional topological orders, such as the quantum anomalous Hall effect.

Here, we combine time- and angle-resolved photoemission spectroscopy (trARPES) and time-resolved magneto-optical Kerr effect (trMOKE) to reveal this distinct mechanism contributing to the surface magnetism in $MnBi_2Te_4$(MBT): A quasi-2D state mediates the surface 2D RKKY interaction via p-d coupling on the top MBT layer, Fig. 1(a). While trARPES resolves the dynamics of the exchange gap in the q-2DS with meV-scale precisions, Fig. 1(b), trMOKE observes the evolution of the magnetization. We construct a 2D RKKY model involving localized Mn $3d$ moments and itinerant p electrons, which accounts for the rapid dynamics of the magnetization and the exchange gap. Furthermore, it can reconcile several open problems in MBT. These include the vanishing gap at the Dirac point of the TSSs [5] and the nonzero residual magnetization in even-layer MBT flakes [6]. Our work highlights the special magnetic interactions on the surface of MBT and establishes the physics foundation for effective ultrafast manipulation of magnetism in tandem with topological orders.

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[4] J. Wang, B. Lian, S.-C. Zhang, *Phys. Scr.* **T164**, 014003 (2015)
[5] C. Yan et al., *Phys. Rev. B* **104**, l041102 (2021)
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9:15am **PCSI-ThM1-10 Infrared Absorption of α-Sn**, *Jaden R. Love,* C. Armenta, A. Moses, S. Zollner, New Mexico State University; *A. Engel,* University of California Santa Barbara; *C. Palmstrom,* University of California at Santa Barbara
Alpha-tin (α-Sn) is a zero-bandgap semiconductor with an inverted s-antibonding electron band. We discuss the presence of a strong E_0 peak in the extinction coefficient appearing at 0.41 eV in infrared spectroscopic ellipsometry measurements. We also discuss the changes seen in the dielectric function at low temperatures. The E_0 peak is attributed to allowed interband transitions from the Γ_7^- VB ("electron") to the Γ_8^{+v} heavy hole VB or the Γ_8^{+c} light "hole" CB [1].

Previous mid-IR ellipsometry measurements of α-Sn grown pseudomorphically by molecular beam epitaxy on InSb or CdTe have a room temperature dielectric function with an E_0 peak at 0.41 eV. The strength of the E_0 peak is affected by hole doping of the α-Sn layer. Unintentional doping with In from the substrate layers were influenced by variations in substrate surface preparation or by growing on a different substrate (CdTe). The effects are noticeable at low temperatures. The E_0 peak for α-Sn grown on InSb demonstrated temperature invariance for both the amplitude and energy while the E_0 peak amplitude forα-Sn grown on CdTe diminishes with decreasing temperature [1].

An MBE was used to grow new 30 nm α-Sn layers on InSb (001) substrate terminated with Sb [2]. By terminating the surface with Sb the amount of background In doping is reduced, therefore limiting the allowed transitions between bands. This limitation leads to a reduction in the peak amplitude at low temperatures. Temperature dependent ellipsometry spectra were taken from 5K – 295K and show that the E_0 peak is larger at high temperatures for α-Sn layers with reduced doping.

This work was supported in part by: AFOSR (FA9550-24-1-0061), ARO (W911NF-22-2-0130), NSF (DMR-2423992), and SCALE-RH (W52P1J-22-9-3009).

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9:20am **PCSI-ThM1-11 Coulomb Disorder in Cd_3As_2 Thin Films**, *Ian Leahy,* A. Rice, J. Nelson, National Renewable Energy Laboratory; *H. Ness,* King's College London, UK; *M. van Schilfgaarde, K. Alberi,* National Renewable Energy Laboratory
Efforts to move topological semimetals (TSMs) toward applications requires understanding of defects and disorder in thin film analogues. Coulomb disorder has important consequences for the properties of topological semimetals (TSMs) [1, 2]. In TSMs, Coulomb disorder is introduced through the presence of charged native defects which become screened contingent on the Fermi energy (E_F) or carrier density (n). The resulting disorder potential is characterized by an average magnitude eV_0 and correlation length ξ. In the limit of weak disorder, when $eV_0 < E_F$, nonsaturating linear magnetoresistance can emerge in many TSMs – generated from scattering from the disorder potential. In Cd_3As_2, we have demonstrated the link between this linear magnetoresistance and the disorder potential [3,4]. Here, we utilize a series of (001)-Cd_3As_2 bulk-like thin films (gapless bulk) to study the effects of Coulomb disorder on the electrical transport for a range of carrier densities. The ultralow carrier densities we obtain have two main effects on the Coulomb disorder: i) the magnitude of the disorder potential increases as screening is reduced and ii) the Fermi energy is reduced, becoming more comparable to eV_0. The combination of these effects serves to move Cd_3As_2 into a strong Coulomb disorder regime with decreasing carrier density ($E_F \sim eV_0$), as shown in Figure 1. The solid black line is calculated for Cd_3As_2 using Ref. 1 and circles are placed in line with sample carrier densities. As eV_0/E_F increases, we find a striking crossover in the magnetic field dependence of the resistivity from linear to quadratic. We connect this change in magnetoresistance to strong Coulomb disorder scattering [5,6].

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9:25am **PCSI-ThM1-12 Gate-Tunable Ferromagnetism in Epitaxially Grown Semimetal-Ferromagnetic Semiconductor Heterostructures**, *Emma Steinebronn,* S. Islam, Penn State University; *A. Grutter, C. Jensen, J. Borchers,* NIST; *W. Yanez-Parreno,* Penn State University; *S. Ghosh,* University of Minnesota; *J. Chamorro, T. McQueen,* Johns Hopkins University; *C. Liu,* Penn State University; *A. Mkhoyan,* University of Minnesota; *N. Samarth,* Penn State University
The coexistence of time-reversal and inversion symmetry in Dirac semimetals (DSMs) is responsible for topologically protected, spin-

degenerate bulk states with Dirac dispersion. Breaking either of these symmetries results in a Weyl semimetal with broken Kramers degeneracy [1]. We explore this concept by using molecular beam epitaxy to interface a canonical DSM, Cd_3As_2, with a ferromagnetic semiconductor, $In_{1-x}Mn_xAs$, with perpendicular magnetic anisotropy (Fig 1 (a), (b)) [2]. Measurements of the anomalous Hall effect (AHE) in top-gated $Cd_3As_2/In_{1-x}Mn_xAs$ devices show that the ferromagnetic Curie temperature is highly gate-tunable (Fig. 1 (c)-(f)). We map out the AHE in these heterostructures as a function of sample structure and chemical potential.To gain additional insights into the exchange interactions at the heterointerface, we carry out polarized neutron reflectometry (PNR) measurements down to cryogenic temperatures. Preliminary analysis of the PNR data indicates a complex magnetic profile, with potential for a net magnetization within the Cd_3As_2. Work supported by NSF-DMR-2407130 and No. DGE1255832.

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9:30am PCSI-ThM1-13 Growth of Cd₃As₂ on GaAs(110) Substrates, *Anthony Rice, I. Leahy, A. Norman, K. Alberi,* National Renewable Energy Laboratory

Cd_3As_2, a prototypical Dirac Semi-metal, provides an excellent platform for studying physics of topological materials. With a single band crossing that is well isolated from trivial bands and is near the intrinsic Ferm level, straightforward methods such as electrical measurements are viable options for studying these states in this material. Additionally, thin film growth methods have been extremely successful, including growth on III-V and II-VI substrates in [112] and [001] orientations. No effort to date has been reported on attempts at [110] oriented films, which could place the c-axis in-plane, allowing for measurements along it via lateral electrical measurements, and also introduce a new orientation for measurements such as ARPES to probe.

Here, Cd_3As_2 films are grown with MBE on GaAs[110] substrates using similar II-VI buffer structures as other reports on [111] and [001] oriented GaAs substrates. A thin layer of Zn_3As_2 is inserted between III-V and II-VI layers to remove tilting of layers which was observed in X-ray diffraction. Unlike previous efforts [1], no substrate miscut or lattice-matched layers are required to obtain mobilities above 10,000 cm^2/V-s. While out of plane lattice constants are consistent with [110] oriented films, transmission electron microscopy reveal 2 domains of c-axis orientation, consistent with either a-axis orienting in-plane. Despite these domains, no difference is observed in electron mobility parallel or perpendicular to these domains, however a large difference in the fractional magnetoresistance is observed. This difference can be explained by differences in defect spacings along these directions and using the guiding center of diffusion model. Possible routes toward single domain films will also be discussed.

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[1] A. D. Rice, K. Park, E. T. Hughes, K. Mukherjee, and K. Alberi. Phys. Rev. Materials 3, 121201(R)

PCSI

Room Keahou I - Session PCSI-ThM2

Oxide Semiconductor Materials II

Moderator: Erwin Kessels, Eindhoven University of Technology

10:00am PCSI-ThM2-19 Opportunities and Challenges of Complex Oxide Membranes, *Bharat Jalan,* University of Minnesota, USA   **INVITED**
In this presentation, I will discuss the challenges involved in synthesizing three-dimensional (3D) perovskite nanomembranes and the innovative approaches our group has developed to overcome these obstacles. Utilizing hybrid molecular beam epitaxy (MBE) with a metal-organic precursor, titanium isopropoxide, we successfully grew epitaxial $SrTiO_3$ (STO) and $BaTiO_3$ (BTO) films directly on graphene layers that were transferred onto bulk STO substrates. These films were then exfoliated and transferred onto various other substrates. Additionally, I will showcase a sacrificial layer method that enables the creation of oxide membranes with a room temperature dielectric constant of approximately 300. The talk will conclude with an exploration of the potential applications of 3D nanomembranes in materials physics and device engineering.

10:40am PCSI-ThM2-27 UPGRADED: The Thermal Decomposition Process of Metalorganic Precursors Used in Hybrid Molecular Beam Epitaxy, *B. Fazlioglu Yalcin,* The Pennsylvania State University*; C. Sanga, I. Erpay,* Istanbul Technical University, Turkey*; D. Yilmaz, A. van Duin,* The Pennsylvania State University*; N. Nayir,* Istanbul Technical University, Turkey*; **Roman Engel-Herbert**,* Paul-Drude Institute for Solid State Electronics, Germany

The hybrid molecular beam epitaxy approach for the growth of oxides – i.e. the co-supply of atomic and molecular species in their elemental and metalorganic form – has allowed accessing a self-regulated growth window for complex oxides thin films with a range of chemistries, including titanates, vanadates, stannates, and ruthenates [1,2]. While it is widely accepted that the favorable growth kinetics is enabled by the volatility of the metalorganic molecules supplied, their thermal decomposition and surface reaction kinetics is complex and far from understood. For example, while it is generally assumed that the thermal decomposition of the widely employed metalorganic molecule titanium(IV)-isopropoxide (TTIP) used for the growth of titanates by hybrid MBE takes place by dissociating C-O bonds via the β-hydride elimination process, alternative reaction pathways, in particular in proximity of solid surface with different chemistries, such as SrO and TiO_2 terminated growth fronts, might be relevant as well.

We present reactive force field molecular dynamics (ReaxFF-MD) and density functional theoretical calculation along with metadynamics simulations to shed light on the reaction kinetics of TTIP at the atomic scale. The initial organic ligand pyrolysis step was found to be spontaneous and occurred primarily by breaking a C-O bond, albeit not always via β-hydride elimination. Bond dissociation in subsequent thermal decomposition stages typically occurred with partial hydronation of the remaining Ti-containing fragment. The complete reaction scheme for the thermal decomposition of TTIP will be presented along with the reaction barriers and thermodynamic driving force for the different bond dissociation events. The computational approach provides a predictive and computationally inexpensive framework to identify chemical reaction pathways relevant to hybrid MBE film growth processes at the atomic scale under realistic, while experimentally relevant conditions.

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