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 MoSe₂/WSe₂ bilayers with small twist angles, where electrons mostly reside in the MoSe₂ and holes nominally in the WSe₂ 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 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 nonequilibrium (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 INVITED

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 as a 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 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.


3D Heterostructure Design

Moderator: Edward Yu, The University of Texas at Austin
2:35pm PCSI-1SuA-2 Optical Properties of Semiconducting Moiré Crystals, Xiaolin Elaine Li, Uniu of Texas at Austin INVITED

Sunday Afternoon, January 19, 2020

PB5 Room Canyon/Sugarloaf - Session PCSI-1SuA

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 (1×1) phase (i.e., unreconstructed surface) [1]. Indeed, the Ge surface remains in the (1×1) 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.


PB5 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, Hassad 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) [2,3], 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. In the family of RE-Vs, GdSb shares the common features of antiferromagnetic type II ordering and unusually high magneto-resistance. Due to the absence of orbital momentum in the 4f configuration of Gd + 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 In₁₋ₓAlₓSb and Be-doped In₁₋ₓGaₓSb 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 1×1, 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 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.


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4:50pm PCSI-2SuA-29 MBE Growth of Zn₁₋ₓCdₓTe on Cd₃As₂, Anthony Rice, K Alberi, National Renewable Energy Laboratory

The Dirac semimetal Cd₃As₂ 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$_{1-x}$As$_{x}$, limiting the ability to develop full heterostructures. One barrier to epitaxy on Cd$_{1-x}$As$_{x}$ is the high vapor pressure of Cd$_{1-x}$As$_{x}$ (1e-7 mbar at only 135 °C ), which is well below the ideal growth temperature of most semiconductors [1].

The Zn$_x$Cd$_{1-x}$Te$_y$ (111) system provides one promising option for overgrowth given that it can be lattice matched to the (112) surface of Cd$_{1-x}$As$_{x}$ and has a relatively low optimal growth temperature (240-300°C). Reflective high-energy electron diffraction (RHEED) patterns of epilayers grown on Cd$_{1-x}$As$_{x}$ 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$_{1-x}$As$_{x}$-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$_{1-x}$As$_{x}$ 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$_{1-x}$As$_{x}$ 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$_{1-x}$As$_{x}$ into a variety of device structures.


4:55pm PCS1-25uA-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$_x$Ti$_{1-x}$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$_x$Ti$_{1-x}$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-voltage characterization of these heterostructures will be presented.

5:00pm PCS1-25uA-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 (ALE) 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.

**PCSI**

**Room Canyon/Sugarloaf - Session PSCI-SuE**

**Single Photon Detectors**

*Moderator*: Christopher Palmstrom, University of California, Santa Barbara

*7:30 pm 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].


*8:10 pm 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, Kagakun University

8:30am PCSI-1MoM-1 MOCVD Epitaxy and Doping for β-Ga2O3 and (Al,Ga)2O3, Hongping Zhao, The Ohio State University

Invited
Ultrawide bandgap (UWBG) gallium oxide (Ga2O3) 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 Ga2O3 represents the thermodynamically stable crystal among the known five phases (α, β, γ, δ, ε). The breakdown field of β-Ga2O3 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-Ga2O3 a promising candidate for high power electronic device and solar blind photodetector applications. Single crystal β-Ga2O3 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-Ga2O3 thin films and its ternary alloy (Al,Ga)2O3. Control of background and n-type doping in β-Ga2O3 will be discussed. Record carrier mobilities of 184 cm²/Vs at room temperature and 4984 cm²/Vs at low temperature (45 K) were measured for β-Ga2O3 thin films with room-temperature doping concentrations of 2.5x10¹⁰ and 2.7x10¹⁰ cm⁻², respectively [1]. Growth and fundamental understanding of (Al,Ga)2O3 are still lacking. The limit of Al incorporation in beta-phase Ga2O3 has not been observed or experimentally verified, although it was predicted up to 60% of Al composition could be incorporated into β-Ga2O3. N-type doping capability as a function of Al composition in (Al,Ga)2O3 is another important fundamental question. Carrier transport properties in (Al,Ga)2O3 will be discussed.

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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 CeO2(111) with controlled degrees of Ce reduction and structural structures can be prepared on Ru(0001) single crystal substrate [2]. Metal-doped ceria mixed oxide interfaces were prepared by depositing Ti or Mn over CeO2(111) thin films. C co-doping of Ce with metal dopants can produce well-ordered Ce, CeO4(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).


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 micron-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].


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10:00am PCSI-1MoM-19 Effects of Annealing on Electronic Defects in β-Ga2O3 Revealed by Linearly-Polarized Photoluminescence (LPLP), 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-Ga2O3 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 grown 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 $^{137}\text{Cs}$ 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.


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 decry, 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.


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The molecular arrangement and the interfacial electronic properties of cobalt phthalocyanine (CoPc) on the deactivated B-Si(111)-V3 x V3 R 30° surface are analyzed using scanning tunneling microscopy and spectroscopy as well as photoemission studies. Our data demonstrate that for a low coverage of CoPc the molecules lie at with the p-orbital of the Si surface atom forming a hybrid state with the d$_x$ 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; 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-Free Halide Perovskites (FA,MA)SnI$_3$, 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 = H(NH$_2$)$_2$; MA = CH$_3$NH$_3$) 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.
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 biphase cobalt oxide composites that strike a careful balance of necessary chemical, optical, and electrical properties [1]. This coating consists of nanocrystalline CoOx 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 stability, the use of expensive catalysts (e.g. platinum) and higher operation temperature for gas sensing (>250°C) 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 (O2−, O− 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 have 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 uncover the scientific phenomena and optimization of device performance.

References:
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.


3:10pm PCSI-1MoA-15 Iuliacumite: A Novel Two-Dimensional Chemical Short Range Order in a Wurtzite Single Monolayer InAs$_{25}$Sb$_{25}$, 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 Pissard, 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 Dumin-Borkowski, P Ebert, Forschungszentrum Jülich, Germany; B Granddier, 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$_{25}$Sb$_{25}$, 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$_{25}$Sb$_{25}$ 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 $^{28}$Si 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.


Atomically precise placement of phosphorus dopants using scanning tunneling microscopy-based hydrogen deactivation 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.

This work was supported by the Laboratory Directed Research and Development Program at Sandia National Laboratories, and was performed, in part, at the Center for Integrated Nanotechnologies, a U.S. DOE, Office of Basic Energy Sciences user facility. Sandia National Laboratories is managed and operated by National Technology and Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy under contract DE-NA-0003525. The views expressed do not necessarily represent the views of the U.S. DOE or the United States Government.

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-photon 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.

Monday Evening, January 20, 2020

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 / SrTiO


8:10pm PCSI-MoE-9 Advances and Possibilities of the Materials Innovation Platform with Examples from Spin-ARPES, Daniel Beaton, Scienta Omicron Inc.

8:15pm PCSI-MoE-10 Superconductivity at Surfaces Studied by Scanning Tunneling Microscopy, Yukio Hasegawa, The University of Tokyo, Japan

8:30pm PCSI-MoE-11 Near-Surface Quantum Hall Effect in Atomically Thin Dirac Semimetals, Wei Chen, Institute for Quantum Matter, University of Maryland

8:45pm PCSI-MoE-12 Quantum Non-equilibrium Dynamics in 2D Topological Superconductors, Junyeong Choe, College of Natural Sciences, Korea Advanced Institute of Science and Technology

9:00pm PCSI-MoE-13 Quantum Hall Effect and Emergent Moving Skyrmion in Colloidal Spin Ice, Sunyoung Kang, College of Natural Sciences, Korea Advanced Institute of Science and Technology

9:15pm PCSI-MoE-14 Quantum Spin-Orbit and Electric Fields: A Lever for Surface Spintronics, Joseph Shinar, Department of Physics and Astronomy, University College London

9:30pm PCSI-MoE-15 Realizing Topological Surface States in Monolayer FeSe / SrTiO

9:45pm PCSI-MoE-16 High-κ Organic Superconductors: Toward Room Temperature Applications, Takanori Kunii, University of Tokyo, Japan

10:00pm PCSI-MoE-17 A New Perspective on the Strongly Correlated Quantum Critical Point in Two-Dimensional Transition Metal Oxides, Wataru Hirobe, KEK-PS Division, High Energy Accelerator Research Organization

10:15pm PCSI-MoE-18 Toward Exploring the Interplay between 2D Phase Fluctuations and the Interfacial Magnetic Field, David Pappas, National Institute of Technology

10:30pm PCSI-MoE-19 Quantum Optoelectronics in 2D Materials, Kyle Shen, B Faeth, S Yang, D Schiom, Cornell University

10:45pm PCSI-MoE-20 Topological Phase Transitions in 2D Magnetic Spin Ice, Yukio Hasegawa, The University of Tokyo, Japan

11:00pm PCSI-MoE-21 Toward Exploring the Interplay between 2D Phase Fluctuations and the Interfacial Magnetic Field, David Pappas, National Institute of Technology

11:15pm PCSI-MoE-22 Toward Exploring the Interplay between 2D Phase Fluctuations and the Interfacial Magnetic Field, David Pappas, National Institute of Technology
Diamond nanoprobes with single engineered NV centers allow enhancing the spatial resolution of 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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9:55am 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 films 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].

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.

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.

4. Åberg et al, IEEE J. of Photov, 6, 185 (2016)
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 specific 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.

In this work, we utilize microspheres on planar substrates to manipulate the emission properties of monolayer WSe$_2$ by Optical Environment Control – Cavities, Coupling and Substrate Manipulation, J Lee, Hyunseung Lee, Ajou University, Republic of Korea

Atomic thin layer of transition metal dichalcogenides (TMDs) such as monolayer WSe$_2$ exhibit direct bandgaps ranging from visible to near-infrared with strong excitonic 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 WSe$_2$. 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 WSe$_2$ 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.

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.
Wednesday Morning, January 22, 2020

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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, **Alex 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. 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 operation mechanism involving organic and inorganic materials, and nanostructured architectures 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 TaS$_2$-SnS Heterostructures with Flexible Stacking Architectures, **Dennice Roberts**, National Renewable Energy Laboratory; D Bordgett, University of Oregon; B Gorman, Colorado School of Mines; J Perkins, A Zakutayev, S Baurer, 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 selnide heterostructures. An example of such tunable properties is seen in the SnSe$_n$-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 inserted into the precursors. Electronic behavior as a function of number of SnS layers is measured.


11:45am PCSI-2WeM-40 Globally Aligned Single-Wall Carbon Nanotube Films through Electrostatic Ordering, **Joshua Walker**, University of Wyoming; J Fagan, A Bacchi, 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 repeatedly and automatically produce globally aligned SWCNT films. Using polarized spectroscopy, we show that high, two-dimensional nematic ordering (S$_{2n}$ ≈ 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 TiO$_2$, Thin Films by Laser Heating, **S Ahmed, J Ritter, M 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 $7 \times 10^{-7}$ change in resistance, from 10 kΩ to $>100$ GΩ. The heated area became transparent due to the loss of free-carrier absorption. Scanning electron microscope (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 Kujanpäivä**, 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, WS$_2$ or MoS$_2$, 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 MoS$_2$, WS$_2$ 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 heterostructures and other architectures based on ‘mix and match’ principle in precisely controlled fashion. Location specific synthesis of materials also provides access to the precursor 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.

Acknowledgement:

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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 silicides and between Si and Sb. These defect states do not easily match to conventional MIGS and this mixes states of metallic 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, $S=\phi_M-\phi_F$ 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.


Figure 1 Showing Fermi level de-pinning and orientation dependence

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

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 Voc values in past heterojunction solar cells, suggesting that this internal junction may, in fact, be limiting efficiencies. Interestingly, while its influence in R(T) is independent of contact materials such as In, Ag, Fe, Co, and Ni, CoS2 compounds dominate this junction and allow 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 CoS2 contacts as a way to both mitigate this junction and advance understanding of electronic transport in FeS2. This work was supported by the customers of Xcel Energy through a grant from the Renewables Development Fund.


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 conditions has been difficult to achieve. 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, Li 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 \textit{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 size increases, the work function increases proportionally. However, the work function is reduced doubly while the lattice size 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.
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 rock salt 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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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 Ga$_2$O$_3$ 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$_2$O$_3$ 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 2p orbitals, and a self-trapping effect of free holes. Recently, we succeeded in developing a nitrogen (N)-ion-implantation doping process for Ga$_2$O$_3$ to form an energy barrier in a device structure [1] and then fabricating vertical Ga$_2$O$_3$ 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$_2$O$_3$. We performed N-ion implantation doping into an n-Ga$_2$O$_3$ layer to fabricate a current-controlled Ga$_2$O$_3$ transistor. The electrical characteristics of Ga$_2$O$_3$ 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.

This work was partially supported by Council for Science, Technology and Innovation (CSTI), Cross-ministerial Strategic Innovation Promotion Program (SIP), “Next-generation power electronics” (funding agency: NEDO).


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. Unlike prior studies of growth of III-Vs on v-groove structures, which have focused on lattice mismatched heteroepitaxy of III-IVs (GaAs, InP, etc.) on Si(111), 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.

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.


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 isostuctural 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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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 SrAl2O4 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 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.

SrAl2O4 (SAO) is a water soluble, cubic oxide (space group Pa-3), with lattice constant 15.9Å. This crystal has 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 SrTiO3 (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 0° 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(001)/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 at 88%. 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 8-2θ 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(200) 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.

In this study, we use the topological insulator Bi$_2$Se$_3$ as a prototypical vdW material for the exploration of growth mechanisms. 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$_2$Se$_3$):Se buffer layer results in the formation of Bi$_2$Se$_3$ 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.

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5:40pm PCSI-2WsA-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-2WsA-49 Novel Growth Mechanisms in van der Waals Epitaxy: 3D Morphologies of Bi$_2$Se$_3$, 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$_2$Se$_3$ 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$_2$Se$_3$):Se buffer layer results in the formation of Bi$_2$Se$_3$ 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.
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, LPCN, 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 (TMDC) 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 boronitride (hBN), we achieve very high optical quality, 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-IP 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.


9:55am PCSI-1ThM-18 Modeling of Interfaces in All-Solid-State Li-ion Batteries, Yue Qi, Michigan State University

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 atomistically-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. 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. 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 a new dendrite resistant criteria by comparing the basic material properties for a number of solid electrolytes including LiZO, LiP$_2$S$_4$, 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.


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