PCSI

Room Canyon/Sugarloaf - Session PCSI-1SuA

2D Heterostructure Design

Moderator: Edward Yu, The University of Texas at Austin

2:35pm **PCSI-1SuA-2 Optical Properties of Semiconducting Moiré Crystals**, *Xiaoqin Elaine Li*, Univ of Texas at Austin **INVITED**
In van der Waals (vdW) heterostructures formed by stacking two monolayers, lattice mismatch or rotational misalignment introduces an in-plane moiré superlattice. The periodic atomic alignment variations between the two layers impose both an energy and optical selection rule modulations as illustrated in Fig. 1A-B. Optical properties of such moiré superlattices have just begun to be investigated experimentally [1-5]. In this talk, I will discuss how the properties of the interlayer excitons in a twisted transition metal dichalcogenide (TMD) heterobilayer are modified by the moiré potential. Specifically, we studied $MoSe_2/Wse_2$ bilayers with small twist angles, where electrons mostly reside in the $MoSe_2$ and holes nominally in the Wse_2 monolayer because of the type-II band alignment. We observe multiple interlayer exciton resonances with either positive or negative circularly polarized emission (Fig. 1C). We attribute these resonances to the ground and excited exciton states confined within the moiré potential. The twist angle dependence, recombination dynamics, and temperature dependence are consistent with this interpretation. These results highlight the versatile and tunable optical properties of semiconducting moiré crystals.

3:15pm **PCSI-1SuA-10 Berryogenesis: Spontaneous Out-of-Equilibrium Plasmonic Magnetism**, *Justin Song*, Nanyang Technological University Singapore, Singapore **INVITED**
Spontaneous symmetry breaking lies at the heart of the description of interacting phases of matter. Here we argue that a driven interacting system subject to a linearly polarized (achiral) driving field can spontaneously magnetize (acquire chirality). In particular, we find when a metal is driven close to its plasmon resonance, it hosts strong internal ac fields that enable Berryogenesis: the spontaneous generation of a self-induced Bloch band Berry flux, which supports and is sustained by a circulating plasmonic motion, even for a linear polarized driving field. This non-equilibrium phase transition occurs above a critical driving amplitude, and depending on system parameters, can enter the spontaneously magnetized state in either a discontinuous or continuous fashion. Berryogenesis relies on nontrivial interband coherences for electronic states near the Fermi energy generated by ac fields readily found in a wide variety of multiband systems. We anticipate that graphene devices, in particular, which can host high quality plasmons, provide a natural and easily available platform to achieve Berryogenesis and spontaneous non-equilibrium (plasmon-mediated) magnetization in present-day devices, e.g., those based on graphene plasmonics. If we have time, we will also discuss other manifestations of non-trivial quantum geometry in Dirac systems.

3:55pm **PCSI-1SuA-18 UPGRADED: Investigation of Graphene/Ge(110) Interface**, *Miriam Galbiati*, Technical University of Denmark, Denmark
Investigating the interfacial properties between graphene and traditional semiconductors is crucial to develop novel electronics [1]. In this framework, the Graphene/Ge(110) has received a great deal of attention over the last couple of years [2–7]. These studies focus on the structure of Graphene/Ge(110) interface and notably on the possible reconstructions of Ge surface as shown by scanning tunnelling microscopy (STM). However, no insights into the electronic properties of this interesting system are today available.

Here, we investigate the evolution of the system´s interface upon annealing in vacuum at different temperatures. We use low-temperature STM to probe the surface structure with atomic precision. At each stage, images at different applied biases are collected and interestingly, graphene becomes transparent at high biases. When growing graphene by chemical vapour deposition, hydrogen that is used during growth passivates the Ge surface, stabilizing the (1x1) phase (i.e., unreconstructed surface) [5]. Annealing the sample at 350°C leads to desorption of hydrogen and STM and low energy electron diffraction (LEED) reveal that the surface of Ge(110) reconstructs into a (6x2) phase, never observed for bare Ge. Upon further annealing above 700°C, STM shows that the Ge surface modifies back into the (1x1) phase. At this point, due to the lack of hydrogen, the (1x1) is stabilized by graphene forming chemical bonds with Ge atoms underneath [2]. Indeed, the Ge surface remains in the (1x1) phase even if further annealing at temperature above 350°C is performed. To gain insights into the electronic properties, we perform angle resolved photoemission spectroscopy (ARPES) after each thermal annealing step. The ARPES data show how graphene's doping changes upon thermal annealing, signature of a different interaction with the Ge substrate.

[1] J. Lee, Science, 344(2014).

[2] J. Tesch, Carbon, 122(2017).

[3] G.P. Campbell, Phys. Rev. Mater., 2(2018).

[4] J. Tesch, Nanoscale, 10(2018).

[5] D. Zhou, J. Phys. Chem. C., 122(2018).

[6] H.W. Kim, J. Phys. Chem. Lett., 9(2018).

[7] B. Kiraly, Appl. Phys. Lett., 113(2018).

PCSI

Room Canyon/Sugarloaf - Session PCSI-2SuA

Epitaxial Growth of Quantum Materials and Structures

Moderator: Seung Sae Hong, Stanford University

4:30pm **PCSI-2SuA-25 UPGRADED: Epitaxial Growth and Electronic Characterization of GdSb**, *Hadass Inbar, S Chatterjee, M Pendharkar, Y Chang, M Bocheff, T Guo, T Brown-Heft,* University of California, Santa Barbara*; A Fedorov,* Lawrence Livermore National Laboratory*; D Read,* Cardiff University*; C Palmstrom,* University of California, Santa Barbara
In recent years, the class of rare-earth monopnictides (RE-Vs) has received renewed interest due to predictions of topological semimetal states[1] and observations of extremely large magnetoresistance (XMR)[2], phenomena holding great promise in novel physics devices and magnetic sensing technologies. The wide range of lattice constants and simple rock salt structure of RE-Vs also allows to easily incorporate them epitaxially with III-V semiconductors. Coupled to III-Vs, RE-Vs have potential applications as buried ohmic contacts, THz emitters and detectors, thermoelectrics, reaction barriers, and plasmonic heterostructures.[3] In the family of RE-Vs, GdSb shares the common features of antiferromagnetic type II ordering and unusually high magneto-resistance.[4] Due to the absence of orbital momentum in the $4f^7$ configuration of Gd^{3+} and the simple magnetic phase diagram, GdSb can serve as a model system for the study of the effect of biaxial strain on band dispersion in RE-Vs, and the interplay between magnetism and XMR.

In this talk, we will demonstrate the first epitaxial growth and characterization of GdSb thin films with thickness varied from 3-30 nm and biaxial strains ranging from -2% to +2% lattice-mismatch. We utilize molecular beam epitaxy to grow GdSb films on $In_{1-x}Al_xSb$ and Be-doped $In_{1-x}Ga_xSb$ buffer layers deposited on undoped and Zn-doped GaSb (001) substrates for magnetotransport and angle-resolved photoemission spectroscopy measurements, respectively. Reflection high-energy electron diffraction patterns observed during growth and *in-situ* X-ray photoelectron spectroscopy and scanning tunneling microscopy (STM) were used to determine the formation of a rock salt phase with the characteristic surface reconstruction of 1X1, indicating the absence of interfacial reactions between the GdSb films and underlying buffer layers. Surface morphology was examined with STM to confirm the growth of continuous films at thicknesses down to 3nm. To determine the in-plane lattice constant and strain of the GdSb thin films we have recorded reciprocal space maps on asymmetric reflections. The thickness dependence in lattice-matched buffers and the effect of biaxial strain on magnetotransport behavior and the bandstructure of GdSb will also be discussed.

[1] Duan, Xu, et al. Commun. Phys. 1 (1) (2018): 71.

[2] Tafti, F. F., et al. Nat. Phys. 12 (3) (2016): 272.

[3] Bomberger, Cory C., et al. JVST B 35 (3) (2017): 030801.

[4] Li, D. X., et al. Phys. Rev. B 54 (15) (1996): 10483.

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4:50pm **PCSI-2SuA-29 MBE Growth of $Zn_xCd_{1-x}Te$ on Cd_3As_2**, *Anthony Rice, K Alberi,* National Renewable Energy Laboratory
The Dirac semimetal Cd_3As_2 has become a scientifically useful material, as it provides access to a variety of interesting phenomena ranging from topological superconductivity to massless Dirac fermions. It is also potentially useful for energy-related applications due to its high electron mobility and large phonon-phonon scattering. While thin film growth has become an increasingly popular route of synthesis, there have been no

reports of epitaxial growth on Cd_3As_2, limiting the ability to develop full heterostructures. One barrier to epitaxy on Cd_3As_2 is the high vapor pressure of Cd_3As_2 (1e-7 mbar at only 135 ° C), which is well below the ideal growth temperature of most semiconductors [1].

The $Zn_xCd_{1-x}Te$ (111) system provides one promising option for overgrowth given that it can be lattice matched to the (112) surface of Cd_3As_2 and has a relatively low optimal growth temperature (240-300° C). Reflective high-energy electron diffraction (RHEED) patterns of epilayers grown on Cd_3As_2 exhibit a (2x1) reconstruction, even with a growth interruption. These patterns are consistent with As-terminated CdTe observed following high temperature annealing under As [2]. CdTe epilayers growth at Cd_3As_2-compatible substrate temperatures (~120° C) are rough, but further growth at 240° C yields smoother surfaces, as seen in atomic force microscopy. X-ray diffraction confirms Cd_3As_2 remains following the higher temperature growth step, suggesting complete coverage is achieved. Higher temperature anneals under As further smooth and passivate this surface, while similar anneals under Te result in disappearance of a RHEED pattern and loss of the Cd_3As_2 layer. Introduction of moderate Zn content into CdTe results in complete surface coverage but also very large features, likely a result of very low Zn adatom mobility at these temperatures. Our results provide a starting point for incorporating Cd_3As_2 into a variety of device structures.

[1] V.J. Lyons and V.J. Silvestri, J. Phys. Chem. **64**, 2266 (1960)

[2] Y. Nakazawa, M. Uchida , S. Nishihaya, S. Sato, A. Nakao, J. Matsuno , and M. Kawasaki, APL Mater. **7**, 071109 (2019)

4:55pm **PCSI-2SuA-30 Interfaces and Growth of NbTiN-AlN Heterostructures on Sapphire as Epitaxial Josephson Junctions**, *Chris Richardson, A Thomas, A Alexander, C Weddle,* Laboratory for Physical Sciences*; B Arey, M Olszta,* PNNL

Plasma assisted Molecular beam epitaxy (PAMBE) is used to grow niobium titanium nitride alloys ($Nb_xTi_{1-x}N$) and wide bandgap nitride (AlN) superconductors directly on c-plane sapphire wafers. This combination of nitride materials provides sufficient degrees of freedom that synthesis of an epitaxial Josephson junction may be possible while satisfying the device requirements for superconducting quantum circuits. Thin films of various $Nb_xTi_{1-x}N$ alloys are grown using the abrupt metamorphic growth paradigm and show the ability to tune the lattice parameters and critical temperatures of the superconducting films. Surface topology, degree of twinning, and superconducting loss are used to evaluate the fitness of these layers.

A prototype NbTiN/AlN/NbTiN (superconductor-insulator-superconductor) Josephson junction structure has been grown. The structural, superconducting, and current-votlage characterization of these heterostructures will be presented.

5:00pm **PCSI-2SuA-31 Growth of AlN Barriers in Al/AlN/Al SIS Josephson Junctions by Low Temperature Atomic Layer Epitaxy**, *Charles R. Eddy, Jr.,* U.S. Naval Research Laboratory*; D Pennachio, J Lee, A McFadden,* University of California, Santa Barbara*; S Rosenberg,* U.S. Naval Research Laboratory*; Y Chang, C Palmstrom,* University of California, Santa Barbara

Superconductor-Insulator-Superconductor (SIS) structures are of increasing interest for the creation of Josephson junctions that can serve as the basis for quantum qubit transmons, which hold significant promise for quantum computing technologies. Traditionally, these devices have been developed using amorphous AlO_x in $Al/AlO_x/Al$ structures and have enabled fundamental demonstrations of transmon performance. However, improved performance may be expected with an epitaxial insulator. Even in these structures, the nature of the superconductor/substrate interface and the superconductor/ambient interface limits coherence and, consequently, qubit performance.

In an effort to address this challenge, we employ low temperature atomic layer epitaxy (ALEp) to grow crystalline AlN insulators on crystalline aluminum films. Smooth epitaxial aluminum films are grown by evaporation on cryogenically-cooled, buffered GaAs(001) substrates [1]. These epitaxial surfaces are "frozen" using a low temperature nitridation atomic layer process (ALP) before the samples are ramped to 300° C for low temperature ALE of AlN using semiconductor grade trimethylaluminum and UHP argon and nitrogen inductively coupled plasmas (ICPs). In this study, we evaluate the structural effects of variations in the initial nitridation ALP, growth conditions of ALEp AlN barriers, and SIS barrier thickness using transmission electron microscopy. We have found that at one end of the spectrum, a simple 5 cycle nitridation ALP of epitaxial aluminum at ~90° C, where each cycle is a 30 second exposure to 300W UHP argon/nitrogen

(200/75 sccm) ICP , consumes a significant fraction of the aluminum to make an amorphous AlN insulator that is roughly 2 nm thick. When this surface is subjected to another low temperature Al evaporation, the top Al films are a mixture of amorphous and polycrystalline. When the same nitridation ALP is employed and followed by 5nm of ALEp AlN growth at 300° C, a similar amount of the aluminum film is consumed and an amorphous ALEp AlN layer results. Finally, when the nitridation ALP is reduced to a single cycle of nitridation, less of the aluminum film is consumed and the 5nm AlN ALEp film shows polycrystallinity with small regions demonstrating sharp, potentially epitaxial interfaces. This result suggests that proper ALP nitridation of the epitaxial aluminum can support epitaxial growth of AlN by ALE. Further studies of the influence of number of cycles, cycle duration, plasma chemistry and plasma power on both the nitridation ALP and AlN ALEp will be presented.

[1] S. Gazibegovic et al., Nature 548, 434 (2017).

Sunday Evening, January 19, 2020

PCSI

Room Canyon/Sugarloaf - Session PSCI-SuE

Single Photon Detectors

Moderator: Christopher Palmstrom, University of California, Santa Barbara

7:30pm **PSCI-SuE-1 Theory of Single Photon Detection by a Photoreceptive Molecule and a Quantum Coherent Spin Center**, *N Harmon,* University of Evansville; *Michael Flatté,* University of Iowa
INVITED

The long spin coherence times in ambient conditions of color centers in solids, such as nitrogen-vacancy (NV−) centers in diamond, make these systems attractive candidates for quantum sensing. Quantum sensing provides remarkable sensitivity at room temperature to very small external perturbations, including magnetic fields, electric fields, and temperature changes. A photoreceptive molecule, such as those involved in vision, changes its charge state or conformation in response to the absorption of a single photon. We show the resulting change in local electric field modifies the properties of a nearby quantum coherent spin center in a detectable fashion. Using the formalism of positive operator values measurements (POVMs), we analyze the photo-excited electric dipole field and, by extension, the arrival of a photon based on a measured readout, using a fluorescence cycle, from the spin center. We determine the jitter time of photon arrival and the probability of measurement errors. We predict that configuring multiple independent spin sensors around the photoreceptive molecule would dramatically suppresses the measurement error[1].

[1] N. J. Harmon and M. E. Flatté, arXiv:1906.01800

8:10pm **PSCI-SuE-9 From Dark Matter Detection to Artificial Intelligence: Uses for Superconducting Nanowire Single Photon Detectors**, *Sae Woo Nam,* National Institute of Standards and Technology, UUSA **INVITED**
Single-photon detectors are an essential tool for a wide range of applications in physics, chemistry, biology, communications, computing, imaging, medicine, and remote sensing. Ideally, a single photon detector generates a measurable signal only when a single photon is absorbed. Furthermore, the ideal detector would have 100% detection efficiency, no false positive (dark counts), and transform-limited timing resolution. Since the first reported detection of a single photon using a superconducting nanowire in 2001[1], steady progress has been made in the development and application of superconducting nanowire single photon detectors (SNSPD or SSPD) with ideal properties. The performance of these detectors is fundamentally related to characterizing and understanding the materials used in these quasi-1D wires that are able to detect photons. I will briefly describe progress in detector developments, use of these detectors in new applications, and opportunities for future work.

PCSI
Room Canyon/Sugarloaf - Session PCSI-1MoM

Oxides
Moderator: Tohru Honda, Kogakuin University

8:30am **PCSI-1MoM-1 MOCVD Epitaxy and Doping for β-Ga₂O₃ and (AlₓGa₁₋ₓ)₂O₃**, *Hongping Zhao,* The Ohio State University **INVITED**
Ultrawide bandgap (UWBG) gallium oxide (Ga_2O_3) represents an emerging semiconductor material with excellent chemical and thermal stability. It has a band gap of 4.5-4.9 eV, much higher than that of the GaN (3.4 eV) and 4H-SiC (3.2 eV). The monoclinic β-phase Ga_2O_3 represents the thermodynamically stable crystal among the known five phases (α, β, γ, d , ε). The breakdown field of β-Ga_2O_3 is estimated to be 6-8 MV/cm, which is much larger than that of the 4H-SiC and GaN. These unique properties make β-Ga_2O_3 a promising candidate for high power electronic device and solar blind photodetector applications. Single crystal β-Ga_2O_3 substrates can be synthesized by scalable and low cost melting based growth techniques. Metalorganic chemical vapor deposition (MOCVD) growth technique was used to develop high quality β-Ga_2O_3 thin films and its ternary alloy (AlₓGa₁₋ₓ)₂O₃. Control of background and n-type doping in β-Ga_2O_3 will be discussed. Record carrier mobilities of 184 cm^2/V·s at room temperature and 4984 cm^2/V·s at low temperature (45 K) were measured for β-Ga_2O_3 thin films with room-temperature doping concentrations of $2.5×10^{16}$ and $2.75×10^{16}$ cm^{-3}, respectively [1]. Growth and fundamental understanding of (AlₓGa₁₋ₓ)₂O₃ are still lacking. The limit of Al incorporation in beta-phase Ga_2O_3 has not been understood or experimentally verified, although it was predicted up to 60% of Al composition could be incorporated into β-Ga_2O_3. N-type doping capability as a function of Al composition in (AlₓGa₁₋ₓ)₂O₃ is another important fundamental question. Carrier transport properties in (AlₓGa₁₋ₓ)₂O₃ will be discussed.

[1] Z. Feng, AFM Bhuiyan, M. R. Karim, H. Zhao, Appl. Phys. Letts, 114, 250601 (2019).

9:10am **PCSI-1MoM-9 Atomic Structure and Electronic Properties of the Non-Polar In₂O₃ and β-Ga₂O₃(100) Surfaces**, *C Schulze, R Zielinski, J Hofmann, C Bruckmann,* Technische Universität Berlin, Germany*; Z Galazka,* Leibniz-Institut für Kristallzüchtung Berlin, Germany*; **Holger Eisele,** Technische Universität Berlin, Germany
In_2O_3 and β-Ga_2O_3 belong to the transparent conducting oxides (TCOs), being promising candidates for a wide field of applications like in solar cells, in detectors, and for high-power devices. In order to achieve high efficiency in electronic and opto-electronic devices a variety of prerequisites are necessary, as e.g., high crystal quality with low defect densities, adjustable conductivity by doping, controllable surfaces and interfaces, etc. Especially the doping mechanisms and the resulting high electron mobility are still under broad discussion for sesquioxide material: Mainly oxygen vacancies are under strong debate about their functionality [1]. We use scanning tunneling microscopy (STM) and spectroscopy (STS) in order to analyze the atomic structure of the non-polar surfaces. Since non-polar surfaces typically show no intrinsic surface states within the fundamental band gap of semiconductor materials, it is furthermore possible to study bulk and doping states using these methods [2].

Both semiconductors, In_2O_3(111) and β-Ga_2O_3(100) show at their respective non-polar surface a 1×1 surface unit cell without reconstruction upon *in situ* cleavage. We found the unreconstructed surface unit cell in the case of In_2O_3(111) in empty state images with atomic resolution. In respective room-temperature STS spectra we can identify the conduction band contribution, the direct and the indirect valence band as well as at least 3 intrinsic states being located within the band gap. Due to the variation of the growth parameter we can assign at least some of these states to charge transfer levels of impurities and vacancies. Since the Fermi level is located within the fundamental band gap, we can exclude an intrinsic electron accumulation for the freshly cleaved surface, while in air aged samples show a strongly different behavior, i.e. metallic appearance as in the case of a surface electron accumulation.

The β-Ga_2O_3(100) surface also shows atomic resolution in empty state images. Even more, we can identify single dopant atoms. In the corresponding STS spectra we can assign the conduction band contribution and again charge transfer levels, originating most likely from vacancies of the three differently coordinated oxygen atom positions within the unit

cell. Even more, we can identify a charge transfer level, which we can assign to Si doping. Due to our findings from differently doped samples we conclude that the conductivity from unintentionally doped β-Ga_2O_3(100) can be assigned to background doping by Si.

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9:15am **PCSI-1MoM-10 Growth and Structures of Metal Dopant-Ceria Mixed Oxide Interfaces**, *E Ginting, L Du, Jing Zhou,* University of Wyoming
Ceria has been widely studied as an oxidation-reduction catalyst due to its unique redox properties and oxygen storage capacity [1]. The addition of other metal elements such as Ti and Mn into ceria could better enhance its thermal stability and improve its redox properties and oxygen storage capacity. To understand the chemistry of doped-ceria mixed oxides, it is of crucial importance to determine their surface structures at the fundamental level. We present our study on the growth of ceria thin films with Ti and Mn dopants and the understanding of their structures using X-ray photoelectron spectroscopy, low-energy electron diffraction, as well as scanning tunneling microscopy. Well-ordered CeO_x(111) with controlled degree of Ce reduction and atomic structures can be prepared on a Ru(0001) single crystal substrate [2]. Metal-doped ceria mixed interfaces were prepared by depositing Ti or Mn over CeO_x(111) thin films. C o-deposition of Ce with metal dopants can produce well-ordered Ce₁₋ₓMₓO₂₋δ(111) mixed oxide films (M=Ti, Mn) [3]. Dopant types and compositions can influence the surface structures, electronic structures, and redox properties of ceria. Effects of Mn and Ti dopants in ceria were investigated for Ni as steam reforming of ethanol catalysts for energy production . Compared to pure ceria, addition of metal dopants in ceria can provide unique anchoring sites and interaction for deposited Ni, which can significantly stabilize Ni as small metal nanoparticles upon heating. Additionally, modified structures and electronic properties of ceria by dopants offer alternative adsorption and reaction sites and provide promotional effects in the resistance of the coke formation over deposited Ni nanoparticles in the adsorption and reaction of ethanol. The research is sponsored by the National Science Foundation (Award Number: CHE1151846).

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[2] Y. H. Zhou, J. M. Perket, A. B. Crooks, J. Zhou, *J. Phys. Chem. Lett.***1, (9)**, 1447-1453 (2010).

[3] Y. H. Zhou, J. Zhou, *J. Phys. Chem. Lett.***1, (11)**, 1714-1720 (2010).

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9:20am **PCSI-1MoM-11 Freestanding Crystalline Oxide Membranes and Heterostructures**, *Seung Sae Hong,* Stanford University **INVITED**
The ability to create and manipulate materials in two-dimensional (2D) form has repeatedly had transformative impact on science and technology. In parallel with the exfoliation and stacking of intrinsically layered crystals, the atomic-scale thin film growth of complex materials has enabled the creation of artificial 2D heterostructures with novel functionality and emergent phenomena, as seen in perovskite oxides. We present a general method to create freestanding complex oxide membranes and heterostructures with millimeter-scale lateral dimensions and nanometer-scale thickness [1]. This facilitates many new opportunities we are beginning to explore, and here we focus on probing the nanomechanical response and the application of extreme strain states [2].

[1] D. Lu, D. J. Baek, S. S. Hong, L. F. Kourkoutis, Y. Hikita, and H. Y. Hwang, Nat. Mater. **15**, 1255 (2016).

[2] S. S. Hong, M. Gu, M. Verma, V. Harbola, B. Y. Wang, D. Lu, A. Vailionis, Y. Hikita, R. Pentcheva, J. M. Rondinelli, and H. Y. Hwang, *in revision*.

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10:00am **PCSI-1MoM-19 Effects of Annealing on Electronic Defects in β-Ga₂O₃ Revealed by Linearly-Polarized Photoluminescence (LPPL)**, *R Sun, Y Ooi, P Ranga,* University of Utah*; M Saleh, K Lynn,* Washington State University*; S Krishnamoorthy, **Mike A. Scarpulla**,* University of Utah
β-Ga_2O_3 is of high interest for high voltage and high-power DC and microwave applications. Annealing in different ambient environments can be used to manipulate the point defect populations as a function of depth, both to understand populations induced by growth processes and then to use this understanding to optimize properties for applications. Here, we report on our studies of electronic defects using unique linearly-polarized photoluminescence (LP-PL). We utilize annealing in different atmospheres to manipulate defects. We find intriguing differences between responses of bulk crystals and epilayers gown on various substrates, elucidating the

unanticipated confounding effects of substrates. We use these comparisons to help to sort out the myriad possible hypotheses for which combinations of defects produce the observed changes. We attempt to unify our results with prior literature and interpretations.

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PCSI
Room Canyon/Sugarloaf - Session PCSI-2MoM

Hybrid Materials
Moderator: Joseph Berry, National Renewable Energy Laboratory

11:00am **PCSI-2MoM-31 Hybrid Perovskite-Based High Energy Photon Detectors**, *Wanyi Nie,* Los Alamos National Laboratory **INVITED**
Radiation spectroscopy is widely needed in security, medical treatment, nuclear material monitoring as well as space science. It quantifies the gamma-ray energies by single radiation photon counting devices. The key is to precisely count gamma-ray photons using highly sensitive detectors. Solid-state detectors employing high density semiconductors to convert gamma-ray photon signal directly into electrical pulses offers promising solution. It outperforms scintillator technologies in count rate and sensitivities with high energy resolutions.

In this talk, I will introduce our recent progress on methylammonium lead halide perovskite single crystal detectors. We show that the single crystal detectors can efficiently count single gamma-ray photon events with electrical pulses. We further investigate the operational principles of the bromide-perovskite solid-state detectors and find using high work function contacts can block out the dark noise from thermally injected electrons and thus allow for efficient pulse collection at higher electrical fields. As a result, we observe strong and reproducible electrical pulses when exposing the detector under several radioactive sources corresponding to gamma-rays at various energies. However, we also discover that the bromide-perovskite detector suffers from voltage instability and slow response which cannot generate reliable energy resolved spectrum. Replacing the bromide by iodide in the crystal, we are able to operate the detector at much higher voltage and deliver sharp electrical pulses at room temperature. By counting the pulses under gamma-ray photons, we constructed the spectrum for ^{137}Cs that clearly shows the expected Compton scatter structure along with signals from photo-electric effect. Our results lay the foundation towards the robust operation of efficient perovskite- detector.

11:40am **PCSI-2MoM-39 Pb-based Metal-Organic Frameworks for Efficient Perovskites Light-emitting Diodes Applications**, *Hsinhan Tsai, W Nie,* Los Alamos National Laboratory
Hybrid perovskites materials have demonstrated an extraordinary potential for clean, sustainable energy technologies and low-cost optoelectronic devices. In spite of the unprecedented progress in photovoltaics over the past decay, perovskites light-emitting diodes (PeLEDs) emergent as one of the most promising light emitters with performances exceeded 20% EQE efficient and low energy consumption devices. One of the key challenges that exists in the field today is the stability and reliability of devices under operation conditions. This vulnerability remains an open question, which might determine the fate of this remarkable material despite excellent properties.

A fundamental requirement for achieving highly efficient light emission and stability operation used in PeLEDs is to design molecular structures that facilitate recombination of the electrically or optically generated electron and hole pair to emit photons. Here, we demonstrate a new type Pb-based metal-organic frameworks (MOFs) perovskites as LED emitter with naturally formed quantum and dielectric confinement, where efficient radiative recombination is expected. We show that the Pb-based MOFs have a PeLEDs performance with over 5% EQE and extended charge localization due to the structure confinement and consequently improved the carrier transport and radiative recombination.

[1] Zhao et al, *Nat. Photonics*, **12**, 783–789 (2018).

[2] Xu et al, *Nat. Photonics*, **13**, 418–424 (2019)

[3] Tsai et al, *Adv.Mater.,***30**, 1704217 (2018).

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11:45am **PCSI-2MoM-40 Arrangement and Electronic Properties of Cobalt Phthalocyanine Molecules on B-Si(111)-√3 × √3 R 30°**, *Susi Lindner, M Franz, M Kubicki, S Appelfeller, M Dähne, H Eisele,* Technische Universität Berlin, Germany
The molecular arrangement and the interfacial electronic properties of cobalt phthaloycyanine (CoPc) on the deactivated B-Si(111)-√3 × √3 R30° surface are analyzed using scanning tunneling microscopy and spectroscopy as well as photoemission studies. Our data demonstrate that for a low coverages of CoPc the molecules lie at with the p_z orbital of the Si surface atom forming a hybrid state with the d_{z2} orbital of the transition metal. This hybridization is observed in an additional contribution to the valence band spectrum. Furthermore, this additional hybridization state is detected in the tunneling spectrum. For higher CoPc coverages, the CoPc molecules are tilted with respect to the Si surface forming highly ordered organic molecular films. The spectroscopic data of the thick film demonstrates that the electronic properties resemble those of pure CoPc.

11:50am **PCSI-2MoM-41 Amino-Acids Detection with Modulation Doped and Surface Nanoengineered GaAs Schottky Diodes**, *T Alkhidir, M Abi Jaoude,* KUST, United Arab Emirates*; D Gater,* University College London, United Kingdom*; C Alpha,* Cornell University*; **Abdel Isakovic**,* Colgate University
Most current techniques for analyzing amino acids require substantial instrumentation and significant sample pre-processing. We designed, fabricated and tested scalable diode-based microdevice that allows for direct sensing and quantification of amino acids. The device is based on modulation doped GaAs heterostructure with a Schottky contact on one side. While relatively high mobility and small dielectric constant of GaAs are naturally helpful in this problem [1][2], we present how etching procedure allows for substantial modification of the surface properties, thereby further boosting the sensing performance. We present data for several qualitatively different amino acids (e.g. belonging to different classes, such as non-polar with aliphatic R-group, polar uncharged R- and charged R-group) with specific examples of Glycine, Cysteine and Histidine, respectively.

The conductance for the GaAs-amino acid interface measured using scanning tunneling microscope (STM) was previously reported to have distinct spectral features [3][4]. In this talk, we show that measuring differential conductance of GaAs diode whose surface is in a direct contact with an amino acid, can still lead to a useful (and easier to obtain) information, previously available only via effective but cumbersome STM and molecular electronics type of approaches. We employ standard multivariate data analysis techniques extract reliably distinct (> 97%) single amino acid specific features. We also present how sensitivity of detection can be achieved within broadly varied pH levels (pH from 4 to 9, so far). Density functional theory (DFT) was used to examine which adsorption processes were likely responsible for surface conductance modification.

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11:55am **PCSI-2MoM-42 Carrier Collection and Transport at Interface of Lead-FreeHalide Perovskites (FA,MA)SnI₃ Solar Cells**, *William Jo,* Ewha Womans University, Republic of Korea
Charge extraction at carrier transport layers adjacent to perovskites is crucial for the optimization of perovskite solar cells. In particular, Sn–perovskites with no lead elements are known to struggle from charge extraction. Here, we report effects of organic ligands like FA and MA (FA = $HC(NH_2)_2^+$; MA = $CH_3NH_3^+$) on charge separation at the interface between electron transport layers and perovskites. TiO_2 mesoporous covering the tin-perovskites show significant changes in electronic structure and built-in potentials according to the ratio of FA to MA. Through a local probe with potential and current mapping, charge transport has been intensively examined. The best cell in this study is obtained as 5.37% at FA : MA = 3 : 1 with only iodine at the halide sites. Even though the value itself is not comparable with lead halides but it could pave a new direction to improve lead-free perovskite solar cells.

PCSI

Room Canyon/Sugarloaf - Session PCSI-1MoA

Catalysis/Nanowires

Moderators: Charles R. Eddy, Jr., U.S. Naval Research Laboratory, Hongping Zhao, The Ohio State University

2:00pm PCSI-1MoA-1 Engineering Active and Stable Semiconductor Photoelectrodes by Atomic Layer Deposition, *Ian Sharp,* Walter Schottky Institut/Technische Universität München, Germany   **INVITED**

The capture of solar energy and its direct conversion to chemical fuel in artificial photosystems provides a promising route to sustainably meet global energy demands and to overcome our current reliance on fossil fuels. However, development of practical photosystems has been impeded by a lack of semiconductor light absorbers that are simultaneously efficient and stable under the reactive conditions required for driving desired chemical transformations. To address this issue, new strategies based on atomic layer deposition (ALD) of conformal corrosion protection layers onto photoelectrode surfaces have recently been developed and yield highly robust systems. Here, we provide an overview of such approaches, discuss outstanding challenges that must be addressed, and highlight a multi-functional water splitting catalyst that is specifically engineered to be interfaced with semiconductor light absorbers. In particular, plasma-enhanced ALD is used to create biphasic cobalt oxide composites that strike a careful balance of necessary chemical, optical, and electrical properties [1]. This coating consists of nanocrystalline Co_3O_4 spinel that is physically robust and provides a stable interface with the chemically sensitive light absorber. This is combined with a chemically labile and disordered $Co(OH)_2$ surface layer that can be easily activated to provide high catalytic activity (Fig. 1). Functional characteristics of the working interface are probed by advanced *in situ* electrochemical X-ray photoelectron spectroscopy, which reveals how the interface transforms from the resting to the active state [2]. Application of the protective catalyst to Si photoanodes results in long-term stable operation with high photochemical activity. These results demonstrate that PE-ALD is a powerful method for synthesizing multi-functional catalysts that support desired chemical transformations, permit efficient interfacial charge transport, and minimize parasitic light absorption due to their conformal nature even at very low thicknesses.

2:40pm PCSI-1MoA-9 Surface States Induced Catalyst-free CO Sensing at GaN and AlGaN/GaN Heterostructures, *Monu Mishra,* Indian Institute of Technology Delhi; *G Gupta,* National Physical Laboratory, India

III-Nitride semiconductors owing unique material properties have proven their potential in the detection of light, chemical, biomolecules and toxic/explosive gases. Despite of numerous advantages *viz.* biocompatibility, high temperature/frequency tolerance and harsh/adverse environmental condition sustainability, the use of expensive catalysts (e.g. platinum) and higher operation temperature for gas sensing (>250ºC) has plagued the development of GaN based cost-effective sensor technology. Upto the best of our knowledge, literature lacks research articles on the development of catalyst-free CO sensors operating at room-temperature using GaN or AlGaN/GaN structures which indicates the necessity of dedicated scientific attention in this area. Therefore, we report the fabrication of nanoflowers-decorated GaN and AlGaN/GaN heterostructure based catalyst-free CO sensors operating at lower (including room) temperature. A set of planar as well as nanostructured GaN & AlGaN/GaN thin films were employed for sensors fabrication which exhibited significant CO sensing associated with its superior surface and interface properties. For in-depth understanding, the obtained results were thoroughly analyzed and correlated to investigate the underlying science/phenomenon which revealed that CO sensing on GaN (and AlGaN/GaN) is governed by the chemical nature of ambient-oxidation induced amorphous oxide (O_2^-, O^{2-} orOH^- species) layer grown on the surface. These surface state act as donor/acceptor states and perturbed the CO adsorption and charge transfer mechanism significantly. Besides, electron accumulation at AlGaN/GaN interface also influenced the critical parameters like schottky barrier height, ideality factor etc. which govern the effective carrier transport and ultimately the device performance. In conclusion, we have observed that the surface and interface states has a strong impact on the efficiency of GaN and AlGaN/GaN based fabricated CO sensors. However, being a first study of its kind, further research is required to explore to uncover the scientific phenomenon and optimization of device performance.

References:

1. M. Mishra, N. K. Bhalla, A. Dash and G. Gupta, Nanostructure GaN and AlGaN/GaN heterostructure for catalyst-free low-temperature CO sensing, Appl. Surf. Sci. 481, 379 (2019).

2:45pm PCSI-1MoA-10 Cu₂O Nanoparticles for Ennhancing Gas Phase Photocatalysis over Metal Oxide Semiconductor Nanostructures, *Hikaru Masegi,* Keio University, Japan

【 Background and Purpose 】 Gas phase photocatalysis over metal oxide (widegap) semiconductor materials has been attracting attention as one of the environmentally friendly technologies such as air purification and clean and renewable energy conversion. In addition, monitoring gas phase photocatalysis is of great use for discussing the basic reaction mechanisms [1]. Since a large part of the metal oxide semiconductor materials are n-type, the development and utilization of p-type materials are quite promising in order to facilitate charge separation and enhance photocatalytic activities via pn-heterojunctions. In this work, we focused on p-type Cu_2O nanoparticles (CNPs) and performed electrochemical fabrication of composites of CNPs and anodized n-type nanotubular arrays such as hematite (α-Fe_2O_3) and TiO_2. Then, the gas phase photocatalysis over the prepared nanocomposites was examined to understand roles of CNPs for the enhanced photocatalytic functions.

【 Experimental 】 As an example, hematite nanotubular arrays (FNTs) were fabricated by anodizing pure iron foils in ethylene glycol containing NH_4F, and crystallized by annealing in oxygen atmosphere. After that, CNPs were deposited onto the anodized samples by pulse electrodeposition in a deposition bath containing $CuSO_4$ and lactic acid. The CNPs were deposited by applying a potential of -0.6 $V_{Ag/AgCl}$ for 0.5 s (on pulse) and 0 $V_{Ag/AgCl}$ for 5 s (off pulse). Then, the H_2 amount from decomposition of gas phase water/methanol mixture was evaluated by gas chromatography.

【Result and Discussion】 CNPs with an average diameter of 200 nm were deposited on the FNT surface with a pore diameter of 20 nm (See Fig.1). As for their photocatalytic properties, the H_2 amount produced with the CNP/FNT sample increased monotonically with longer time of the visible light irradiation (380-800 nm), and the maximal H_2 yield was 0.08 μmol/cm² after 6 hours of visible light irradiation (See Fig.2). In addition, H_2 was not detected either with only FNT or only CNP. H_2 production with the FNT/CNP sample may be attributed to Z-scheme mechanism. Besides, we also confirmed that CNPs can work as cocatalysts for photocatalytic TiO_2 nanotubular arrays.

2:50pm PCSI-1MoA-11 UPGRADED: Self-Selective Formation of 1D and 2D GaBi Structures on GaAs, *Y Liu,* Lund University, Sweden; *S Benter, J Knutsson, S Lehmann,* Lund University; *E Young, N Wilson, C Palmstrom,* University of California, Santa Barbara; *A Mikkelsen, Rainer Timm,* Lund University, Sweden

Bismuth (Bi) incorporation and alloying in III-V semiconductors such as InAsBi and GaAsBi has become a popular topic during recent years, due to a number of promising properties including band gap engineering, a large spin-orbit splitting, and predicted band inversion and topological behavior in the case of high Bi concentrations [1,2]. However, the realization of alloys with high Bi content by epitaxial growth has remained challenging [3].

We follow a different approach and deposit Bi onto the surfaces of GaAs and InAs planar substrates and nanowires (NWs), aiming for a surface layer of high Bi content. We use scanning tunneling microscopy and spectroscopy (STM/S) for systematically studying Bi adsorption and incorporation for different Bi deposition temperatures and post-deposition annealing parameters. Nanowires give us an extra degree of freedom, since they can be grown containing both segments of cubic zincblende (Zb) and of hexagonal wurtzite (Wz) crystal phase, resulting in a variety of surface facets. Previously, we studied the deposition of Sb on GaAs NWs with STM/S and observed a preferential incorporation of Sb atoms into Zb {110} surface facets as compared to {11-20} Wz facets [4].

Here, we observe the incorporation of Bi atoms in the topmost layer of the GaAs surface through group-V exchange, replacing As atoms, upon Bi deposition on GaAs NWs at a temperature of 250°C. The NWs had been cleaned before by annealing in atomic hydrogen, which has been shown previously to remove the native oxide layer [4]. On the NW Zb segments, Bi atoms are scattered at random positions (though generally on As lattice sites), with an increase in density towards step edges of the surface terraces. On the Wz segments, however, the incorporated Bi tends to form one-dimensional GaBi chains and extended two-dimensional GaBi islands along the <0001> edges of surface terraces. A model for the incorporation of Bi through the step edges will be discussed, including differences

observed between {11-20} and {10-10} Wz facets and for different densities of surface steps. Importantly, the ordered 1D and 2D GaBi structures are exclusively found on the Wz segments, which can be tailored in size through NW growth conditions, forming atomically sharp interfaces to Zb segments [5]. This lays the path towards the formation of ordered GaBi structures with atomic-scale precision.

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3:10pm PCSI-1MoA-15 Iuliacumite: A Novel Two-Dimensional Chemical Short Range Order in a Wurtzite Single Monolayer InAs$_{1-x}$Sb$_x$ Shell on InAs Nanowires, *Michael Schnedler,* Forschungszentrum Jülich, Germany*; T Xu, I Lefebvre, J Nys,* Université Lille, CNRS, Centrale Lille, ISEN, Université Valenciennes, France*; S Plissard,* Université Lille, CNRS, Centrale Lille, ISEN, Université Valenciennes, Germany*; M Berthe,* Université Lille, CNRS, Centrale Lille, ISEN, Université Valenciennes, France*; H Eisele,* Technische Universität Berlin, Germany*; R Dunin-Borkowski, P Ebert,* Forschungszentrum Jülich, Germany*; B Grandidier,* Université Lille, CNRS, Centrale Lille, ISEN, Université Valenciennes, France

The reduced dimensionality of semiconductor nanowires (NWs) offers the unique opportunity to grow materials with crystal structures, which are otherwise unstable. One of the most prominent example is the growth of wurtzite (WZ) structure InAs NWs, although stable InAs bulk material prefers the zincblende (ZB) structure. In contrast, other III-V materials, notably InAs$_{1-x}$Sb$_x$, prefer to keep their ZB bulk structure even in NWs or nanostructures with reduced dimensionality. However, lateral overgrowth of these ternary III-V semiconductor alloys on sidewall facets of WZ structure III-V nanowires offers the prospect to nevertheless obtain reliably a WZ structure shell, despite being unstable. Thereby new polytype structures of ternary III-V semiconductor alloys can be achieved, offering additional degrees of freedom for adjusting the band structure in, e.g., core-shell nanowires. Therefore, we designed a two-dimensional single monolayer InAs$_{1-x}$Sb$_x$ WZ structure shell on sidewall facets of InAs nanowires and investigated the chemical ordering using atomically resolved scanning tunneling microscopy. We identify the existence of a short-range chemical ordering in this WZ structure single monolayer shell. The new type of two-dimensional ordering, called Iuliacumite, is characterized by an ordering vector in [0001] and an anti-ordering vector in <11-20> direction. The ordering is driven by a strong repulsive interaction of neighboring Sb atoms along the <11-20>-oriented atomic chains on the *m* plane sidewall facets.

PCSI
Room Canyon/Sugarloaf - Session PCSI-2MoA

Dopants in Semiconductors
Moderator: John Robertson, University of Cambridge

4:20pm PCSI-2MoA-29 Control of Spin-Orbit Coupling in Single Acceptor States in Silicon, *Sven Rogge,* University of New South Wales, Australia **INVITED**

Spins in silicon are suitable candidates for scalable quantum information devices, because of their long coherence times and inherent compatibility with current CMOS processing techniques. While quantum information devices in donor-based systems have been shown to be promising [1], the small dipole moment of donor spins make interaction of multiple qubits challenging to implement. The presence of spin-orbit coupling in acceptors however, could allow for fast quantum-gate manipulations [2] and effective long-range inter-qubit coupling [3]. Recent acceptor qubit proposals [4] suggest the possibility of maintaining the dipole moment between the spin-orbit states, without suffering from short coherence times.

In the first part of the presentation we show that long coherence times can be achieved for acceptor spins in bulk isotopically purified strained ^{28}Si. By coupling the bulk ^{28}Si crystal to a superconducting coplanar waveguide (CPW) resonator, we measured a coherence time (T2) of 0.7 ms for the acceptor spin ensemble in bulk ^{28}Si crystal under strain, in contrast to 0.04 ms for the same crystal without externally applied strain. The coherence time for the strained 28Si crystal was extended to 8.5 ms with the Carr-Purcell-Meiboom-Gill (CPMG) sequence [5]. This value for this coherence time is over 4 orders of magnitude higher than previously found in boron-

doped silicon devices [6] and demonstrates the potential of boron-based acceptor spins in silicon as a candidate for scalable, electrically-driven qubits with long coherence times.

In the second part of the talk we focus on addressing single acceptors [7]. In general, J = 3/2 systems are much less studied than S = 1/2 electrons, and spin readout had not yet been demonstrated for acceptors in silicon. We present acceptor hole spin dynamics by dispersive readout of single-hole tunneling between two coupled acceptors in a nanowire transistor [8]. We identify mJ = ±1/2 and mJ = ±3/2 levels, and we use a magnetic field to overcome the initial heavy-light hole splitting and to tune the J = 3/2 energy spectrum. We find regimes of spin-like (+3/2 to −3/2) and charge-like (±1/2 to ±3/2) relaxations, separated by a regime of enhanced relaxation induced by mixing of light and heavy holes. The demonstrated control over the energy level ordering and hybridization are new tools in the J = 3/2 system that are crucial to optimize single-atom spin lifetime and electrical coupling.

5:00pm PCSI-2MoA-37 UPGRADED: Low-Temperature Epitaxial Silicon Growth and Confinement of Delta Doped Si:P Nanostructures, *Scott Schmucker*, E Anderson, J Lucero, E Bussmann, P Lu, A Katzenmeyer, T Luk, T Beechem, L Tracy, T Lu, A Grine, D Ward, D Campbell, P Gamache, M Gunter, S Misra, Sandia National Laboratories

Atomically precise placement of phosphorus dopants using scanning tunneling microscopy-based hydrogen depassivation lithography (Figure 1) on silicon (Si:P) has implications for both high-performance digital electronics and quantum devices. Devices are fabricated by dissociative chemisorption of donor precursor molecules into patterned reactive areas in a hydrogen resist. A silicon capping layer, needed to encapsulate the device, is deposited at temperatures low enough to prevent dopant movement, but high enough to minimize defect generation.

Here, we explore the origin and influence of atomic defects in both the dopant layer and Si overgrowth, techniques available for characterization of these defects, and the relationship between surface passivation and device fidelity. Using a combination of optical spectroscopy, electrical transport, and transmission electron microscopy (TEM) (Figure 2), we relate P confinement and defect density in Si epitaxy to parameters of the fabrication process, surface chemistry, and the electronic characteristics of the resulting devices.

5:20pm PCSI-2MoA-41 The Electronic Bandstructure of Atomically Sharp Dopant Structures in Silicon, *Justin Wells,* Norwegian University of Science and Technology, Norway **INVITED**

Recently, it has become possible to control the placement of dopants in silicon with atomic precision, and this has given rise to a plethora of atomic scale and quantum proto-devices [1-3]. In this talk, I will present our ongoing work on understanding the electronic bandstructure of these dopant profiles in silicon.

Angle Resolved Photo-Electron Spectroscopy (ARPES) is the method of choice for observing the bandstructure, however observing the bandstructure of buried structures is extremely challenging. We have demonstrated that it is nonetheless possible to use ARPES to measure the bandstructure of dopant structures which have been created several nm beneath the surface [4]. It is also possible to see electron-phonon and electron-impurity interactions [5], quantum confinement of both the valence band and conduction band [6] and more. I will present these findings together with an overview of the current in understanding and controlling the electronic structure of dopant assemblies in semiconductors.

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PCSI
Room Canyon/Sugarloaf - Session PCSI-MoE

Superconductivity I
Moderator: David Pappas, National Institute of Technology

7:30pm **PCSI-MoE-1 Fluctuating High Temperature Superconductivity in Monolayer FeSe / SrTiO₃**, *Kyle Shen, B Faeth, S Yang, D Schlom,* Cornell University   **INVITED**
The nature and origin of the enhanced superconductivity in monolayer FeSe / $SrTiO_3$ has been attracted tremendous interest due to its unique character as an interfacially enhanced high- T superconductor. FeSe / $SrTiO_3$ exhibits a spectroscopic gap opening temperature (T_{gap}) between 60 to 70 K, nearly one order of magnitude higher than that of bulk FeSe (T_c = 8K), and in excess of related electron-doped FeSe-based bulk compounds. This dramatic enhancement remains the largest amongst known superconductors, positioning monolayer FeSe / $SrTiO_3$ as an ideal platform for investigating fundamental questions about interfacial superconductivity. In particular, the combination of its high-T_c and inherently two-dimensional (2D) nature makes FeSe / $SrTiO_3$ suited for exploring the interplay between 2D phase fluctuations and the interfacial enhancement of superconductivity, a better understanding of which could enable the future design and engineering of artificial higher- T_c superconductors. In this work, we employ a combination of *in situ* electrical resistivity and angle-resolved photoemission spectroscopy (ARPES) measurements of monolayer FeSe / $SrTiO_3$ to reveal an unprecedentedly large pseudogap regime between the initial formation of incoherent Cooper pairs (T_{gap} ~ 70K) and the onset of a zero resistance state (T_0 ~ 30 K). Through measurements of the V(I) characteristics, we identify this large pseudogap regime as originating from two-dimensional superconducting fluctuations, establishing the critical role that reduced dimensionality plays in the superconductivity of monolayer FeSe / $SrTiO_3$.

8:10pm **PCSI-MoE-9 Advances and Possibilities of the Materials Innovation Platform with Examples from Spin-ARPES**, *Daniel Beaton,* Scienta Omicron Inc.
The quest for device applications based on quantum materials, such as topological insulators, density wave systems, or superconductors, requires strict control of the environments these materials are exposed to during production and also while under investigation. It is most straightforward to gather all parts of the experiment, from sample growth to state-of-the-art analysis, in one connected UHV system. This approach in creating a so-called Materials Innovation Platform (MIP) has proven to be extraordinarily valuable in recent years.

In this presentation, I will focus on one such configuration; a combination Molecular Beam Epitaxy (MBE) system and Angle Resolved PhotoEmission Spectroscopy with spin detection capability (Spin-ARPES). The advantages of this set-up will be explored, as well as highlighting some of the very recent electronic band structure research performed with such a system. Two specific examples will be reviewed: Yang *et al.*[1] investigation of the impact of photogenerated carriers on the superconducting transition temperature; and advances high efficiency spin-ARPES[2]. The work by Yang *et al.*, enabled by the *in-situ* growth and analysis possibility, shows rapid, reliable, reproducible switching between normal and superconducting states, which demonstrates the possibility of making energy-efficient quantum optoelectronics devices. Future possibilities of Spin-ARPES and laser-ARPES in combination with MIP will also be discussed in relation to how this approach can allow more complete and precise studies of quantum materials.

[1] Yang et al., Nature Communications (2019)10:85, https://doi.org/10.1038/s41467-018-08024-w

[2] Data courtesy: Prof. Dengsung Lin, Dept. of Physics, NTHU, Taiwan

8:15pm **PCSI-MoE-10 Superconductivity at Surfaces Studied by Scanning Tunneling Microscopy**, *Yukio Hasegawa,* The University of Tokyo, Japan   **INVITED**
Superconductivity that emerges in metallic surface states is one of the ultimately thin two-dimensional (2D) superconductors. One of the advantages, if compared with other 2D superconductors, is that atomically well-ordered structures can be easily formed in macroscopic dimensions because of the thermal stability through the self-organized structural reconstruction. Basic properties such as atomic structure and electronic states are well characterized by standard surface science techniques including scanning tunneling microscopy (STM), and can be modify in a

controlled manner through the deposition and adsorption of additional materials.

One ubiquitous feature of the 2D atomically-thin electronic systems is the natural presence of atomic steps on its substrate. Atomic steps are considered to strongly affect electron transport as they decouple neighboring surface terraces [1]. We have demonstrated that the steps of the √3x√3-In/Si(111) surface superconductor behave as a Josephson junction and hold elongated vortices called Josephson vortices along the steps [2]. On striped incommensurate (SIC) phase of Pb/Si(111) the steps are found to block the propagation of the superconducting proximity effect and enhance it when they are located within the coherence length [3].

In two-dimensional superconductors usual orbital pair breaking of the superconductivity by in-plane magnetic field can be suppressed, allowing the Zeeman pair breaking to determine the critical magnetic field. There is however no protection against perpendicular magnetic fields. Using STM, we found that in narrow terraces of the Pb/Si(111) surface whose width is less than the coherence length superconductivity is protected against perpendicular magnetic fields. It is presumably due to the suppression of orbital pair breaking by the step confinement. Since the density and the coupling strength of the steps can be controlled, our study opens a way to design 2D superconductors that maintain the pair correlation under magnetic field in all directions.

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PCSI
Room Canyon/Sugarloaf - Session PCSI-1TuM

Magnetism
Moderator: Michael Flatté, University of Iowa

8:30am PCSI-1TuM-1 Quantum Microscopy of Nanoscale Materials and Devices, *Christian Degen*, ETH Zurich, Switzerland   **INVITED**
Diamond nanoprobes with single engineered NV centers allow enhancing scanning probe microscopy with quantum metrology. In this talk, I will introduce the basic concepts and technology of diamond nanoprobes, and give illustrative examples of applications in nanoscale imaging of magnetism and currents.

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9:10am PCSI-1TuM-9 UPGRADED: Mechanical Control of Valley Magnetization and Berry Curvature Dipole in Monolayer MoS₂, *Joolee Son*, Ajou University, Republic of Korea; *K Kim*, Pohang University of Science and Technology, Republic of Korea; *Y Ahn*, Ajou University, Republic of Korea; *H Lee*, Pohang University of Science and Technology, Republic of Korea; *J Lee*, Ajou University, Republic of Korea
Atomically thin honeycomb crystals have recently emerged as promising platforms to investigate electron's valley degree of freedom for the development of functional valley-based devices. Electron control by valley index has been demonstrated using electrical, optical and magnetic means, owing to the opposite signs of the Berry curvature between two valley centers. Here we report a different kind of valley-based electron control that is based on the Berry curvature dipole. We demonstrate the generation of net valley magnetization under an in-plane electric field, regulated by the strain-induced modification of the Berry curvature distribution, which produces the Berry curvature dipole. The generation of valley magnetization is optically detected by using the Kerr rotation microscopy on monolayer MoS_2 embedded in flexible van der Waals heterostructures as functions of tunable strain. The measured valley magnetization is well explained by the calculated values of the strain-induced Berry curvature dipole. Our work demonstrates strain as a new functionality for potential novel flexomagnetic and valley information processing devices using monolayer TMD materials.

9:30am PCSI-1TuM-13 Room Temperature Ferromagnetic Monolayer MnGaN-2D Investigated by Spin-polarized Scanning Tunneling Microscopy/ Spectroscopy and First-principles Density Functional Theory, *Y Ma, T Erickson*, Nanoscale & Quantum Phenomena Institute; *K Meng, F Yang*, The Ohio State University; *D Hunt, A Barral, V Ferrari*, CAC-CNEA, Argentina; *A.R. Smith*, Nanoscale & Quantum Phenomena Institute
Development of spintronic applications based on semiconductor materials combined with magnetic dopants has been a topic of great interest for many years. More recently has been the rapid growth of interest in 2-dimensional materials with both semi-conductive and/or magnetic properties. We have reported the direct observation of the room-temperature ferromagnetism for MnGaN-2D using spin-polarized scanning tunneling microscopy and spectroscopy combined with firstprinciples calculations.[1] This 2D material is directly grown on the surface of N-polar GaN(0001) using molecular beam epitaxy and consists of 1/3 ML of Mn atoms incorporated into the surface Ga adlayer and forming a √3 x √3 - *R*30° structure as seen in Fig. 1.

Density functional theory shows that this monolayer structure has *perpendicular* magnetic anisotropy with a highly spin-polarized and spin-split manganese density of states. We verify the magnetic properties using SQUID magnetometry. In addition, we explore changes in the energy of the Mn peak DOS as seen in tunneling spectroscopy and discover theoretically that it is caused by surface strain. Different models, including isotropic, anisotropic, and defect-induced strain models are explored, and it is concluded that the Mn-N bond length is the critical parameter. The local strain is then directly observed in atomic scale STM images as a non-Gaussian distribution of lattice parameters, and disordering is seen in the 2D pair correlation as well. This strain may be the effect of the manner in which the surface is prepared, thus opening the possibility of atomic-scale engineering of magnetic anisotropy.

[1] Y. Ma, A.V. Chinchore, A.R. Smith, M.A. Barral, and V. Ferrari, *Nano Letters* **18**, 158 (2018).

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9:35am PCSI-1TuM-14 UPGRADED: Local Exchange Resonance in DC Magnetoresistance of Spin-Polarized Current Through a Dopant, *Stephen McMillan*, University of Iowa; *N Harmon*, University of Evansville; *M Flatté*, University of Iowa
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. In this work we consider 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]. The stochastic Liouville formalism is employed to calculate the current through the individual dopant. We predict a substantial increase in resistance at finite magnetic fields due to the formation of a non-trivial bottleneck in the spin-correlated transport. Resonance between the Zeeman and exchange coupling leads to a cancelation in the coherent evolution of the dopant spin resulting in an on-site polarization opposing that of the SP-STM. This feature provides a precise method for measuring the dopant exchange coupling to a nearby electronic spin and by direct analog hyperfine coupling in the presence of nuclear spins. This technique does not require the use of ac electric or magnetic fields and is sensitive to exchange or hyperfine energies well below the thermal energy of the system.

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9:55am PCSI-1TuM-18 Room Temperature Ferromagnetism in GaSb Thin Films Doped with Mn, *A Pulzara Mora, Camilo Andres Pulzara Mora*, Universidad Nacional de Colombia, Colombia
The design and development of Hall Effect magnetic field sensors with III-V semiconductor materials and magnetic alloys (Mn) is a current topic - due to its applications in different branches of physics like spintronics. Semiconductor materials such as GaSb are important because of their applications in modern Nano-electronics, infrared emitting lasers with a 0.7 eV bandgap and especially in photovoltaic systems and their optical response to wavelengths longer than silicon-based solar cells [1][2]. When the Mn is introduced in the matrix of these semiconductors, we have new opportunities in the context of spintronics, owing that in the alloys the spatial distribution of electrons and holes can be controlled easily, resulting in the magnetic properties of these materials.

The structural, electrical and magnetic properties of GaSbMn thin films were studied. The samples were grown by Magnetron Sputtering on heated Si (111) substrates. In order to incorporate Mn in low concentrations in the GaSb matrix, the substrate temperatures were varied from 300°C to 400°C. X-ray diffraction patterns show that they have a polycrystalline structure. We find that at 300°C GaSbMn grows as a smooth, phase-pure film, whereas at higher temperatures (400°C) the films become increasingly rough, but more crystalline with segregated MnSb and Mn impurities, shown also by Scanning Electron Microscopy. High temperature SQUID magnetometry measures Curie temperatures of 350 K for the film grown at 300°C, and above 500K for 400°C. The GaSbMn exhibits a well-defined magnetic hysteresis loop above room temperature. These loops show that the superparamagnetic

(or weak ferromagnetic) behavior of the GaSbMn layers depends on the Mn content. Magnetotransport measurements show well developed anomalous Hall effect (AHE) hysteresis loops that persist up to room temperature. This result shows that the magnetic properties are very sensitive to experimental parameters such as working pressure and growth temperature [3][4].

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10:00am PCSI-1TuM-19 Magnetotransport Studies in Hybrid 2D/0D Nanostructures, *Ethel Perez-Hoyos, Y Luo, A Dehankar, J Xu, D Pharis, J Winter, R Kawakami, E Johnston-Halperin*, The Ohio State University
We introduce a device fabrication strategy that takes advantage of stacking techniques developed for van der Waals heterostructures to construct

hybrid 2D/0D composite magnetic nanostructures, with potential application in the study of spin and charge disorder as well as magnetic-proximity effects. The structures in this study are comprised of superparamagnetic iron oxide nanoparticles (SPIONs) and monolayer graphene. The SPIONs are deposited first using a Langmuir-Blodgett technique, yielding rafts of highly ordered nanoparticles. Characterization via magnetic force microscopy (MFM) reveals magnetic order at multiple length scales and SQUID magnetometry identifies both glassy antiferromagnetic and ferromagnetic response. Single graphene monolayers are mechanically stacked on the SPIONs layer, and characterized via low temperature magneto-transport. Initial measurements show good electron mobility in the graphene layer and indications of exchange coupling between the graphene and the SPIONs layer.

PCSI
Room Canyon/Sugarloaf - Session PCSI-2TuM

Superconductivity II
Moderator: Kyle Shen, Cornell University

11:00am **PCSI-2TuM-31 Fabrication of High Coherence Superconducting Qubits**, *J Long, H Ku, X Wu,* NIST*; R Lake,* BlueFors*; **David Pappas,** NIST*
INVITED

Scaling up qubit circuits and achieving high coherence relative to gate speed is imperative to realizing the full power of quantum computing. In this work we demonstrate superconducting transmons with coherence times ranging from 25 to 90 μs, significantly longer than typical gate speeds, which range from 10 to 200 ns for single and two-qubit interactions.

The circuits were fabricated on intrinsic Si(001) substrates (Fig. 1_. The metallization (gold) was NbTiN. The meander feedline (from Port 1 to Port 2), inductively couples to resonators (R1-R6, only R1 labeled for clarity) which are then capacitively coupled to concentric capacitor plates. The plates are connected together with a Josephson junction that was fabricated using a two-step overlap process [1] to form transmon qubits, Q1-Q6. Some of the methods used to enhance the coherence include using a nitride pre-treatment of the substrate prior to metallization, post-treatment of the circuit with buffered oxide etch, and extensive wire-bonding. Variations of coherence between qubits was about a factor of 2, and can be understood in some one case (the shortest) as being due to damage during wire-bonding. Fluctuations are hypothesized to be due to coupling of the qubits to two-level systems around the junctions [2].

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11:40am **PCSI-2TuM-39 UPGRADED: Interface Chemistry and Decoherence Processes in Superconducting Quantum Circuits**, *D. Frank Ogletree,* Lawrence Berkeley National Lab*; V Altoe, X Liu, A Minor, S Cabrini, S Griffin,* Molecular Foundry, LBNL*; A Bannerjee,* Lawrence Berkeley National Lab*; J Kriekebaum, I Siddiqi,* University of California, Berkeley

Artificial atoms based on superconducting circuit elements including Josephson tunnel junctions and strip-line resonators can be used as "qubits" for quantum computation and simulations, and as platforms for studying quantum cavity electrodynamics and other quantum phenomena. The performance of these systems depends critically on achieving coherent lifetimes that are significantly longer than initialization and readout times. Significant progress has been made in increasing coherence over the last decade or two by better electromagnetic circuit design to control losses and cross-talk, by improved radio-frequency electronics [1], and by advances in shielding and measurement techniques [2]. Further progress can come from improvements in materials and fabrication and better control of interface chemistry [3].

We will report initial results on interfacial studies combining SEM, analytical STEM, and x-ray spectroscopy to understand substrate, vacuum and internal interfaces in both Al Josephson junctions and Nb resonator structures.

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PCSI

Room Canyon/Sugarloaf - Session PCSI-TuE

The Future of PV

Moderator: Kirstin Alberi, National Renewable Energy Laboratory

7:00pm **PCSI-TuE-1 Progress in Hybrid Perovskite Photovoltaics and Optoelectronics**, *Joseph Berry*, National Renewable Energy Laboratory
INVITED

Photovoltaic devices based on hybrid organic-inorganic perovskite absorbers have reached outstanding performance over the past few years, surpassing power conversion efficiency of over 25% for single junction and present multiple paths to tandems with efficiencies beyond 30%. These efficiencies have been achieved largely via the use of solution processing of the active layer coupled to more traditional vacuum processing for contacts and interface layers. This talk will start with recent progress and challenges in hybrid perovskite solar cells (HPSCs) with an emphasis on the role of materials integration challenges needed to enable device performance, tandem processing and stability. While, this talk will highlight recent progress at NREL, the challenges of tandems based on HPSC devices, work to develop hybrid materials for other applications and to understand their basic physical properties will also be discussed. Details of material structure, synthesis, the resulting interfaces and the role of processing in creating controlling material properties will discussed. Data on the optoelectronic, spintronic and ferroelectric properties as characterized by an array of analytical tools including time resolved spectroscopy, structural studies and device level evaluation will be presented. Links from these fundamental materials properties to technologically relevant advances and suggestions for overarching research themes will be touched upon.

7:40pm **PCSI-TuE-9 On the Path Towards Tandem Junction Nanowire Based Solar Cells**, *Magnus Borgström*, Lund University, Sweden **INVITED**
Semiconducting nanowires have been recognized as promising materials for high-performance electronics and optics where optical and electrical properties can be tuned individual. Especially, nanowires have been identified as a means to high efficiency solar cells [1, 2] using significantly reduced materials consumption due to strong geometrically enhanced light absorbing properties [3].

In order to further optimize the performance of NWPV, and integrate them on Si in a tandem junction configuration, nanowires with dimensions corresponding to optimal light harvesting capability are necessary. We developed nano imprint lithography for patterning of catalytic metal particles with a diameter of 200 nm in a hexagonal pitch of 500 nm. We found that a pre anneal and nucleation step was necessary to keep the particles in place during high temperature annealing to remove surface oxides. We intend to transfer these grown nanowires to a Si platform (existing PV), either by direct growth on Si PV, or by nanowire peel off in polymer, followed by transfer and electrical contacting, or by aerotaxy and alignment for transfer to Si. We used electron beam induced current measurements as a tool to optimize the electrostatic potential profile in nanowires, leading to 15% efficient InP nanowire solar cells, even though only covering about 10 % of the substrate surface. The optimal band gap in combination with Si is about 1.7 eV, where we identify GaInP and GaAsP as materials for development of nanowire *pn* junctions, the heart in a solar cell.

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PCSI

Room Canyon/Sugarloaf - Session PCSI-1WeM

Optical Properties of 2D Materials

Moderator: Wanyi Nie, Los Alamos National Laboratory

8:30am **PCSI-1WeM-1 Metals at the Atomic Limit**, *Joshua Robinson,* Penn State University **INVITED**

The last decade has seen an exponential growth in the science and technology of two-dimensional materials. Beyond graphene, there is a huge variety of layered materials that range in properties from insulating to superconducting that can be grown over large scales for a variety of electronic devices and quantum technologies, such as topological quantum computing, quantum sensing, and neuromorphic computing. In this talk I will discuss our pioneering work in confinement heteroepitaxy (CHet) that enables the creation of 2D forms of 3D materials (e.g. 2D-Ga, In, Sn) and *decouples* the growth of the metals from other 2D layers, thereby enabling a new platform for creating artificial quantum lattices (AQLs) with atomically sharp interfaces and designed properties. As a specfic example, we synthesize plasmonic layers that exhibit >2000x improvement in nonlinear optical properties, and 2D-superconductors combined with topological insulators as the building block of next generation "2D" topological superconductors. Confinement heteroepitaxy opens up avenues for enabling a virtual "legoland" of hybrid quantum materials.

9:10am **PCSI-1WeM-9 Tuning the Spontaneous Emission of Monolayer WSe$_2$ by Optical Environment Control – Cavity Coupling and Substrate Manipulation**, *J Lee, Hyunseung Lee,* Ajou University, Republic of Korea

Atomically thin layer of transition metal dichalcogenides (TMDs) such as monolayer WSe2 exhibit direct bandgaps ranging from visible to near-infrared with strong exitonic effect. Thanks to its optical characteristics, these materials can be used for integrated functional devices such as light emitting devices, photodetectors and optical modulators. In these applications, device performances can be improved by engineering the material thicknesses and doping levels, applying external fields, or modulating optical environment. In particular, tailoring the optical environment has been demonstrated by coupling monolayer TMDs to various types of optical microcavities such as Bragg reflectors or photonic crystals.

In this work, we utilize microspheres on planar substrates to manipulate the emission properties of monolayer WSe2. First, we show the enhancement of the photoluminescence (PL) emission which is controlled by the size of the coupled microsphere which ranges from 2 to 7 μm. Time-resolved PL measurement supports the cavity-induced emission rate enhancement of monolayer WSe2 coupled to a microsphere. The PL enhancement is further increased by increasing the thickness of the oxide layer between the microsphere and silicon substrate, which is supported by finite-time domain method (FDTD) simulations. Both microsphere coupling and substrate manipulation provide convenient pathways to modulate 2D material-based photonic devices.

9:15am **PCSI-1WeM-10 First Principles Study on Optical Properties of Monolayer Bismuthene under an Electric Field**, *Wei-Chieh Liu,* L Xu, M Lin, Hanyang University, South Korea; *T Leung, H Hsu,* National Taipei University of Technology, Republic of China

Monolayer bismuthene has extraordinary optoelectronics, catalytic and biocompatible properties, and potential as a 2D topological insulator. When monolayer bismuthene is deposited in a sufficiently thin layer on an object, it possesses a stable low-buckled hexagonal structure and it has the property of semiconducting, which could be a promising low-dimensional thermoelectric material. Monolayers bismuthene is p-type semiconductors, but the hole concentration arising from the intrinsic defects is very low and hard to control. In this work, the band structure, density of states and optical constant of monolayer bismuthene have been calculated using first-principle calculations based on density functional theory (DFT). The results are compared to those calculated from the tight-binding model. With an applied external electric field, it is found that the electric and optical properties will be dramatically changed. Monolayer bismuthene can be calculated may generate some applications in optoelectronics, either combined with other 2D materials or topological materials.

9:20am **PCSI-1WeM-11 Formation of Coherent Phase Domain Heterojunctions in Single Layer MoS$_2$ on Au(111)**, *Fanglue Wu, Z Liu,* Texas A&M University; *M Chandross,* Sandia National Laboratories; *Q Moore,* Texas A&M University; *N Argibay, J Curry,* Sandia National Laboratories; *J Batteas,* Texas A&M University

Two-dimensional (2D) transition metal dichalcogenides (TMDs) have attracted tremendous attention over the past decade due to their exciting mechanical, electronic and frictional properties [1-5]. Heterojunctions of semiconductors and metals are the fundamental building blocks of modern electronics. Coherent heterostructures between dissimilar materials can be achieved by composition, doping or heteroepitaxy of chemically different elements. Here we report, the formation of coherent single-layer MoS heterostructures (Figure 1), which are chemically homogenous with matched lattices, but show electronically distinct semiconducting (1H phase) and metallic (1T phase) character, when deposited by mechanical exfoliation on Au(111). The facile exfoliation technique here eliminates tape residues usually found in many exfoliation methods, and yields single-layer MoS with millimeter (mm) size. Raman spectroscopy, X-ray photoelectron spectroscopy (XPS), scanning tunneling microscopy (STM) and scanning tunneling spectroscopy (STS) have collectively been employed to elucidate the structural and electronic properties of MoS monolayers on Au substrates. Our work provides a basis to produce macroscale two-dimensional heterostructures, which represent unique candidates for future electronic devices and applications.

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9:25am **PCSI-1WeM-12 UPGRADED: Effects of Electromechanical Coupling in Locally Strained Monolayer MoS$_2$**, *Alex De Palma,* G Cossio, K Jones, J Quan, The University of Texas at Austin; *X Li,* Univ of Texas at Austin; *E Yu,* The University of Texas at Austin

Strain in atomically thin transition metal dichalcogenides (TMDs) has a broad range of consequences, and can be used for tuning of their optical and electronic properties [1, 2]. In particular, the use of localized strain to engineer these effects, such as in exciton funneling, has been demonstrated [3]. Additionally, TMDs exhibit intrinsic piezoelectricity in monolayer and few layer form originating from a lack of centrosymmetry [4]. The presence of piezoelectricity in TMD systems with strain and strain gradients can also have appreciable effects, which have only begun to be explored. Understanding these effects is necessary for engineering of TMD-based structures in which strain is present.

In this work, we examine the effects of piezoelectricity on MoS$_2$ in the presence of strain and strain gradients. Samples consisting of monolayer MoS2 suspended over 800nm-diameter cavities were fabricated by exfoliation and transfer of MoS$_2$ onto a patterned substrate. Suspended MoS$_2$ was deformed via atomic force microscope (AFM) indentation, and Photoluminescence (PL) measurements were simultaneously performed as a function of indentation force to determine the effects of the strain gradient on exciton bandgap and exciton diffusion (Fig. 1a, b). Additionally, we show through calculations that spatially varying strain, can be a source of electrostatic potentials due to the piezoelectric effect. According to a mechanical model for indentation [5], the charge density can be as high as 10^{12} e/cm^2 at the points of highest strain gradient - significant enough to generate electrostatic potential variations on the order of ±0.1V over the MoS$_2$ (Fig. 1c). The relationship between strain and the potential generated by piezoelectricity, and the impact of this effect on excitons, will be discussed.

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PCSI
Room Canyon/Sugarloaf - Session PCSI-2WeM

Material Modification and Self Assembly
Moderator: Sven Rogge, University of New South Wales, Australia

11:00am PCSI-2WeM-31 Neuromorphic Computing with the Redox Transistor, *Alec Talin,* Sandia National Laboratories   **INVITED**
Efficiency bottlenecks inherent to conventional computing in executing neural algorithms have spurred the development of novel devices capable of 'in-memory' computing. Commonly known as 'memristors', a variety of device concepts including conducting bridge, vacancy filament, phase change and other types have been proposed as promising elements in artificial neural networks for executing inference and learning algorithms. In my talk, I will review the recent advances in memristor technology for neuromorphic computing and discuss strategies for addressing the most significant performance challenges, including non-linearity, high read/write currents, and endurance. As an alternative to two-terminal memristors, I will introduce the three-terminal electrochemical memory based on the redox transistor (RT) which uses a gate to tune the redox state of the channel.[1] Decoupling the 'read' and 'write' operations using a third terminal and storage of that information as a charge-compensated redox reaction in the bulk of the transistor enables high-density information storage. These properties enable low-energy operation without compromising analog performance and non-volatility. I will discuss the RT operating mechanisms using organic and inorganic materials, approaches for array integration, and prospects for achieving the device density and switching speeds necessary to make electrochemical memory competitive with established digital technology.

11:40am PCSI-2WeM-39 Kinetically-Driven Assembly of TaS₂-SnS Heterostructures with Flexible Stacking Architectures, *Dennice Roberts,* National Renewable Energy Laboratory; *D Bardgett,* University of Oregon; *B Gorman,* Colorado School of Mines; *J Perkins, A Zakutayev, S Bauers,* National Renewable Energy Laboratory
Chalcogenide heterostructures enable access to a remarkable range of materials properties by virtue of structural flexibility at the nanoscale. An interesting approach to the preparation of such heterostructures utilizes layered amorphous precursor films designed to mimic a desired superlattice heterostructure product, and has been successful in creating a wide range of metastable selenide heterostructures. An example of such tunable properties is seen in the $SnSe-VSe_2$ system, where changing layer sequencing can both enhance and quench charge density wave (CDW) transitions, as well as modify their onset temperatures.[1] Such CDWs in TaS_2 are hysteretic and have been proposed for phase change memory applications,[2] and so incorporating TaS_2 into superlattice structures known to enhance CDW transitions might further enhance this material towards these applications.

Previous work from our group developed a framework for preparing amorphous sulfide precursor films by RF sputtering.[3] Here we present the first crystalline sulfide heterostructures prepared using this precursor approach, composed of tunable numbers of SnS sandwiched between monolayers of TaS_2 in a superlattice. We also demonstrate the utility of combinatorial synthesis for creating precursors of several different stacking sequences in a single deposition. Structural measurements confirm smooth films with superlattice ordering as well as the presence of constituent TaS_2 and SnS layers. Superlattice architecture is confirmed by high resolution transmission electron microscopy (TEM) and EDS, resolving atomically precise sequencing of SnS and TaS_2 monolayers in the arrangement experimentally instilled into the precursors. Electronic behavior as a function of number of SnS layers is measured.

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11:45am PCSI-2WeM-40 Globally Aligned Single-Wall Carbon Nanotube Films through Electrostatic Ordering, *Joshua Walker,* University of Wyoming; *J Fagan, A Biacchi,* National Institute of Standards and Technology; *V Kuehl,* University of Wyoming; *T Searles,* Howard University; *A Hight Walker,* National Institute of Standards and Technology; *W Rice,* University of Wyoming
The one-dimensional nature of single-wall carbon nanotubes (SWCNTs) creates unique, anisotropic optical, electrical, and thermal characteristics.

To utilize these anisotropic properties, researchers must be able to easily and reproducibly fabricate aligned SWCNT structures. To be most useful, SWCNT alignment protocols must incorporate solution-based nanotubes, as they provide the highest quality (chiral enrichment, length sorting, tube filling, etc.) nanotubes [1] which are necessary for applications.

We expanded [3] upon the slow-filtration SWCNT alignment technique [2] through automation and parallelization. Such advances not only provided increased film reproducibility and throughput, but also enabled a rapid optimization of the complex parameter space to produce the highest aligned films to date. Furthermore, this work provides researchers with a new capability to investigate the underlying physics driving alignment. We find that by controlling flow rate, flattening the meniscus, and membrane buffing, we can repeatably and automatically produce globally aligned SWCNT films. Using polarized spectroscopy, we show that high, two-dimensional nematic ordering ($S_{2D} \approx 0.9$) of SWCNTs can be achieved [3]. Experiments altering the ionic strength and membrane surface charging suggest that this ordered SWCNT phase is driven by linear charging on the membrane and inter-nanotube electrostatic interactions.

11:50am PCSI-2WeM-41 Defining Insulating Regions on TiO₂ Thin Films by Laser Heating, *S Ahmed, J Ritter, **Matt McCluskey**,* Washington State University
Optically defining conducting and insulating regions on an oxide thin film could provide a means for writing and rewriting transparent electronic circuits. Titania (TiO_2) films are straightforward to deposit and exhibit *n*-type conductivity that depends strongly on the concentration of oxygen vacancies, which act as shallow donors. Heating in a reducing atmosphere, such as vacuum or hydrogen, increases the density of oxygen donors and hence the conductivity. Conversely, heating in an oxygen atmosphere reduces the oxygen vacancy concentration and makes the sample insulating. While electrons in the rutile phase are small polarons, those in anatase TiO_2 behave as free electrons. This property makes the anatase structure preferable for applications requiring high electrical conductivity.

In the present work, 300 nm thick anatase TiO_2 films were sputtered on fused silica substrates. Heating under a rough vacuum (30 mTorr) produced conducting films with free-carrier absorption in the visible and IR. A green laser (532 nm wavelength, 1-5 W power) was then focused on regions of the sample, in the open air. Localized laser heating resulted in a 7 order-of-magnitude increase in resistance, from 10 kΩ to >100 GΩ. The heated area became transparent due to the loss of free-carrier absorption. Scanning electron microscopy (SEM) and optical transmission spectroscopy indicate that laser heating does not degrade the films. The process is reversible – conductivity is restored after annealing in vacuum again. The effect of interface heat conduction will be discussed.

11:55am PCSI-2WeM-42 Towards Mask Free Direct Write fabrication of Micro- and Nanoscale Architectures on Different Substrates via Aqueous Ink Precursors and CVD Synthesis, *Irma Kuljanishvili, D Alameri, D Karbach, R Dong, L Moore,* Saint Louis University; *R Divan, Y Liu,* Argonne National Laboratory
Low-dimensional materials such as 2D graphene, boron nitride or other layered van der Waals atomic crystals, WS2 or MoS2, and 1D nanowires (NWs) and nanoribbons such as ZnO, and other semiconducting materials, have drawn significant attention in the past decade due to their nanoscale geometry and unique physical, chemical, optical properties as These low dimensional materials when assembled/interfaced in vertical or lateral arrangements often lead to the largely enhanced properties, and new functionalities. While the preparation of layered architectures usually involves multi-step fabrication processes it also relies predominately on a mask assisted lithographic techniques.

Here we present a mask-free controlled selective preparation of 1D and 2D nanostructures of MoS2, WS2 and ZnO in the variety of geometric assemblies by employing parallel direct- write patterning (DWP) of aqueous ink precursors on substrates and devices at predefined locations. In a two-step process (1st patterning and 2nd growth) our unconventional fabrication approach enables simple and flexible production of hetero-structures and other architectures based on "mix and match" principle in precisely controlled fashion. Location specific synthesis of materials also provides access to as-grown interfaces and rapid testing of materials quality, crystallinity and chemical composition can be easily confirmed by several non-destructive surface probe tools such as Raman Spectroscopy, PL, AFM, XRD etc. Our 'bottom-up' approach offers simple and flexible route to rapid testing of prototype nano-architectures and platforms, via multiplexing and the ease of probing device interfaces their viability and

robustness and the potential for further development of specific targeted applications.

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PCSI

Room Canyon/Sugarloaf - Session PCSI-1WeA

Devices and Contacts
Moderator: Alex Demkov, The University of Texas

2:00pm **PCSI-1WeA-1 Towards Fermi Level De-pinning at Contacts**, *John Robertson,* Cambridge University, UK*; Y Guo,* Wuhan University, China*; Z Zhang,* Cambridge University, UK   **INVITED**
Fermi level pinning at Schottky barriers (SB) strongly limits the reduction of contact resistances and thus scaling of modern electronic devices and future 2D semiconductor devices. We find that some complex semiconductor-metal interfaces with bonding configurations parallel to the interface create a type of localized interface or 'defect state' beyond the metal induced gap state (MIGS) model. Examples are interfaces between Si and metal disilicides and between Si and Sb. These defect states do not easily match to conventional MIGS and this mixes states of metal character into the surface pinning level. This creates Fermi level de-pinning and a variation of SB height with interface orientation.

The MIGS model [1] has successfully described many aspects of Schottky barrier behavior, including the slope of barrier height (SBH) with metal work function, $S=\partial\varphi/\partial F_M$ and the charge neutrality level. However, it does not include several factors like interface bonding [2]. The MIGS model would say the S factor should depend only on metal work function, not type of metal (elemental or silicide/TiN) or on the face orientation, despite these being seen experimentally [2,3] and found in DFT supercell calculations [4]. We show that both metal silicides and Sb break the MIGS due to the presence of 'defect-like' states [5] at their interfaces, due to states which cannot be easily captured by the limited MIGS basis set of bulk semiconductor states. A metal-like character enters the effective CNL pinning energy, which also gives the orientation dependence. The chemically different case of Si:Sb behaves similarly to the silicides. These two factors are signifiers of Fermi level de-pinning, to find other examples.

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Figure 2 Showing 'defect state at Si:silicide (111), (100) interfaces causing the de-pinning and orientation dependence

Figure 1 Showing Fermi level depinning and face dependence in Si: silicide interfaces

2:40pm **PCSI-1WeA-9 Observation, Characterization, and Mitigation of the Internal *p-n* Junction in Pyrite FeS$_2$, a Potential Low-cost Solar Absorber**, *Bryan Voigt,* W Moore, J Walter, B Das, M Maiti, M Manno, University of Minnesota*; E Aydil,* New York University*; C Leighton,* University of Minnesota
Pyrite FeS$_2$ is widely acknowledged as an ideal semiconductor for thin film solar cells due to its earth-abundance, low toxicity, low cost, suitable band gap (0.95 eV) and minority carrier diffusion length, and high visible light absorptivity. Power conversion efficiencies of FeS$_2$ heterojunction solar cells, however, have never exceeded 3% due to low open-circuit voltages (V_{OC} <0.3 V). One hypothesis emerging from recent temperature (T)-dependent transport of single crystals is that this low V_{OC} is due to a conductive pyrite surface with a carrier type (*p*-type) inverted from bulk (*n*-type) [1,2]. This could create a leaky (*i.e.*, low-V_{OC}) internal junction, thus limiting solar cell efficiencies. These studies established conduction through a 1-3 nm-thick, *p*-type surface upon freeze-out of *n*-type bulk carriers [1,2]. Two parallel resistors representing the surface and bulk can describe the T-dependence of resistivity [1] and the non-linear Hall effect observed near the crossover between bulk- and surface-dominated conduction [2]. Notably, what has neither been observed nor characterized, however, is the internal junction implied by this *p*-surface and *n*-bulk. Here, we directly observe this internal junction for the first time. In-plane sheet resistance (R_S) measurements of polished crystals doped heavily *n*-type *via* sulfur vacancies are shown to display an effect where metallic-like transport abruptly transitions to rapidly increasing R_S below ~175 K, eventually transitioning to surface conduction (at T <100 K).

We show that this very unusual T-dependence can be well described by incorporating an exponentially-T-dependent junction resistance into the parallel resistor model. Junction barrier heights extracted from the model are typically 0.15 − 0.30 eV, in good agreement with typical V_{OC} values in past heterojunction solar cells, suggesting that this internal junction may, in fact, be limiting efficiencies. Interestingly, while its influence in $R_S(T)$ is independent of contact materials such as In, Ag, Fe, Co, and Ni, CoS$_2$ contacts mitigate this junction, allowing the first characterization of bulk properties to low T. Access to low T unveils rich phenomena, such as the onset of a smaller donor activation energy below 175 K, non-linear Hall effect near 100 K, and an unusual resistivity anomaly at T ≤10 K, showcasing CoS$_2$ contacts as a way to both mitigate this junction and advance understanding of electronic transport in FeS$_2$. This work was supported by the customers of Xcel Energy through a grant from the Renewables Development Fund.

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2:45pm **PCSI-1WeA-10 UPGRADED: Photo-Driven Dipole Reordering: Key to Carrier Separation in Metalorganic Halide Provskites**, *Philipp Ebert,* Forschungszentrum Jülich, Germany*; H Hsu,* National Taiwan University, Republic of China*; B Huang,* Academia Sinica, Republic of China*; S Chin,* National Taiwan University, Republic of China*; C Hsing, D Nguyen,* Academia Sinica, Republic of China*; M Schnedler,* Forschungszentrum Jülich, Germany*; R Sankar,* Academia Sinica, Republic of China*; R Dunin-Borkowski,* Forschungszentrum Jülich, Germany*; C Wei,* Academia Sinica, Republic of China*; C Chen, Y Chiu,* National Taiwan University, Republic of China
Photo-driven dipole reordering of the intercalated organic molecules in halide perovskites has been suggested to be a critical degree of freedom, potentially affecting physical properties, device performance, and stability of hybrid perovskite–based optoelectronic devices. However, thus far a direct atomically-resolved dipole mapping under device operation condition, i.e. illumination, is lacking. Here, we map simultaneously the molecule dipole orientation pattern and the electrostatic potential with atomic resolution using light-illuminated cross-sectional scanning tunneling microscopy and spectroscopy.

Our experimental observations demonstrate that a photo-driven dipole reordering, initiated by a photo-excited separation of electron-hole pairs in spatially displaced orbitals, leads to a fundamental reshaping of the potential landscape in halide perovskites, creating separate one-dimensional transport channels for holes and electrons. We anticipate that analogous light-induced polarization order transitions occur in bulk and are at the origin of the extraordinary efficiencies of organometal halide perovskite-based solar cells as well as could reconcile apparently contradictory materials' properties.

3:05pm **PCSI-1WeA-14 First Principles Study on Electronic Properties of Graphene Nanostructures for High Current Density Cathode**, *Nan Zhao, L Xu, M Lin,* Hanyang University, South Korea*; T Leung,* National Chung Cheng University, Republic of China*; H Hsu,* National Taipei University of Technology, Republic of China
Graphene is a crystalline allotrope of carbon with two-dimensional properties. Its carbon atoms are densely packed in a nano-scale hexagonal pattern. Graphene has many unusual properties. It is about 200 times stronger than the strongest steel. It can efficiently conduct heat and electricity and is nearly transparent. In this work, we study the electronic properties of graphene using first principles or *ab initio* calculations based on density functional theory (DFT) in order to explore its applications in field emission devices. The change of work function due to the lattice deformation of graphene is investigated using a supercell including a vacuum layer which is thick enough so that the layer interaction is negligible. It is found that the work function is very sensitive to the lattice size. As the lattice site increases, the work function increases proportionally. However, the work function is reduced doubly while the lattice site is reduced. The local work function of graphene has also been determined and this can be used to predict field emission current from Fowler-Nordheim equation more accurately. For realistic applications, this approach has been used to calculate the work function of carbon nanoribbons with different widths and terminating edges with and without passivation.

3:10pm **PCSI-1WeA-15 Band Offset Modulation in Si-EuO Heterostructures *via* Controlled Interface Formation**, *W Li, A Posadas,* The University of Texas at Austin; *Alex Demkov,* The University of Texas

In a Si-based spintronic device, Si serves as the spin channel material. Owing to its small spin-orbit coupling, Si has a long spin relaxation lifetime and long spin coherence length, making it an excellent choice. Because the rock salt lattice of EuO is compatible with the *fcc* lattice of Si (see Fig. 1), and EuO is thermodynamically stable on Si, Si/EuO heterostructures have a real potential for use in Si-based spin-FETs. Combining first principles calculations and experiment, we investigate the atomic and electronic structure of the Si/EuO interface. We consider the thermodynamic stability of interface structures with different levels of oxidation to identify the most probable configuration. By comparing the calculated band alignment and core level shifts with measured values, we validate the theoretically constructed interface model. EuO has unusual electronic properties in that its charge neutrality level appears to be inside the conduction band [1,2]. In Fig. 2 we show a contour plot of the partial density of states (PDOS) as a function of energy and position along the *z* direction normal to the plane of the interface. In the contour plot one can clearly see the band edges of Si and EuO and read off the VBO, which is +0.19 eV. We find that the band offset can be tuned by altering the relative energy positions of the Si and EuO conduction bands via interface oxidation, which can be used to tune this materials system for specific applications in spintronics [3].

Figure 1. Top view of rock salt EuO and face centered silicon lattices. Purple ball represents Eu, red O and blue Si. It can be seen that rocksalt and face centered lattices match well. It can also be rotated by 45°.

Figure 2. Contour plot of PDOS for spin-up channel in the valence band and band gap regions. The dark blue region is the band gap and the yellow region is the valence band top.

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3:15pm **PCSI-1WeA-16 First Principles Study on Electronic Properties of Magnetite for Spin Polarized Emission under an Electric Field**, *Liang liang Xu, N Zhao, M Lin,* Hanyang University, South Korea; *T Leung,* National Chung Cheng University, Republic of China; *H Hsu,* National Taipei University of Technology, Republic of China

Magnetite is a mineral and one of the main iron ores. With the chemical formula Fe_3O_4, it is one of the oxides of iron. Magnetite is the earliest discovered magnet, around 1500 B.C. It crystallizes in the inverse cubic spinel structure (Fd3m) above the so-called Verwey transition temperature, which is about 120 K. In this work, we study the electronic properties of magnetite (100), (110), and (111) surfaces under external electric fields using first principles or *ab initio* calculations based on density functional theory. With an electric field applied, the surface properties could be modified. For example, the (111) surface with an O_2 termination, the half-metal behavior becomes metal behavior under a critical electric field. With a +U calculation, most of the surfaces with different terminations show half-metallic, different from those predicted by a without +U calculation. We can use an electric field to control the metallic properties to be metallic or half-metallic. Un addition, the effective work function changes under different field strength. By calculating the local work function, we can know the distribution of work function on a certain surface. The effective work functions of magnetite Fe_3O_4 on different surfaces have been determined. The local work function has been found to have the correspondences with the atoms' positions and charge densities. It is proposed that the magnetite as a half-metal can possibly be used as a spin-polarized electron source.

3:20pm **PCSI-1WeA-17 Work Functions of Alkali and Alkaline Earth Metal Surfaces under Electric Fields based on First-Principles Calculations**, *Y Wang, L Xu, Ming-Chieh Lin,* Hanyang University, South Korea; *T Leung,* National Chung Cheng University, Republic of China; *H Hsu,* National Taipei University of Technology, Republic of China

Alkali (Li, Na, K, Rb, Cs) and alkaline earth metal (Be, Mg, Ca, Sr, Ba) are widely used in various fields. In the field emission, the adsorption of alkali

metals and alkaline earth metals to tungsten (W) will greatly change the work function. In this work, we study the work functions and local work functions of alkali and alkaline earth metal (100) (110) (111) surfaces under different electric fields using the first-principles or *ab initio* calculations. The convergence of density-functional-theory (DFT) calculations in the local-density approximation (LDA) and generalized-gradient approximation (GGA) with a plane-wave basis set the projector-augmented wave method as implemented in the Vienna ab-initio simulation package (VASP) has been carefully and systematically tested. For a comparison, the work functions have been calculated with five different pseudo potentials. By applying an electric field on the alkali and alkaline earth metals, we can calculate the effective work function, local work function and investigate the dependence of the effective work function and the local work function on the field strength.

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PCSI
Room Canyon/Sugarloaf - Session PCSI-2WeA

Synthesis of Materials for Devices
Moderator: Alec Talin, Sandia National Laboratories

4:30pm **PCSI-2WeA-31 Nitrogen Doping of Gallium Oxide by Ion Implantation and its Application to Vertical Transistors**, *Masataka Higashiwaki,* National Institute of Information and Communications Technology, Japan; *M Wong,* National Institute of Information and Communications Technology; *K Goto, H Murakami, Y Kumagai,* Tokyo University of Agriculture and Technology, Japan   **INVITED**

β-gallium oxide (β-Ga_2O_3) has a very large bandgap (~4.5 eV) and a breakdown electric field exceeding 6 MV/cm, making it an attractive candidate for next-generation power electronics. However, Ga_2O_3 has a fundamental physical drawback, namely a lack of hole-conductive *p*-type material, because of unavailability of shallow acceptors, a valence band structure mostly formed by O 2*p* orbitals, and a self-trapping effect of free holes. Recently, we succeeded in developing a nitrogen (N)-ion-implantation doping process for Ga_2O_3 to form an energy barrier in a device structure [1] and then fabricating vertical Ga_2O_3 transistors by using a device process based on the N-ion implantation doping [2, 3].

N atoms are theoretically expected to be a deep acceptor in Ga_2O_3. We performed N-ion implantation doping into an *n*-Ga_2O_3 layer to fabricate a current blocking layer by forming a Si-doped–N-doped–Si-doped Ga_2O_3*n-p-n* junction. Note that Si is a shallow donor with an activation energy of about 50 meV in Ga_2O_3. Then, depletion-mode (D-mode) and enhancement-mode (E-mode) vertical Ga_2O_3 transistors with a current aperture were fabricated by using a manufacturable all-ion-implanted process, which is similar to commercial Si and SiC power device technologies, with Si and N doping. Both the D-mode and E-mode devices demonstrated successful transistor action and decent device characteristics.

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5:10pm **PCSI-2WeA-39 Studying the Nucleation of GaP on v-Grooved Si for III-V/Si Device Integration**, *Emily Warren,* National Renewable Energy Laboratory; *T Saenz,* Colorado School of Mines; *A Norman,* National Renewable Energy Laboratory; *J Zimmerman,* Colorado School of Mines

The direct heteroepitaxy of III-V materials on Si for high efficiency optoelectronic and photovoltaic applications has progressed greatly in recent years, but most studies have focused on polished wafers, that are compatible with microelectronics (e.g. CMOS) fabrication, but not photovoltaic technologies. There has been recent interest in growing III-Vs on "v-grooved" surfaces, where nanoscale patterning and facet selective

etching is used to pattern nominally (001) Si surfaces with linear (111)-facetted v-groove structures. This v-grooved geometry suppresses antiphase boundaries (APBs), thereby enabling defect-free nucleation of polar III-V materials on non-polar Si. However, for applications where cost is important, it also brings with it the challenge of creating the v-grooved pattern in a cost-effective way, without an expensive wafer-polishing step.

In this work, we show how v-groove structures can be prepared with cost-effective patterning approaches (nanoimprint lithography and interference lithography) on unpolished Si surfaces.[1] Unlike prior studies of growth of III-Vs on v-groove structures, which have focused on lattice mismatched heteroepitaxy of III-Vs (GaAs, InP, etc.), we have focused on GaP, which has a very small lattice mismatch with Si and enables us to understand the fundamentals of III-V nucleation on partially v-grooved surfaces, where multiple facets are exposed during growth. This is also an excellent platform to investigate the coalescence of selective area growth, a topic that is important for large-area applications such as photovoltaics.[2] We have systematically studied the nucleation conditions for GaP on v-groove Si and identified conditions that enable facet-selective nucleation without the formation of APBs, and lead to smooth, planar coalesced films.

5:15pm PCSI-2WeA-40 Improving Heterointerfaces in Rapidly Grown III-V Electronic Devices using Dynamic Hydride Vapor Phase Epitaxy (D-HVPE), *Dennice Roberts*, J Simon, K Schulte, A Ptak, National Renewable Energy Laboratory

High growth rates and precursor utilization make hydride vapor phase epitaxy (HVPE) a powerful tool for the growth of homoepitaxial III-V materials, particularly GaN and GaAs [1,2]. However, most applications are limited to thick single layers rather than electronic devices that require multiple heterointerfaces. Single-chamber HVPE systems are hampered by the long residence times of vapor phase constituents, typically requiring a growth interrupt to create abrupt interfaces. The non-abrupt nature of interfaces created in single-growth-chamber systems limits the use of HVPE in heteroepitaxial devices. The recent development of dynamic HVPE (D-HVPE) addressed this issue by introducing a second, largely isolated growth chamber, allowing a sample to be shuttled between growth chambers with established steady-state reactions to produce high quality, chemically- and structurally-abrupt interfaces. D-HVPE-grown single- and dual-junction GaAs and GaAs/GaInP solar cell devices show efficiencies approaching that of materials grown by more conventional means such as MOVPE. [3]

Here we present an assessment of improved interface quality between isostructural samples grown by traditional HVPE and D-HVPE in a custom reactor. Time-resolved photoluminescence measurements reveal samples grown by D-HVPE have significantly higher lifetimes than samples grown by HVPE. Trap-assisted recombination is also present in samples grown by traditional HVPE, resulting in different calculated lifetimes at high- and low-level injection. We compare structure and morphological differences and discuss growth mechanisms of D-HVPE grown solar cells.

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5:20pm PCSI-2WeA-41 Real-Time Optical Monitoring of the Epitaxial Growth of Zincblende Semiconductors, *Alfonso Lastras-Martinez*, Universidad Autónoma de San Luis Potosi, México

Non-invasive optical probes such as reflectance anisotropy spectroscopy (RAS) are attractive for real-time monitoring of the epitaxial growth of cubic semiconductors given their high sensitivity and instrumental simplicity. RAS enhances the surface response against the bulk signal by taking advantage of the reduced symmetry of the near-surface region of cubic crystals. Nevertheless, although the surface specificity of RAS has been known for long time, its use for monitoring epitaxial growth had been hampered by the lack of both a rapid spectrometer to follow epitaxial growth and a full understanding of the physics underlining RAS line shapes.

In this talk we demonstrate the power of RAS to elucidate phenomena occurring during the very first stage of the MBE homoepitaxial growth of GaAs (first half monolayer (ML)). We present real-time RAS spectra acquired during growth, taking advantage of a recently developed rapid RAS spectrometer. On the basis of a singular value decomposition analysis, we show that RAS spectra for As-rich surfaces (corresponding to c(4x4) and (2x4) surface reconstructions) comprise two independent components with contrasting evolutions along growth. A first component, associated to the orthorhombic strain induced by surface reconstruction, rises sharply upon starting growth and its amplitude changes sign as the surface reconstruction shifts from c(4x4) to (2x4). All this takes place during the

growth of the first half ML. Afterwards, the amplitude of the first component oscillates following layer-by-layer growth. In contrast, the amplitude of the second component shows relatively small changes along growth which suggests that it is characteristic of As-terminated surfaces, regardless of their specific reconstruction.

5:25pm PCSI-2WeA-42 Pulsed Laser Deposition of Epitaxial $Sr_3Al_2O_6$ as a Water-Soluble Sacrificial Layer for GaAs Deposition, *Imran Khan*, B McMahon, A Norman, A Zakutayev, National Renewable Energy Laboratory

Despite the record high efficiency for GaAs solar cells, its terrestrial application is limited due to both the particularly high costs related to the required single crystal substrates and the epitaxial growth. Significant substrate reuse is one strategy that has been heavily explored by the PV community, however, the usefulness of all the existing techniques is limited due to the need for toxic etchants, substrate re-polishing and/or expensive intermediate process steps. A water-soluble lift off layer could reduce costs by avoiding these potential downsides.

$Sr_3Al_2O_6$ (SAO) is a water soluble, cubic oxide (space group *Pa-3*), with lattice constant 15.84Å. This is close to $(2\sqrt2)a_{GaAs} = 15.99$Å, giving a close lattice match between SAO <100> and GaAs <100> after 45° lattice rotation. We investigated the epitaxial growth of high structural quality SAO on single crystal $SrTiO_3$ (STO) substrates by Pulsed Laser Deposition (PLD), and the feasibility of subsequently growing GaAs epitaxially on top of it.

We identified that pulsed laser deposited SAO on STO is polycrystalline for substrate temperatures lower than 650°C, however the films could be epitaxially crystallized partially by high temperature annealing. Careful optimization of the growth parameters for obtaining epitaxial SAO on STO was explored, and we identified that the SAO film quality is strongly dependent on the growth temperature and O_2 partial pressure. An STO capping layer was grown on the SAO to protect from moisture induced degradation, which was also epitaxial.

XRD spectra for the films with optimized deposition parameters showed SAO (400) and SAO (800) peaks that were epitaxially aligned to the STO (100) and STO (200) substrate peaks. TEM analysis revealed that the grown SAO films are epitaxially crystalline throughout the thickness. The epitaxial growth of the STO capping layer is a qualitative indication for the high quality of the SAO surface. Research activity is ongoing to experiment the practicability of growing GaAs on these sacrificial SAO films.

5:35pm PCSI-2WeA-44 Epitaxial Relationship of Cu3N Grown on YSZ(001) Substrate by Mist CVD Method, *Nao Wakabayashi*, Kogakuin University, Japan

Copper nitride (Cu3N) is Anti-ReO3 type cubic structure. It is reported that the bandgap energy of single crystal Cu3N is about 1.4 eV and this can be applied as a solar energy conversion material [1]. Cu3N has typically grown by physical vapor deposition (PVD) using vacuum pressure [2]. Mist chemical vapor deposition (mist CVD) method is one of the cost-effective growth techniques and is possible to grow in atmospheric pressure [3]. Recently, we have succeeded in the epitaxial growth of Cu3N on *c*-plane sapphire by mist CVD method using NH3 aqueous solution as a solvent. The epitaxial relationship in in-plane direction of this Cu3N film was Cu3N(100)//a-Al2O3(11-20). This indicates that the film had multi-domain structure, since a-Al₂O₃ has not cubic but corundum structure. [4]. In this study, Cu3N was grown on a YSZ(001) substrate by mist CVD method. The epitaxial relationship was evaluated.

Cu3N thin film was grown on a YSZ(100) substrate by vertical-type mist CVD method. Copper (II) acetylacetonate was used as a source material for the growth. The Cu (II) acetylacetonate was solved in NH3 aqueous solution of 28%. The concentration of Cu was 0.1 mol/L. The mist, formed by the 2.4 MHz ultrasonic transducer, was transferred to the reaction area by nitrogen carrier gas. The Cu3N film was grown totally for 2 hours at the temperatures of 300°C.

The XRD θ-2θ pattern, shown in Fig. 1(a), indicates that the film has the epitaxial relationship of Cu3N(001)//YSZ(001) in the growth direction. The XRD f scan patterns, shown in Fig. 1(b), indicates that the film has the epitaxial relationship of Cu3N(100)//YSZ(100) in the in-plane direction. Thus, we have succeeded in the suppression of multi-domain structure, which is observed in the growth on a-Al₂O₃, using the YSZ substrate with cubic structure.

In the presentation, different growth phenomena for Cu3N on a-Al2O3 and YSZ substrates are also discussed.

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5:40pm **PCSI-2WeA-45 UPGRADED: Halogen Surface Chemistries for Atomically Precise Manufacturing on Si(100)**, *Kevin Dwyer, M Dreyer, K Gaskell,* University of Maryland*; R Butera,* Laboratory for Physical Sciences
Atomic-scale fabrication of electronic devices in silicon has been widely demonstrated using a scanning tunneling microscope (STM) and hydrogen-based surface chemistries to precisely place phosphorous donor atoms on the surface. Incorporation of PH_3 precursors into lithographic patterns formed from a hydrogen resist in a Si surface can produce metallic wires, quantum dots defined by electrostatic gates, and single donor atom qubits for quantum information (QI) research[1]. However, interest in acceptor dopants and hole-based devices necessitates the development of alternate precursor and/or resist chemistries for device fabrication. Halogen chemistry is potentially more favorable for acceptor incorporation than hydrogen[2], and to that end we explore halogen-based resists including Cl, Br, and I, along with metal-halide precursors to deposit acceptor dopants.

Here, we present results on the complete surface passivation of Si(100) using Cl, Br, and I, and demonstrate STM lithography at cryogenic and elevated temperatures [3]. We further study the stability of halogen-terminated Si(100) in ambient environments using x-ray photoelectron spectroscopy (XPS) to facilitate transport of samples outside of ultra-high vacuum environments. Finally, we present results of metal-halide adsorption on Si(100) as a viable path towards acceptor doping.

6:00pm **PCSI-2WeA-49 Novel Growth Mechanisms in van der Waals Epitaxy: 3D Morphologies of Bi_2Se_3**, *Theresa Ginley, S Law,* University of Delaware
Van der Waals (vdW) materials, such as graphene, transition metal dichalcogenides, and bismuth chalcogenides, are an increasingly popular research topic due to their wide variety of applications. They are characterized by strongly bonded layers in the *a-b* plane and weak vdW bonds between layers in the *c*-direction. Careful control of vdW materials could create designer stacks of 2D materials or unlock the unique physics of 3D topological insulators, resulting in improved optoelectronic, spintronic, and valleytronic technologies. Growth via Molecular Beam Epitaxy (MBE) is a promising avenue for improved material quality due to its' highly customizable growth conditions. Unlike traditional MBE, which relies on the strong interaction between the growth material and a lattice matched substrate, vdW epitaxy takes advantage of the weak vdW bonds to grow on substrates with vastly different crystal structures. Unfortunately, vdW epitaxy cannot be fully explained via the well-known mechanics of traditional MBE. Growth of atomically smooth layers remains challenging as vdW materials tend to grow in terraced "wedding cake" morphologies. Also, vdW materials favor the (001) orientation with the vdW gaps parallel to the growth surface. Other orientations have been reported via MBE but require extensive substrate pretreatment or prepatterning. Improved understanding of the growth mechanisms involved in vdW epitaxy could allow for improved material quality as well as exotic growth morphologies.

In this study, we use the topological insulator Bi_2Se_3 as a prototypical vdW material for the exploration of growth mechanics. We chose to grow on GaAs(001) substrates as the interaction of adatoms with the post deoxidization reconstructed surface may provide greater insight than a less complex growth surface, such as previous work on sapphire substrates. It was found that growth at a substrate temperature of 425°C produced a significant amount of growth in the elusive (0015) orientation, with domains aligned along the GaAs[110] axis (Sample A). It is believed that bismuth aggregation due to thermal degradation as well as fast diffusion of bismuth along GaAs[110] combine to push growth into this orientation. A film grown on a 10nm $(Bi_{0.5}In_{0.5})_2Se_3$ buffer layer results in the formation of Bi_2Se_3 platelets with sheer walls and flat tops (Sample B). Based on this research it is believed that vdW growth dynamics are dominated by the relative strength of film/adatom and substrate/adatom interactions. The morphologies reported here differ significantly from those reported on sapphire, implying that substrate interaction is key to understanding novel morphologies in vdW materials.

PCSI

Room Canyon/Sugarloaf - Session PCSI-1ThM

2D Materials - Strain and Heterostructures

Moderator: Joshua Robinson, The Pennsylvania State University

8:30am **PCSI-1ThM-1 Electron Transport in Strain-Engineered Graphene**, *Nadya Mason,* University of Illinois at Urbana Champaign   **INVITED**
There is wide interest in using strain-engineering to modify the physical properties of 2D materials, for both basic science and applications. Deformations of graphene, for example, can lead to the opening of band gaps, as well as the generation of pseudo-magnetic fields and novel electronic states. We demonstrate how controllable, device-compatible strain patterns in graphene can be engineered by depositing graphene on corrugated substrates. We discuss several techniques for creating corrugated substrates [1,2], focusing on periodic spherical curvature patterns in the form of closely packed nanospheres. We show how the smaller nanospheres induce larger tensile strain in graphene, and we explain the microscopic mechanism of this [3]. We also present experimental results demonstrating how a nearly periodic array of underlying nanospheres creates a strain superlattice in graphene, which exhibits mini-band conductance dips and magnetic field effects that depend on the magnitude of induced strain [4]. This control of the strain degree of freedom provides a novel platform both for fundamental studies of 2D electron behavior and for prospective applications in 2D electronic devices.

9:10am **PCSI-1ThM-9 UPGRADED: Revealing Exciton Masses and Dielectric Properties of Monolayer Semiconductors with High Magnetic Fields**, *Mateusz Goryca, J Li, A Stier,* Los Alamos National Laboratory; *T Taniguchi, K Watanabe,* National Institute for Materials Science, Japan; *E Courtade, S Shree, C Robert, B Urbaszek, X Marie,* Universite de Toulouse, INSA-CNRS-UPS, LPCNO, France; *S Crooker,* Los Alamos National Laboratory
In semiconductor physics, many of the essential material parameters relevant for optoelectronics can be experimentally revealed via optical spectroscopy in sufficiently large magnetic fields. For the new class of monolayer transition-metal dichalcogenide (TMD) semiconductors, this field scale can be substantial – many tens of teslas or more – due to the relatively heavy carrier masses and the very large electron-hole (exciton) binding energies. For that reason many fundamental parameters of TMDs were – up to now – still assumed from density functional theory calculations and have not been experimentally measured.

Here we report circularly-polarized absorption spectroscopy of the monolayer semiconductors MoS_2, $MoSe_2$, $MoTe_2$, WS_2, and WSe_2 in very high magnetic fields up to 91 T. By encapsulating exfoliated monolayers in hexagonal boronnitride (hBN), we achieve very high optical quality structures that allow to follow the diamagnetic shifts and valley Zeeman splittings of not only the 1s ground state of the neutral exciton but also its excited 2s, 3s, ..., ns Rydberg states. The energies and diamagnetic shifts provide a direct determination of the effective (reduced) exciton masses and the dielectric properties of these monolayer semiconductors. Unexpectedly, the measured exciton masses are significantly heavier than predicted for Mo-based monolayers. Moreover, we also measure other important material properties, including exciton binding energies, exciton radii, and free-particle bandgaps. These results provide essential and quantitative parameters for the rational design of optoelectronic van der Waals heterostructures incorporating 2D semiconductor monolayers.

9:30am **PCSI-1ThM-13 Optical Determination of Ice-Induced Interfacial Strain on Single-Layer Graphene**, *Subash Kattel, J Murphy, S Pasco, J Ackerman, V Alvarado, W Rice,* University of Wyoming
Ice formed on a material creates a strain that is indicative of its adhesive strength with another material. Previous determinations of ice adhesion strength, a critical parameter for understanding icing physics, have proven to be highly dependent on experiment-specific conditions, such as surface roughness, icing conditions, water purity, etc. In this work, we use Raman spectroscopy to contactlessly and non-destructively measure temperature-dependent ice-induced strain for the first time. To isolate the ice-material interface, we probe the vibrational modes of single layer graphene (SLG) from 20°C to -30°C with and without ice as shown in Figure 1(a). Along with the well-known temperature-dependent Raman shift of SLG, a clear, ≈2 cm^{-1} change in the 2D-frequency (2650 cm^{-1}) developed upon ice formation is shown in Figure 1(b). We found this change in the Raman shift occurred even between supercooled water and ice at the same temperature. This small, change in the Raman shift of SLG corresponds to a 0.013% strain, which we show through spatial Raman mapping has a rich variation over the ice-SLG interface, as depicted in Figure 2. This point-by-point spatial mapping of the ice-induced strain enables precise correlation with surface roughness evaluation methods and theoretical models . Our results demonstrate that vibrational spectroscopy of 2D monolayers can precisely and locally measure strain at ice-material interfaces.

9:35am **PCSI-1ThM-14 UPGRADED: Electron Pairing by Remote-Phonon Scattering in Oxide-Supported Graphene**, *D Shin,* The University of Texas; *M Fischetti,* The University of Texas at Dallas; *Alex Demkov,* The University of Texas
Using first principles calculations we have shown that placing graphene on a (111)-oriented perovskite $SrTiO_3$ (STO) surface provides a possible doping mechanism [1]. Further theoretical analysis presented here suggests that coupling of electrons in graphene to interfacial hybrid plasmon/optical modes via remote-phonon scattering may result in an effective attractive electron-electron interaction that, in turn, could lead to electron pairing and superconductivity [2]. Specifically, we consider top-gated graphene supported by STO as shown in Fig.1. Using the full dynamic polarizability within the random phase approximation (RPA) for the entire system (including the hybrid modes arising from the coupling of the graphene plasmons to the optical phonons of the STO substrate and gate insulator), we estimate the superconducting transition temperature in the strong-coupling limit. In Fig. 2, we show the estimated superconducting critical temperature as a function of carrier density for different oxide thicknesses. As the carrier density increases, the critical temperature increases. The critical temperature is higher in the system of thicker HfO_2 oxide since the electron-IPP interaction is stronger with thicker top-gate oxide.

Figure 1. Schematic of a model used in our calculation. Here the STO substrate is assumed to be semi-infinite and the graphene layer is laterally infinite in the vacuum region between HfO_2 and STO.

Figure 2. Estimated superconducting critical temperature as a function of carrier density and the two indicated values of the oxide thickness in the strong-coupling limit.

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9:55am **PCSI-1ThM-18 Modeling of Interfaces in All-Solid-State Li-ion Batteries**, *Yue Qi,* Michigan State University   **INVITED**
Paring solid electrolytes with Li metal anode and high voltage cathodes form promising all-solid-state Li-ion batteries with higher energy density and ultimately safety. With the rapid development of fast Li-ion conducting solid electrolytes, the major bottleneck for all-solid-state Li-ion batteries lies at the high interfacial resistance and Li dendrite growth. This talk will focus on new mechanism understanding obtained by atomisticly-informed multi-scale modeling approaches.

The high interfacial resistance is due to two main factors: physical contact and chemical effect. The chemical effect was captured by a new density functional theory (DFT) based model, which predicts the potential map inside a solid-state battery and determines the potential drop, electrostatic dipole, and space-charge layer at the electrode/solid-electrolyte interface.[1] This new physics insight unified the seemingly contradictory experimental observations and led to new device design rules to promote interfacial ion transport in future solid-state batteries.[2] The physical contact was described by combining contact mechanics and 1D Newman battery model. The model suggested how much pressures should be applied to recover the capacity drop due to contact area loss.

To simulate Li dendrite growth inside polycrystalline solid electrolytes, we coupled DFT calculations with the phase-field method. This model successfully explained the experimentally observed dendrite intergranular growth and revealed that the trapped electrons at grain boundaries and surfaces may produce isolated Li-metal nucleation, leading to a sudden increase of Li-dendrite penetration depth. Based on the model, we developed new dendrite resistant criteria by comparing the basic material properties for a number of solid electrolytes including LLZO, Li_3PS_4, LATP, and LiPON. [3][4]

These modeling advancements will be integrated into a new framework to guide the development of all-solid-state Li-ion batteries.

[1] M.W. Swift and Y. Qi, Phys. Rev. Lett. 122, 167701 (2019)

[2] H.-K. Tian and Y. Qi, J. Electrochemical Society 164 (11), E3512-E3521

[3] H.-K. Tian, B. Xu, and Y. Qi Journal of Power Sources 392 (2018) 79–86

[4] H.-K. Tian, Z. Liu, Y. Ji, L.-Q. Chen, and Y. Qi, Chemistry of Materials 31 (2019) 7351-7359

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