PCSI
Room Ballroom South - Session PCSI-SuA
Topological Materials I & Pervovskites

Moderators: Scott Crooker, Los Alamos National Laboratory, Peter Krogstrup, Niels Bohr Institute

3:00pm **PCSI-SuA-1 Topological Superconductivity and Majorana Zero Modes on β-Bi$_2$Pd Thin Films**, ***Can-Li Song***, Tsinghua University, China **INVITED**

The search for Majorana fermions in solid state system is one of paramount research targets in physics today. Majorana fermions are an exotic class of fermions (which are their own antiparticles) and predicted to exist in topological superconductors. By growing β-Bi$_2$Pd epitaxial films on SrTiO$_3$ substrates with state-of-the-art molecular beam epitaxy, we here demonstrate a topologically nontrivial superconductivity on β-Bi$_2$Pd thin films. Majorana zero modes, supported by such a superconducting state, are identified by directly probing quasiparticle density of states within the vortex cores under magnetic field with a cryogenic scanning tunneling microscope. The superconductivity and Majorana zero modes (MZMs) exhibit resistance to intrinsic point and linear defects, characteristic of a time-reversal-invariant topological superconductor. Our discovery of the topological superconductivity and MZMs in single material of β-Bi$_2$Pd thin films represents one of the major advances in topological quantum physics.

3:30pm **PCSI-SuA-7 Origin of the Helicity Dependent Photocurrent in Electrically Gated (Bi$_{1-x}$Sb$_x$)$_2$Te$_3$ Thin Films**, ***Yu Pan***, *N Samarth, C Liu, Q Wang,* Penn State University; *A Yeats, D Awschalom,* University of Chicago

Experimental studies of three-dimensional topological insulators have shown that circularly polarized photons can robustly generate a directional helicity-dependent photocurrent at room temperature [1]. Surprisingly, the phenomenon is readily observed at photon energies that excite electrons to states far from those within the spin-momentum locked Dirac cone. The underlying mechanism for the helicity-dependent photocurrent is thus far from obvious and still a mystery. We resolve the puzzle by carrying out a comprehensive study of the helicity dependent photocurrent in (Bi1-xSbx)2Te3 thin films (Figure 1) as a function of the incidence angle of the optical excitation, its wavelength and the gate-tuned chemical potential (Figure 2). Our observations allow us to unambiguously identify the circular polarized photo-galvanic effect as the dominant mechanism for the helicity-dependent photocurrent. Additionally, we relate the directional nature of the photocurrent to asymmetric optical transitions between the topological surface states and bulk bands. This is rigorously inferred from a first principles calculation that reproduces the distinctive experimental dependence of the helicity-dependent photocurrent on gate voltage and excitation wavelength. The insights provided by our study are important for engineering opto-spintronic devices whose functionality relies on optical steering of spin and charge currents.

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3:45pm **PCSI-SuA-10 High-efficiency Hybrid Perovskite Based Optoelectronic Devices with Technologically Relevant Stability**, ***Aditya Mohite***, Los Alamos National Laboratory **INVITED**

Hybrid (inorganic-organic) perovskites have demonstrated an extraordinary potential for clean sustainable energy technologies and low-cost optoelectronic devices such as solar cells; light emitting diodes, detectors, sensors, ionic conductors etc. In spite of the unprecedented progress in the past six years, one of the key challenges that exist in the field today is the large degree of processing dependent variability in the structural and physical properties. This has limited the access to the intrinsic properties of hybrid perovskites and led to multiple interpretations of experimental data. In addition to this, the stability and reliability of devices has also been strongly affected and remains an open question, which might determine the fate of this remarkable material despite excellent properties. In this talk, I will describe our recently discovered approach for thin-film crystal growth as a general strategy for growing highly crystalline, bulk-like thin-films of both three-dimensional (3D) and layered two-dimensional (2D) hybrid perovskites that overcomes the above issues by allowing access to the intrinsic charge and energy transport processes within the perovskite thin-films and results in reproducible and stable high performance optoelectronic devices.

Briefly, photovoltaic devices fabricated using 3D hybrid perovskites show hysteresis-free response, with high degree of reproducibility, with an average efficiency of planar devices approaching ~18%. Photo-physical, electrical characterization and theoretical modeling attribute the improved performance to reduced defects (bulk and interface) and improved charge-carrier mobility in large-grain devices. Finally, I will also describe some new results on Ruddlesden-Popper phase perovskites based devices. In our first few attempts, we fabricated solar cells with efficiency approaching 13% as compared to the previous best of 4.5%. This phenomenal increase in efficiency is attributed to the near single-crystalline quality thin-films with a strongly preferential out-of-plane alignment of the inorganic perovskite component that facilitates efficient charge transport. Photovoltaic devices exhibit no hysteresis or degradation in performance under continuous operation and withstand an illumination intensity up to 4-Suns. Importantly, these devices with layered perovskites exhibit extraordinary, technologically relevant stability with no loss in performance with for ~2000 hours under humidity and 1-SUN full spectrum illumination.

4:15pm **PCSI-SuA-16 The Origin of High Photovoltaic Efficiencies in Large-grain Organic-Inorganic Perovskites**, ***Jean-Christophe Blancon***, *W Nie, A Neukirch, S Tretiak,* Los Alamos National Laboratory; *L Cognet,* Institut d'optique & CNRS; *A Mohite, J Crochet,* Los Alamos National Laboratory

Organometallic perovskites have attracted considerable attention after promising developments in energy harvesting and other optoelectronic applications. Notably, the recent synthesis of high-crystallinity thin films with grain sizes of hundreds of microns has offered a new opportunity for the development of efficient solar cells with high reproducibility and photo-stability [1][2]. However, it is crucial to obtain a deeper understanding of the intrinsic photo-physics and transport properties of perovskites with relevant structural characteristics. Here, we will present an investigation of the dynamics of photogenerated charge carriers in large-area grain organometallic perovskite thin films via confocal time-resolved photoluminescence spectroscopy. Our findings show that the bimolecular recombination of free charges is the dominant decay mechanism at excitation densities relevant for photovoltaic applications [3]. Bimolecular coefficients were found to be on the order of 10^{-9} cm^3/s, comparable to typical direct-gap semiconductors, yet significantly smaller than what is theoretically expected. We also will provide evidence that there is no degradation in carrier transport in these thin films due to electronic defects through modeling of the photoluminescence kinetics and open circuit voltage characteristics of a photovoltaic cell. We conclude that suppressed electron-hole recombination and transport that is not limited by defects provide a microscopic model for the superior performance of large-area grain hybrid perovskites for photovoltaic applications.

$^+$ Author for correspondence: jblancon@lanl.gov

[1] W. Nie, et al., Science **347**, 522 (2015).

[2] W. Nie, et al., Nat. Commun. **7**, 11574 (2016).

[3] J.-C. Blancon, et al., Adv. Func. Mater. **26**, 4283 (2016).

4:20pm **PCSI-SuA-17 Origin of Photo-absorption and Photo-emission in Two-dimensional Ruddlesden-Popper Perovskites**, ***Jean-Christophe Blancon***, *H Tsai, W Nie, A Stier,* Los Alamos National Laboratory; *L Pedesseau,* INSA de Rennes; *C Stoumpos, M Kanatzidis,* Northwestern University; *J Even,* INSA de Rennes; *S Crooker, J Crochet, A Mohite,* Los Alamos National Laboratory

Two-dimensional Ruddlesden-Popper layered perovskites (RPLPs) have recently emerged as an alternative to the classic bulk organic-inorganic hybrid perovskites, mainly due to significantly improved photo- and chemical-stability in optoelectronic devices [1][2]. They also offer a richer chemical playground as compared to their 3D counterparts, which promises a wider range of functionalities for this layered material. Few recent encouraging developments in optoelectronic applications, notably in energy harvesting and light emitting [2][3], have already been demonstrated in these two-dimensional layered perovskites. However, further development and optimization of devices will require a deeper understanding of the intrinsic photo-physics and transport properties of the phase-pure RPLP materials. Here we investigate the physical properties of photo-generated charge carriers in phase-pure (BA)$_2$(MA)$_{n-1}$Pb$_n$I$_{3n+1}$ layered perovskite family [4], for which the *n*-number can be experimentally tuned thus the thickness of the perovskite layer. It is found that the photo-absorption and photo-emission properties of thin films with n>2 are dominated by bound excited states associated with edge-states of perovskite layers, which rule the characteristics of thin-film solar cells and light-emitting diodes. On the other hand, optical and electronic properties in RPLP crystals derive from both quantum and dielectric confinements of carriers in the two-dimensional perovskite layers, which are promising for future applications of color-tunable photon sources. Opportunities to control and switch between these states is also relevant for novel technology.

⁺ Author for correspondence: jblancon@lanl.gov

[1] I. C. Smith, et al., Angew. Chem. Int. Ed. **53**, 11232 (2014).

[2] H. Tsai, et al., Nature **536**, 312 (2016).

[3] M. Yuan, et al., Nat. Nanotechnol. **11**, 872 (2016).

[4] C. C. Stoumpos, et al., Chem. Mater. **28**, 2852 (2016).

4:25pm **PCSI-SuA-18 Tin Oxide Atomic Layer Deposition on Hybrid Lead Halide Perovskites for Tandem Photovoltaics***, **Axel Palmstrøm**, K Bush, J Raiford, M McGehee, S Bent,* Stanford University

Hybrid lead halide perovskites are promising candidates for low cost, thin film light absorbers; they have a tunable band gap and have demonstrated efficiencies as high as 22.1%. As such, these materials are of interest for wide-bandgap absorbers in tandem photovoltaics. Hybrid lead halide perovskites have rough surfaces and are sensitive to temperature and oxidative conditions, making many deposition processes incompatible with this material. Typical perovskite solar ells employ spin-deposited organic selective transport layers and evaporated metal contacts on top of the perovskite absorber. These organic selective transport layers have two main drawbacks for tandem solar cells: first, the rough perovskite surface requires thick organic layers for complete coverage, resulting in significant optical losses and second, these organic materials are incompatible with the types of sputter processes used to deposit high quality transparent contacts (such as indium-tin oxide). We apply tin oxide by atomic layer deposition (ALD) as a dual-purpose layer to achieve electron selectivity and sputter protection with high optical transmission.

In this work, we investigate by x-ray diffraction thin film perovskite stability under various ALD reaction conditions on three perovskite materials: $Cs_{0.25}FA_{0.75}Pb_{0.5}Sn_{0.g}I_3$ (1.2 eV), $Cs_{0.17}FA_{0.83}Pb(Br_{0.17}I_{0.83})_3$ (1.6 eV) and $Cs_{0.17}FA_{0.83}Pb(Br_{0.5}I_{0.5})_3$ (1.8 eV). We then investigate the role of a LiF/C_{60} surface passivation layer on the stability and performance with tetrakis (dimethylamino)tin(IV) and water that degradation is driven by metal organic precursor exposure, rather than by moisture, and that LiF/C_{60} improves surface stability. Finally we demonstrate the efficacy of an optimized tin oxide layer for realizing both high efficiency and stability in perovskite-perovskite and perovskite-silicon tandem devices. We achieve an NREL certified 23.6% efficiency and over 1000 hr stability with a monolithic perovskite-silicon tandem architecture

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Room Ballroom South - Session PCSI-SuE

Energy & Van der Waals Heterostructures I

Moderators: Leonard Brillson, Ohio State University, Arend van der Zande, University of Illinois at Urbana Champaign

7:30pm **PCSI-SuE-1 Understanding Surface Chemistry of Atomic Layer Deposition: Toward Renewable Energy Applications***, **Stacey Bent,*** Stanford University **INVITED**

With the intensifying interest in functional nanoscale materials for applications in electronics and energy conversion, methods for fabricating materials with atomic-level control are becoming increasingly important. Atomic layer deposition (ALD) is a method that provides excellent capabilities for depositing thin films, nanoparticles, and other nanoscale materials. This talk will describe research into the surface chemistry occurring during ALD, focusing on the ALD of metal oxides of interest for renewable energy applications. Deposition of binary, ternary, and doped metal oxides at a range of important interfaces has already been demonstrated using ALD. However, a fundamental understanding of the growth process for metal oxides is still lacking. Moreover, it is often difficult to correlate the material properties and growth characteristics with the process parameters due to the limited understanding of the underlying surface chemistry. In this talk, we will describe the results of both *in situ* and *ex situ* studies investigating nucleation in metal oxide deposition, using zinc tin oxide (ZTO) as a model system. Based on a combination of quadrupole mass spectrometry, infrared spectroscopy, low energy ion scattering, and density functional theory, we propose mechanisms explaining the presence of a nucleation delay that occurs when the metal oxide processes are mixed. The application of ALD metal oxides to renewable energy applications will also be presented. We will examine both a photovoltaics application, in which ALD is used to deposit layers in thin film solar cells, and an application in clean fuel synthesis for which ALD produces active electrocatalysts.

8:00pm **PCSI-SuE-7 Li-ion Synaptic Transistor for Low Power Analogue Computing (LISTA)***, **Alec Talin,*** Sandia

Neuromorphic networks that emulate brain plasticity and adaptive learning will revolutionize artificial intelligence and computing. The key element for neuromorphic networks is the artificial synapse, which emulates the function of its biological counterpart using strictly solid-state components. Necessary attributes of an artificial synapse are non-volatile memory and history-dependent analogue states. These synapse characteristics can be realized using two-terminal memristive devices. However, two-terminal memristors cannot readily utilize existing computational algorithms designed for CMOS circuits, thus requiring development of new algorithms. Recently, three-terminal, transistor-like memristive devices utilizing an ionic liquid gate to control source-drain resistance by injection or extraction of oxygen vacancies have been demonstrated at Harvard and IBM. This functionality enables the implementation of spike time dependent plasticity (STDP) by converting the time difference between source (pre-neuron) and drain (post-neuron) spikes into a gate voltage. The exact channel conductance state achieved through a set of voltage pulses determines the synapse weight. The Harvard and IBM approach, however, has two principal drawbacks: 1) it requires a liquid gate to effectively inject or withdraw oxygen vacancies 2) switching is slow (~seconds) even at 160 ^{o}C due to the sluggish motion of oxygen ions in solid lattices at or near room temperature. To address these shortcomings, we describe an alternative synaptic transistor based on insertion/extraction of Li-ions from a Li_xCoO_2 channel. Similarly to oxygen vacancies, Li-ions act as dopants, contributing a mobile electron or hole every Li-ion insertion or extraction, depending on the specific material. Compared to O-vacancies, however, Li-ions move as interstitials with much lower activation energy. Since Li diffusivity at room temperature is relatively high, the ionic liquid gate is replaced in our device by a solid Li electrolyte to realize all-solid state synaptic transistors.

8:15pm **PCSI-SuE-10 The World of 2D: It's All About Interfaces***, **Joshua Robinson,*** Penn State **INVITED**

The last decade has seen nearly 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. Furthermore, heterogeneous stacking of 2D materials also allows for additional "dimensionality" for band structure engineering. In this talk, I will discuss recent breakthroughs in two-dimensional atomic layer synthesis and properties, including novel 2D heterostructures and novel 2D nitrides. Our recent works demonstrate that the properties of 2D materials, especially those grown via CVD, are extremely sensitive to the substrate choice. I will discuss substrate impact on 2D layer growth and properties, doping of 2D materials with magentic elements, selective area synthesis of 2D materials, and the first demonstration of 2D gallium nitride (2D-GaN). Our work and the work of our collaborators has lead to a better understanding of how substrate not only impacts 2D crystal quality, but also doping efficiency in 2D materials, and stabalization of nitrides at their quantum limit.

8:45pm **PCSI-SuE-16 One-dimensional Metals in Twin Grain Boundaries of $MoSe_2$***, Y Ma, H Coy Diaz, S Kolekar,* University of South Florida*; J Avila, M Asensio,* Synchrotron SOLEIL*; J Carmelo,* University of Minho*; **Matthias Batzill,*** University of South Florida

Electrons confined in one-dimension (1D) behave fundamentally different from the Fermi-liquid in higher dimensions. Material line defects are one dimensional but the search and proof of 1D electron behavior in such defects has been so far unsuccessful. In this presentation we show that a line defect in the 2D semiconductor MoSe2 is metallic and hosts 1D electrons. Scanning tunneling microscopy of monolayer MoSe2 films grown by MBE on other van der Waals materials reveal a high density of these line defects (figure). Furthermore, low temperatures STM shows the formation of a charge density wave (Peierl's transition) as is expected for any 1D-metal. Importantly, the high density of these crystallographically aligned defects enables the characterization of the electronic properties by angle resolved photoemission spectroscopy (ARPES) and thus, for the first time, a direct k-space resolved measurement of the electronic structure of a material's line defect. The measured Fermi-wave vector agrees with the measured periodicity of the charge density wave in STM. Further important verification of 1D behavior of these metallic states comes from the Tomonaga Luttinger liquid behavior of the density of states at the Fermi-level. The most 'exotic' property of 1D quantum liquids is, however, the separation of spin- and charge- excitations. Our ARPES measurements (figure) clearly exhibit the splitting of the spectral line into 'spinon' and 'holon' excitations. To understand these distinctive k-dispersion lines one has to go beyond the traditional Tomonaga Luttinger formalism for 1D electrons. Using a 1D Hubbard model with finite-range interactions enables to exactly reproduce our experimental data, demonstrating the observation of spin-charge separation in these line defects. Our results also imply that isolated quantum wires can be formed in twin boundaries of 2D transition metal dichalcogenides, which should enable quantum transport on these individual quantum line defects in the future.

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Room Ballroom South - Session PCSI-MoM

Nanostructured Surfaces/Oxides I/Semiconductor Growth I/New Techniques I

Moderators: Aaron Arehart, The Ohio State University, Stacey Bent, Stanford University, Shane Johnson, Arizona State University, Frances Ross, IBM T. J. Watson Research Center

8:30am **PCSI-MoM-1 Quantum dots created by atom manipulation with the scanning tunneling microscope*, Stefan Fölsch,*** Paul-Drude-Institut für Festkörperelektronik, Germany **INVITED**

Atom manipulation with the scanning tunneling microscope (STM) makes it possible to create ultimately small structures at surfaces. We extended this technique to III-V semiconductor surfaces [1,2] and found that their electrostatic potential landscape can be precisely designed by the controlled positioning of charged adatoms. In this way, quantum dots with identical, deterministic sizes can be created one atom at a time. By using the lattice of the InAs(111)A surface to define the allowed atomic positions, the shape and location of the dots is controlled with effectively zero error. The dots are assembled from +1 charged indium adatoms, leading to the confinement of intrinsic surface-state electrons [3,4]. This approach enables one to construct quantum dots with a perfectly defined level structure, as well as dot assemblies whose quantum coupling has no intrinsic variation but can nonetheless be tuned over a wide range.

In a related experiment, we found that the tunneling conductance of a single organic molecule adsorbed on InAs(111)A can be controlled by the adatom-induced gating potential, with the STM tip and substrate acting as source and drain contacts, respectively [5]. Depending on the potential, the molecular charge state can be tuned from neutral to -1, as well as to bistable intermediate states. Moreover, the molecule changes its orientational conformation upon charging. This coupling between charge and conformation induces a conductance gap more than one order of magnitude larger than normally found, for example, in electron transport through single molecules in the regime of strong electron-vibron coupling. The observed behavior can be rationalized within the framework of charge transport through a gated molecular quantum dot with strongly coupled charge and orientational degrees of freedom.

The discussed results illustrate that atom manipulation in combination with scanning tunneling spectroscopy provides detailed insight into the quantum-physical properties of artificial surface structures at the smallest size scales. Understanding and controlling these properties – and the new kinds of behavior to which they can lead – will be crucial for integrating atomic-scale devices with existing semiconductor technologies.

$^+$ Author for correspondence: foelsch@pdi-berlin.de

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9:00am **PCSI-MoM-7 Distance-Dependence of Chemical Interactions and Image Contrast Reversal in Noncontact Atomic Force Microscopy: A Case Study on Highly Oriented Pyrolytic Graphite*, Omur Dagdeviren,*** *J Goetzen, E Altman, U Schwarz,* Yale University

The structural and chemical nature of surfaces governs a material's ability to interact with its surrounding. Designing nanodevices requires tailoring surfaces to meet specific needs and revealing underlying fundamental principles, which determine surface reactivity at the atomic scale. A particularly interesting case occurs when the surface site exhibits varying attraction with distance. To shed light on this issue, noncontact atomic force microscopy experiments combined with scanning tunneling microscopy experiments have been carried out where the evolution of the atom-specific chemical interaction leads to contrast reversal in the force channel. Due to the importance of sp^2-hybridized carbon surfaces in functional nanostructures, we have used highly ordered pyrolytic graphite surface and metal probe tips as the model system. Our experiments reveal that at larger tip-sample distances, carbon atoms exhibit stronger attractions at hollow sites while upon further approach, hollow sites become energetically more favorable. The analysis suggests the fundamental factors promoting contrast reversal are local varying decay lengths and an onset of repulsive forces that occurs for distinct surface sites at different tip-sample separations. In addition to these, a change of the hybridization state of carbon atoms from sp^2 to sp^3 under the influence of an approaching reactive probe can also result in contrast reversal. Our experiments address the unexpected nature of contrast reversal due to different governing mechanisms, which are determined by local properties of the sample as well as interacting materials. Combined with in-depth computational analysis, such experiments will lead to a deeper understanding of the fundamental effects that govern how materials interact with their surroundings at sub-nanometer scale. Entangling these fundamental principles with design will enable fabrication and synthesis of better nanodevices with graphene and other layered materials as well as nanotubes.

9:05am **PCSI-MoM-8 Epitaxial Graphene Induced Surface Reconstruction in Ge(110)*, Gavin Campbell,*** Northwestern University*; B Kiraly,* Northwestern University, Netherlands*; R Jacobberger,* University of Wisconsin-Madison*; A Mannix,* Northwestern University*; M Arnold,* University of Wisconsin-Madison*; N Guisinger,* Argonne National Laboratory*; M Hersam, M Bedzyk,* Northwestern University

Understanding and engineering the properties of single-crystal surfaces has been critical in developing functional microelectronics at the nanoscale. Previously achieved through covalently bonded adatoms at surfaces, here we report how weakly bonded van der Waals' solids influence the development of new surface reconstructions in the EG/Ge(110) system. Employing scanning tunneling microscopy (STM), in-plane X-ray diffraction (XRD), and crystal truncation rod scattering (CTR) we investigate EG/Ge(110) and present a Ge(110) reconstruction stabilized by the presence of epitaxial graphene unseen in bulk semiconductor surfaces [1]. The combined STM and XRD results show the EG/Ge(110) interface, upon annealing, rearranges into a (6x2) superstructure persistence over large areas of the EG/Ge(110). CTR studies confirm the vdW gap and reveal that graphene sits atop the surface reconstruction with a 0.34 nm spacing. This structure represents a new avenue towards nanoscale engineering, using a vdW atomic layer to induce new stable surface reconstructions.

9:15am **PCSI-MoM-10 Emerging Memory Technologies and the Future of Computing*, Matthew Marinella,*** Sandia National Laboratories **INVITED**

The most significant bottleneck in modern computing is that between the processing and storage of information. Decades of improvement in microprocessor technology have rendered the energy and time requirements for computation insignificant compared to those for reading and writing to off-chip main memory and storage. Improvements in computational efficiency are now swamped at the system level by memory access – and solving this von-Neumann bottleneck is one of the key challenges to enable the next generation of computing. Fortunately, several compelling memory technologies are emerging which may solve this challenge. Chief among these are a class of devices in which the state of the memory is stored as the resistance across its terminals. These technologies include redox resistive memory (ReRAM), conducting bridge memory (CBRAM), phase change memory (PCRAM), ferroelectric tunnel junctions (FTJ), and spin transfer torque (STT-RAM). All of these technologies can be integrated into the back end of line with a standard CMOS logic process. Monolithic integration of memory with logic drastically reduces the latency and energy of memory access. Voltage controlled technologies like ReRAM, CBRAM, and PCRAM can be configured in a dense crossbar with an area as small as $4F^2$ when using an inline select device (where F is the minimum lithographic feature size). When layered, these devices can reach densities of 100 terabits per cm^2, which can enable extraordinarily dense information storage integrated close to the computation. Magnetic and ferroelectric memories are capable of nearly infinite endurance with a very low switching energy, and hence may offer a replacement for the large SRAM cell for caches. It is also possible to use emerging memories to perform logic operations, further increasing the efficiency and performance of a computing system. However, several challenges remain before the full potential of emerging memory technologies will be realized. Chief among these are improving retention, endurance, and bit error rates through better understanding of the basic physics of switching. In addition, the development of suitable in-line select devices will be required to enable maximum density. This presentation will discuss the basic physical mechanisms, state of the art, and future prospects for these key emerging memory technologies and their role in the Beyond Moore era of computing.

Sandia National Laboratories is a multi-mission laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

9:45am **PCSI-MoM-16 Optochemical Sensing using Metal Oxide Nanoparticles: Adsorption and Detection***, **James Whitten**, S Kim, R Somaratne, C Granz, S Sengupta,* The University of Massachusetts Lowell

While a large amount of literature exists related to the use of metal oxide nanoparticles for chemical sensing, most of those studies have involved measuring chemical resistance changes of heated metal oxide nanoparticle films upon exposure to gases or vapors. One disadvantage of this type of sensor is the relatively high electrical power needed for heating the film. However, many metal oxide nanoparticles are photoluminescent, with their emission spectrum related to the presence of defects and surface states. This offers a new opportunity for chemical sensing, since adsorption is expected to affect the emission spectrum. Zinc oxide is a particularly interesting photoluminescent metal oxide with a bimodal room temperature emission spectrum that consists of an excitonic recombination peak at 380 nm and a visible, defect-related peak in the 500-600 nm range. Examples of other photoluminescent metal oxide nanoparticles include zirconium oxide and cerium oxide. The goals of this work are to measure and understand the changes in the photoluminescence spectra of metal oxide nanoparticles upon exposure to various gases and vapors. In addition to atmospheric gases, reactive gases such as sulfur dioxide, methanethiol, hydrogen chloride and chlorine have been investigated. Experiments using nitrogen saturated with various organic vapors have also been performed, including methanol, benzene, toluene and pyridine. Photoluminescence measurements have been carried out in real-time using a custom-built UV LED-based fluorometer, and these have been accompanied by surface science studies on the powders to determine if irreversible chemisorption occurred. It has been found that molecules that chemisorb on ZnO nanoparticles, such as benzene and pyridine, cause an irreversible decrease in the intensity of visible emission peak and an increase in that of the UV peak. For physisorbates, such as methanol, the changes are completely reversible. Density functional theory (DFT) calculations have also been performed in an attempt to correlate the strength of adsorption to the photoluminescence changes.

9:50am **PCSI-MoM-17 Strained MoO_3/MoS_2 Heterostructures: Facile Fabrication,Structure and Electronic Properties***, **Vijay Saradhi Mangu**, S Brueck, F Cavallo,* University of New Mexico

Few atomic-layer-thick MoO_3/MoS_2 heterostructures are receiving increasing attention for application in opto-electronics as a result of their unique mechanical and electrical properties. For instance, this material combination can support a high strain field without undergoing plastic deformation, due to its nano-scale thickness. Strain significantly affects the band structure of MoS_2 and MoO_3, allowing a variety of different electronic heterostructures without altering the chemical composition of the bilayer on nm-scale transverse dimensions. Despite all this interest, the fabrication technology of MoO_3/MoS_2 heterostructures is still relatively primitive, and the fundamental electronic properties of this material combination have not been investigated in detail. We develop a facile process to fabricate few-layer MoO_3/MoS_2 heterostructures on textured substrates, and therefore achieve mechanically strained films. In our approach a ~1-3 mm-thick MoS_2 flake is extracted from a bulk crystal via mechanical exfoliation and transferred to bulk Si patterned into a matrix of ultra-sharp tips. After this process step the MoS_2 flake is only supported by the ultra-sharp tips and hence mostly suspended over the substrate. A thermal annealing step in air/Ar atmosphere results in: (i) formation of MoO_3 at the top and bottom surface of the MoS_2 flake, (ii) delamination of few-layer Mo-compounds at the bottom surface of the transferred flake (i.e., the one in contact with the Si tips), (iii) conformal contact of the delaminated layers to the substrate pattern. We obtain ultra-sharp tips of Mo-compounds with height ranging from 350 to 500 nm, and base of ~350 nm, as measured by scanning electron microscopy (SEM). The remaining portion of the MoS_2 flake stays intact, and it is removed by mechanical exfoliation. We demonstrate that different annealing conditions result in guided self-assembly of a variety of Mo-compounds. Specifically, we vary annealing temperature, air partial pressure, and annealing time to gain some insight on the chemical and physical processes which result in delamination and guided self-assembly of the ultra-thin films. The geometry, structural quality and spatially varying strain are characterized by optical contrast, electron microscopy, Raman and photoluminescence spectroscopies. The effect of different annealing conditions on carrier type and carrier concentration is estimated by X-ray photo-electron spectroscopy.

9:55am **PCSI-MoM-18 Photoinduced Electron Transfer Across Single Crystal Oxide Electrolyte Interfaces***, **Bruce Parkinson**,* University of Wyoming

Oxide single crystals are attractive substrates to study the fundamentals of photoinduced electron transfer process at interfaces. A variety of crystals are available in both synthetic and natural forms, including TiO_2, SnO_2 and ZnO, all of which have different surface chemistries, band gaps and conduction and valence band energies. We have studied the binding and photoinjection yields of various dyes, photoactive polymers, quantum dots and semiconducting nanotubes adsorbed on these carefully prepared atomically flat single crystal surfaces. The atomic flatness of the crystals allows imaging of the adsorbate structures possible using scanning probe microscopies. The experiments can be used to provide fundamental insights into solar energy conversion devices such as the dye-sensitized solar cells where we have developed and verified a physical model for predicting the electron collection yields in these systems [1]. We have also performed simultaneous total internal reflectance and photocurrent spectroscopy measurements on ZnO single crystal electrodes with adsorbed dyes to correlate the absorption spectra of the adsorbed monomer and aggregate species with the photoinjection yields measure with photocurrent spectroscopy and adsorbed dye structures as indicated by atomic force microscopy [2]. Using anatase TiO_2 single crystals we were the first to demonstrate photoinjected electron quantum yields of greater than one as a result of multiple exciton generation in adsorbed PbS quantum dots [3] opening the door for devices that exceed the Shockley/Queisser limit for photovoltaic energy conversion efficiency. Recently we have measured photoinjection from purified semiconducting carbon nanotubes on atomically flat synthetic crystals of SnO_2 [4] where multiple exciton generation and collection is also possible.

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11:00am **PCSI-MoM-31 The Atomic-Scale Mechanisms of Ternary Semiconductor Alloy Growth: Self-limited vs. Accumulating Anion Processes***, **Joanna Millunchick**, G Rodriguez, C Tait, E Anderson,* University of Michigan **INVITED**

Alloys of compound semiconductors are necessary to create heterostructures for optoelectronic and electronic devices. Growth of alloys that vary the cation component, eg: AlGaAs or InGaP, is fairly straight forward because there are few reactions between the cation species. Growth of mixed anion alloys, such as InAsSb and GaSbBi, are more complex because of the strong tendency for the individual anion species to interact. In the case of InAsSb, for instance, the displacement of Sb with impinging As is well documented. Furthemore, it is proposed that Sb atoms are weakly physisorbed on the surface. We investigate this hypothesis by scanning tunneling microscopy coupled with *ab initio* total energy calculations. We show that rather than remaining weakly physisorbed, Sb roughens the surface by increasing the coverage of divots (vacancy clusters) and two dimensional islands. Our calculations show how that As-terminated surface reconstructions may transform into mixed heterodimer terminated configurations, which causes the roughening by pulling atoms from the terrace. Thus we propose an alternative model for interfacial broadening by intermixing rather than by surface segregation. Another example of a complex mixed anion alloy is the Bi-containing materials system. The growth of GaAsBi and GaSbBi often leads to low Bi incorporation, droplets on the surface, and nonuniformity in the composition. We have developed a kinetic Monte Carlo simulation that explicitly takes cation and anion reactions into account that is capable of examining the unique characteristics of Bi-containing III-V semiconductor alloys. A phase diagram for a range of growth rates was generated using this simulation that predicts both Bi content and droplet formation. Furthermore, we propose a new kinetic model that captures the dynamics of incorporation and droplet formation in the growth of these alloys.

11:30am **PCSI-MoM-37 Preparation of InSb Surfaces for Molecular Beam Epitaxy Growth and Re-growth***, **Mihir Pendharkar**, J Lee, P Iyer, B Shojaei, A McFadden, J Schuller, C Palmstrom,* University of California, Santa Barbara

Molecular Beam Epitaxy of III-V semiconductors has allowed for a continued improvement in the understanding of materials and the discovery of novel physical phenomenon. The narrow band gap of InSb coupled with its low electron effective mass have generated significant interest for its applications in high electron mobility transistors and infrared detectors and metasurfaces. Lack of lattice matched wide band gap III-V substrates and the challenging thermal desorption of the InSb surface oxide, has led to the growth of InSb on highly lattice mismatched materials. Performance of functional InSb devices based on mismatched substrates has been limited due to very high defect and dislocation densities.

In this work, preparation of InSb (001) substrates by atomic Hydrogen cleaning, in Ultra High Vacuum, and subsequent growth of InSb epi-layers by Molecular Beam Epitaxy, has been demonstrated. The efficiency of Hydrogen cleaning on the surface of InSb, for removal of the surface oxide, was studied by X-Ray Photo-Electron Spectroscopy (XPS), Reflection High Energy Electron Diffraction (RHEED) and Scanning Tunneling Microscopy (STM). The developed surface preparation technique has allowed for the first demonstration of an InSb quantum well on an InSb substrate, with record electron mobility.

Re-growth of III-V epi-layers of InSb, after ex-situ device fabrication, has also been demonstrated. A combination of wet chemical etching and in-situ atomic Hydrogen cleaning has been used to achieve an epi-ready surface. The demonstrated ability of growth and re-growth on InSb (001) surfaces is expected to be a paradigm shift in the discovery and development of new electronic and photonic devices using (Al,Ga)xIn1-xSb material system as a template.

11:35am **PCSI-MoM-38 Mechanisms of Light-Assisted Epitaxy of III-V and II-VI Alloys***, **Kirstin Alberi**, K Park, D Beaton,* National Renewable Energy Laboratory*; M Scarpulla,* University of Utah

The synthesis of semiconductor epilayers, heterostructures and interfaces is often limited by adatom incorporation processes, dopant solubility and native defect formation. Modern uses of semiconductors therefore depend on our ability to control these processes during growth. Some degree of control is typically achieved by tuning the substrate temperature and chemical potential of the system. However, these variables may be inadequate for substantially manipulating some growth mechanisms. External stimulation of the growth surface through photon irradiation provides an additional process variable. Investigation of the mechanisms by which photon irradiation alters semiconductor growth suggests that the most substantial changes occur via electronic processes. Photogenerated carriers can directly modify adatom incorporation sites through enhanced desorption and passivation of dangling bonds [1,2]. Splitting of the quasi-Fermi levels caused by the presence of non-equilibrium carrier concentrations also affects the formation energy of native defects and built-in electric fields at the growth surface [3]. These mechanisms and the potential to exploit them to solve challenges related to the growth of metastable semiconductor alloys and heterovalent heterostructures as well as the impact on defects will be discussed.

$^+$ Author for correspondence: Kirstin.Alberi@nrel.gov

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[2] D.A. Beaton, C. Sanders and K. Alberi, Effects of incident UV light on the surface morphology of MBE grown GaAs, *J. Crystal Growth*, **413**, 76 (2015)

[3] K. Alberi and M.A. Scarpulla, Suppression of compensating native defect formation during semiconductor processing via excess carriers, *Scientific Reports*, **6**, 27954 (2016)

11:40am **PCSI-MoM-39 *Ab initio*-based Approach to Adsorption of In atom with Strain Relaxation on InAs Wetting Layer Surface Grown on GaAs(001)***, **Ryo Kaida**, T Akiyama, K Nakamura, T Ito,* Mie University, Japan

InAs/GaAs(001) lattice mismatched system has been paid much attentions to fabricate low dimensional nanostructures such as self-assembled quantum dots (QDs) by molecular beam epitaxy (MBE) [1]. Despite the importance of the InAs/GaAs(001) system, there has been few theoretical studies for the QD formation mechanisms because of the difficulty of understanding the behavior of InAs wetting layer (WL) grown on GaAs substrate by *ab initio* calculations. We previously revealed that the growth of InAs and resultant surface structural change cannot proceed without eliminating lattice strain in the InAs WL at 0.96 monolayer (ML) [2]. Furthermore, we recently clarified that misfit dislocation (MD) formation as one of promising candidates for strain relaxation mechanisms starts at the InAs/GaAs(001) interface from 0.5ML during the growth [3]. These findings suggest that the InAs growth and its surface structural change are closely related to the lattice relaxation mechanisms on the InAs WL. In order to clarify the relationship between the growth process and the strain relaxation, lattice relaxation mechanisms on the InAs WL, we investigate the adsorption behavior of In atom on InAs WL surfaces including various lattice strain conditions on the basis of *ab initio* calculations.

Figure 1 shows the calculated adsorption energy of In atom on the (4×3) reconstructed surface consisting of In-As dimers as a function of hypothetical lattice constant of the InAs WL, which corresponds to the strain relaxation of the InAs WL. The calculated adsorption energy on the (4×3) surface with lattice constant a=5.76 Å, which corresponds to InAs WL without strain relaxation, is larger than that for adsorption of In atom under the MBE condition at 730 K (-2.63 eV). This indicates the adsorption does not occur without strain relaxation [3]. In contrast, the adsorption energy of In atom drastically decreases when lattice constant is larger than 6.08 Å, and becomes close to the value for fully relaxed InAs WL of -2.63 eV. The reduction of adsorption energy around a=6.08 Å thus manifests that the adsorption of In atom and resultant surface structural change toward the (2×4) reconstruction [4] can be realized by eliminating lattice strain of the InAs WL such as MD formation.

$^+$ Author for correspondence: 415M605@m.mie-u.ac.jp

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11:45am **PCSI-MoM-40 Atom Probe Tomography of Low-Dimensional Materials: III-As Nanowire Heterostructures and Doped Layered Chalcogenides***, **Lincoln Lauhon**,* Northwestern University **INVITED**

We will describe the application of atom probe tomography (APT) to the analysis of facet driven composition fluctuations in GaAs-AlGaAs nanowire core-shell heterostructures and the distribution of Ag dopant atoms in (PbSe)$_5$(Bi$_2$Se$_3$)$_3$. AlGaAs is a ternary semiconductor whose composition can be tuned smoothly from GaAs to AlAs in molecular beam epitaxial growth. However, transmission electron microscopy and APT of GaAs-AlGaAs core-shell heterostructures have revealed facet dependent segregation.[1] Furthermore, APT analysis has linked quantum dot like emission spectra to composition fluctuations that exceed those expected for a random alloy,[1] despite the absence of a miscibility gap at typical growth temperatures. When the shell growth temperature is reduced from 560 °C to below 400 °C, the *non*-randomness of the alloy distribution in the AlGaAs shell is greatly reduced.[2] These observations will be explained in terms of a facet dependent segregation that is kinetically suppressed at reduced growth temperatures.

van der Waals heterostructures in layered or two-dimensional (2D) materials represent an entirely new class of ultrathin heterostructure. Doping of the constituent 2D materials provides a route to tuning electronic properties and forming new types of heterojunctions between semiconductors, metals, and superconductors. A nanoscale perspective on the dopant distribution can provide important insights into electronic structure and physical behaviors. APT analysis of Ag doped (PbSe)$_5$(Bi$_2$Se$_3$)$_3$ [3] shows that Ag dopes both Bi$_2$Se$_3$ and PbSe layers in (PbSe)$_5$(Bi$_2$Se$_3$)$_3$, and correlations in the position of Ag atoms suggest a pairing across neighboring Bi$_2$Se$_3$ and PbSe layers. Density functional theory (DFT) calculations confirm the favorability of substitutional doping for both Pb and Bi and provide insights into the observed spatial correlations in dopant locations. This work demonstrates the feasibility of APT analysis of 2-D materials.

$^+$ Author for correspondence: lauhon@northwestern.edu

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[2] Bernhard Loitsch, Nari Jeon, Markus Döblinger, Julia Winnerl, Eric Parzinger, Sonja Matich, Ursula Wurstbauer, Hubert Riedl, Gerhard Abstreiter, Jonathan J Finley, Lincoln J Lauhon, and Gregor Koblmüller. *Applied Physics Letters***109**, 093105 (2016).

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12:15pm **PCSI-MoM-46 High Aspect Ratio GaN Nanowires for Tip Metrology and Optical Application***, **Mahmoud Behzadirad**, M Nami, D Feezell, T Busani,* University of New Mexico

GaN has recently received many attentions for their specific optical properties as a wide band gap semiconductor. GaN, in form of single crystal NWs, is taking an important role in future optoelectronic devices as they can increase surface to volume ratio of the active region and enhance the device efficiency [1, 2]. Since the quality of the NWs after growing determine the efficiency of the final device operation, many researches have been devoted to grow high quality NWs [1, 2, 3]. Bottom-up approach has been employed to acquire desire NWs since late 1990s [3], however, it is difficult to control growing parameters in Molecular Beam Epitaxy (MBE) or Metal Organic Chemical Vapor Deposition (MOCVD), and so the fabrication process is complex and expensive. Likewise, growing high aspect ratio NWs with small diameter (<100 nm) is always challenging. On the contrary, top-down approach has demonstrated promising results in creating high aspect ratio structures as an alternative method for NWs fabrication. However, emerging roughness in side wall of the NWs and as a result poor optical property of the device has been an issue in top-down process which hindered wide application of this cost-effective method in device fabrication. Here, we demonstrate two-step (dry-wet etch) top-down fabrication of high aspect ratio (10-18) single crystal GaN NWs with side wall of sub-nanometer roughness. Two methods are employed to inspect NW side wall quality: i) TEM imaging, and ii) optically pumping of NWS. All NWs with different aspect ratio demonstrated very smooth side wall on TEM imaging as well a sharp lasing peak at ~367 nm when they are pumped with 266 nm laser. We also demonstrate how fabricated NWs can outperform standard Si tip in Atomic Force Microscopy, and potentially create more effective optoelectronic devices as they have less roughness compared to other reported works using the same growing method.

12:20pm **PCSI-MoM-47 Nanoscale Chemical Imaging with Photo-induced Force Microscopy***, **Thomas Albrecht**,* Molecular Vista

Correlating spatial chemical information with the morphology of multi-component nanostructures remains a challenge for the scientific community as many such systems are not easily interrogated at the nanometer scale in real space via existing instruments based on optics or electrons. A novel scanning probe technique called Photo-induced Force Microscopy (PiFM) measures the photo-induced polarizability of the sample directly in the near field by detecting the time-integrated force between the tip and sample. Imaging with infrared wavelengths specific to different molecular components, PiFM can resolve the nanometer-scale distribution of individual chemical species in diverse multi-phase and multi-component materials. When coupled to a widely tunable infrared quantum cascade laser system, a rich spectral analysis mode, which we call hyperspectral imaging, can be realized. A hyperspectral image consists of a PiFM spectrum (which correlates well with bulk FTIR spectra for most species) at each pixel of a (n x n) image. By detecting the molecular infrared absorption via mechanical force measurement on a sharp tip, PiFM achieves spatial resolution that surpasses the diffraction limit by an astonishing factor of ~1000 X. The power and utility of PiFM and hyperspectral imaging will be demonstrated by presenting results on several multi-component nanomaterials, including self-assembled block copolymer patterns, star polymers, polymer blends, asphalt binder, organic photovoltaic materials, and a variety of other materials.

12:25pm **PCSI-MoM-48 Z-Scan Photo-Reflectance Characterization of Resonant Optical Nonlinearities of Surfaces***, **Will Chism**,* Xitronix Corporation

Z-scan techniques based upon the distortion of a Gaussian laser beam provide a sensitive means to characterize nonlinear refraction and absorption in a wide variety of materials. In general, Z-scan techniques use the transmittance of a Gaussian laser beam through a finite aperture in the far field to determine the sign and magnitude of nonlinear refraction and absorption. Reflection Z-scan techniques are particularly suited to measure surface nonlinearities of materials with limited transparency. At the same time, photo-reflectance (PR) is a well established technique to study the bandstructure and interfacial electric fields of semiconductors and semiconductor microstructures. In general, PR measures the change in reflectivity of a sample whose surface electric field is modulated by the photo-injection of electron-hole pairs. The physical origin of the PR response is a resonant third order nonlinearity involving one probe photon and two DC field quanta. In this paper, Z-scan techniques are applied to the case of a probe laser beam in a PR setup. In particular, the theory of laser beam propagation as it applies to the probe laser beam in a PR apparatus is described and the use of Z-scan PR to independently characterize resonant nonlinear refraction and absorption in silicon-germanium samples exhibiting large absorption is demonstrated.

PCSI

Room Ballroom South - Session PCSI-MoA

Magnetism/Spintronics I/Organics/Nanostructures

Moderators: Martin Brandt, Walter Schottky Institut, Technische Universität München, Paul M. Koenraad, Eindhoven University of Technology, Netherlands, Daniel Loss, University of Basel, Giovanni Vignale, University of Missouri-Columbia

2:00pm **PCSI-MoA-1 Magnetic Dipole-dipole Sensing at Atomic Scale using Electron Spin Resonance STM***, **Taeyoung Choi**, W Paul,* IBM Almaden Research Center*; S Rolf-Pissarczyk,* Max Planck Institute for the Structure and Dynamics of Matter, Germany*; A Macdonald,* University of British Columbia, Canada*; K Yang,* IBM Almaden Research Center*; F Natterer,* École Polytechnique Fédérale de Lausanne, Switzerland*; C Lutz,* IBM Almaden Research Center*; A Heinrich,* Ewha Woman University, Republic of Korea **INVITED**

Magnetometry having both high magnetic field sensitivity (energy resolution) and nanoscale spatial resolution has been of great interest and an important goal for applications in diverse fields covering physics, chemistry, material science, and biomedical science. The scanning tunneling microscope (STM) has been one of the most versatile tools for atomic-scale imaging, manipulation, and tunneling spectroscopy.

Here, we successfully combine electron spin resonance (ESR) and STM, coherently driving spin resonance of individual iron (Fe) atoms on surfaces (MgO/Ag(100)) [1]. A radio-frequency electric field (~20 GHz), applied at the tunneling junction, modulates the spin state of the Fe atoms. The spin resonance signal is detected by a spin-polarized tunneling current. The ESR signals from individual Fe atoms differ by a few GHz (~10 µeV) while the ESR linewidth is in the range of only a few MHz (~10 neV). Such a high energy resolution enables us to distinguish spin distributions down to single-atom level and to investigate weak magnetic interactions.

When we placed two Fe atoms close together with controlled atom manipulation, we found that the ESR signal from each Fe atom splits into doublet, of which separation depends on the distance between two atoms. Our measurements show $r^{-3.01\pm0.04}$ distance-dependent splitting, in excellent agreement of magnetic dipole-dipole interaction. We utilized this precisely measured dipolar interaction to determine the location and magnetic moment of unknown spin centers with sub-nanometer and one hundredth of Bohr magneton precision [2].

Our ESR-STM may promise the STM as a new and unique platform for a quantum sensor, investigating spin-labeled molecular structures and a quantum information processor, modeling quantum magnetism. We gratefully acknowledge financial support from the IBM and Office of Naval Research.

$^{+}$ Author for correspondence: taeng0@gmail.com

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2:30pm **PCSI-MoA-7 Mechanism of Stabilization and Magnetization of Impurity-doped Zigzag Graphene Nanoribbons***, Y Uchida, S Gomi, H Matsuyama, A Akaishi, **Jun Nakamura**,* The University of Electro-Communications (UEC-Tokyo), Japan

In recent years, a considerable number of studies have focused on the modification of the electronic structure of graphene by nitrogen or boron doping. It has been reported that N atoms prefer to locate near the so-called zigzag edge of graphene, but it is not always understood why this should be so. In addition, every study has suggested a different interpretation of the appearance of impurity levels of dopants located near the zigzag edge of graphene nanoribbons (GNRs). Here, we propose the charge transfer model that satisfactorily explains the structural stability and the electronic structure of the impurity-doped zigzag GNR (ZGNR).

The structural stability and the electronic structure of doped ZGNR have been investigated using first-principles calculations based on the density functional theory. The formation energy of doping increases as a function of the distance between the N (B) atom and the zigzag edge, and two tendencies are observed depending on whether the dopant is an odd or even number of sites away from the zigzag edge. Such an energetic dependence is successfully explained by the charge transfer model; when the N (B) atom dopant is located near the edge, the extra electron (hole) of the N (B) atom transfers to the edge state, resulting in the occupation (vacation) of the originally-unoccupied (occupied) edge state. Since the edge state has amplitude only at odd-numbered sites, only the N-2p_z orbital at odd-numbered sites can resonate with the edge state; thus, the eigenvalue of the edge state for odd-numbered-site doping becomes lower than that for even-numbered-site doping. The gain in the electrostatic energy between the N cation (B anion) and the extra electron (hole) delocalized at the edge decreases with increasing distance of the N (B) atom from the edge, which leads to the trend of increasing formation energy. On the other hand, when the N (B) atom dopant is located sufficiently away from the edge, the extra electron (hole) is no longer transferred to the edge, but occupies the π*-band (π-band), which results in a kinetic energy gain because of the large energy dispersion of the π*-band (π-band) [1].

Such an electron (hole) transfer leads to the compensation (disappearance) of the local spin-magnetic moment at one side of the ZGNR, manifesting in the ferromagnetic ground state of ZGNR. Our findings will open up a route for development of new types of lightweight magnetic materials.

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2:35pm **PCSI-MoA-8 Magnetoresistance and Electrically Detected Magnetic Resonance Study of Leakage Currents in Low-k Dielectrics***, **Ryan Waskiewicz**, M Mutch, P Lenahan,* Penn State University*; S King,* Intel Corporation

Leakage currents in low dielectric constant thin films utilized in present day integrated circuitry are important reliability concerns. We have initiated a study of the defects involved in electron transport through low-*k* films utilizing both electrically detected magnetic resonance (EDMR) and low field magnetoresistance (MR) measurements. The EDMR and MR response involves spin dependent trap assisted tunneling [1]. The investigated sample structures were p-Si/a-SiOC:H/Ti. In the MR measurement, we observe a response very similar to the EDMR response at resonance, but the MR response occurs around zero magnetic field applied and is due to a mixing of singlet and triplet defect electron states. We investigate the gamma radiation response of leakage currents in dense and porous a-SiOC:H thin films, which are utilized in industry. (The changes generated are likely also relevant to high electric field behavior in these films.)Representative EDMR and MR spectra for the porous films as a function of bias during irradiation are illustrated in Fig. 1. Before gamma irradiation, we observe a weak MR response and nearly no EDMR response. Along with changes in leakage currents after 15 Mrad irradiation, we observe a large increase in both MR and EDMR response although the MR response remains larger than then EDMR response. A qualitatively similar response is observed in the dense films (not shown). The response of these films as a function of applied bias has also been studied with both EDMR and MR measurements. The amplitude of both the EDMR and MR responses increase linearly with applied Ti gate bias. At a negative bias, both responses are below detection limits. This bias response allows us to draw some conclusions about defect energy levels, which will be provided during the conference. This bias response also suggests that the defects responsible for the EDMR and MR are the same defect. As a continuation of this study, we will further study the response of these films with stressing and attempt to identify the defect(s) responsible for transport, now tentatively identified as Si dangling bonds before irradiation and C dangling bonds after irradiation [2]. This project is sponsored in part by the Department of Defense, Defense Threat Reduction Agency under grant number HDTRA1-16-0008. The content of the information does not necessarily reflect the position or the policy of the federal government, and no official endorsement should be inferred.

$^{+}$ Author for correspondence: rjw5352@psu.edu

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2:40pm **PCSI-MoA-9 Interface Characterization via Spin Dependent Charge Pumping***, **Mark Anders**, P Lenahan,* Penn State University*; A Lelis,* U. S. Army Laboratory

Electrically detected magnetic resonance (EDMR) has been very useful in the study of point defects in semiconductor/insulator heterojunctions. Nearly all of these EDMR interface studies have utilized spin dependent recombination (SDR). Although SDR EDMR is quite sensitive ($>10^7$ times the sensitivity of EPR). It utilizes a recombination current, so it is only highly sensitive to deep level defects. We show that a new EDMR technique, spin dependent charge pumping (SDCP) [1], overcomes this limitation, allowing EDMR measurements of defects with levels in most of the band gap. SDCP is also significantly more sensitive than SDR based interface methods. In

SDCP, a trapezoidal waveform is applied to the gate which cycles the Fermi level from near the conduction to valence band edges. Interface traps are filled, then emptied which creates a current that allows measurement of defects throughout most of the band gap. Like SDR EDMR, we find the sensitivity of SDCP is very nearly field and frequency independent, allowing for a wide range of resonance frequency and field SDCP measurements from 5600 Gauss to 35 Gauss. In addition, we find that there is a strong SDCP response near zero magnetic field. We believe this response involves physics similar to the low field magnetoresistance observed in organic semiconductors. SDCP at low resonance field and frequencies allows for: (1) partial separation of spin-orbit coupling and hyperfine effects on magnetic resonance spectra, (2) observation of otherwise forbidden half-field effects [2] which make EDMR, at least in principle, quantitative, and (3) observation of Breit-Rabi shifts [3] in superhyperfine measurements. We present results on 4H-SiC nMOSFETs, but the approach utilized should be widely applicable to other heterointerfaces such as Si/SiO$_2$, Si/High-K, and SiGe/insulator systems. Although the abstract length is too short to discuss all results, we illustrate a representative ultra-low resonance frequency (85 MHz) SDCP spectrum in Fig.1. Fig 1(a) illustrates the Breit-Rabi shift of the 10.4 Gauss doublet, a hydrogen complexed E' center spectrum. Fig. 1(b) illustrates the half-field resonance response due to the "forbidden" transitions created by magnetic dipole-dipole moment interaction between defects. Its intensity, in principle, allows a precise quantitative measurement of the defect density via EDMR [4]. The strong response near zero magnetic field can provide some hyperfine information and EDMR-like detection in fully processed devices without the expense and complexity of a resonance spectrometer.

2:45pm **PCSI-MoA-10 Theory of the Nonlocal Anomalous Hall Effect***,* ***Giovanni Vignale****, S Zhang,* University of Missouri-Columbia **INVITED**

The anomalous Hall effect is deemed to be a unique transport property of ferromagnetic metals, caused by the concerted action of spin polarization and spin-orbit coupling. Nevertheless, recent experiments have shown that the effect also occurs in a nonmagnetic metal (Pt) in contact with a magnetic insulator [yttrium iron garnet (YIG)], even when precautions are taken to ensure that there is no induced magnetization in the metal. We propose a theory of this effect based on the combined action of spin-dependent scattering from the magnetic interface and the spin-Hall effect in the bulk of the metal. At variance with previous theories, we predict the effect to be of first order in the spin-orbit coupling, just as the conventional anomalous Hall effect - the only difference being the spatial separation of the spin-orbit interaction and the magnetization. For this reason we name this effect "nonlocal anomalous Hall effect", and we predict that its sign will be determined by the sign of the spin-Hall angle in the metal. The anomalous Hall conductivity that we calculate from our theory is in order of the magnitude agreement with the measured values in Pt/YIG structures.

3:15pm **PCSI-MoA-16 Spin-Polarized Current Injection Induced Magnetic Reconstruction at Oxide Interface***,* ***Gunter Luepke****,* College of William & Mary

Electrical manipulation of magnetism presents a promising way towards using the spin degree of freedom in very fast, low-power electronic devices. Though there has been tremendous progress in electrical control of magnetic properties using ferromagnetic (FM) nanostructures, an opportunity of manipulating antiferromagnetic (AFM) states should offer another route for creating a broad range of new enabling technologies. Here we selectively probe the interface magnetization of SrTiO$_3$/La$_{0.5}$Ca$_{0.5}$MnO$_3$/La$_{0.7}$Sr$_{0.3}$MnO$_3$ heterojunctions and discover a new spin-polarized current injection induced interface magnetoelectric (ME) effect [1]. The accumulation of majority spins at the interface causes a sudden, reversible transition of the spin alignment of interfacial Mn ions from AFM to FM exchange-coupled, while the injection of minority electron spins alters the interface magnetization from C-type to A-type AFM state. In contrast, the bulk magnetization remains unchanged (Fig. 1). We attribute the current-induced interface ME effect to modulations of the strong double-exchange interaction between conducting electron spins and local magnetic moments. The effect is robust and may serve as a viable route for electronic and spintronic applications.

4:30pm **PCSI-MoA-31 Organics Invited 2***,* ***Markus Wohlgenannt****,* University of Iowa **INVITED**

5:00pm **PCSI-MoA-37 Microwave Magnetization Dynamics in Room Temperature Organic-Based Magnets: From Fundamental Studies to Emerging Applications***,* ***Ezekiel Johnston-Halperin****, M Chilcote, A Franson, M Harberts, Y Lu, H Yu,* The Ohio State University*; N Zhu,* Yale University*; I Froning,* The Ohio State University*; X Zhang,* Yale University*; R Adur, C Hammel, A Epstein,* The Ohio State University*; M Flatte,* University of Iowa*; H Tang,* Yale University

Organic and organic-based materials are attractive candidates for applications in magnetoelectronics and spintronics due to their low cost, ease of fabrication, and low spin-orbit coupling (and consequently long spin lifetimes). More recently, advances in these fields have highlighted the potential for dynamic excitations to drive new phenomena such as ferromagnetic resonance generated spin-pumping. Here we present a series of recent breakthroughs in the synthesis, encapsulation, and measurement of organic-based magnets that lay the foundation for all organic magnetoelectronic and spintronic devices. We will discuss advances in encapsulation strategies that allow lifetimes of up to 1 month in air [1], the use of ligand substitution to generate a library of related magnetic materials [2], the growth of all-organic and hybrid organic/inorganic magnetic heterostructures, and measurements of ferromagnetic resonance (FMR) linewidths of ~ 1 Oe [3], comparable to yttrium iron garnet (YIG). Finally, we demonstrate the potential for real world applications in the construction of a V[TCNE]2 based spin-wave resonance device with spectral tuning from 1 – 5 GHz and a quality factor in excess of 3,200 that operates under ambient conditions [4]. These results establish the validity of organic-based magnets for applications in next-generation magnetoelectronics and provide unique leverage on long-standing challenges in the field of organic spintronics.

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5:05pm **PCSI-MoA-38 Characterization of Energy Conversion Behavior in Nanostructured PEDOT Polymer-Graphene Composite***, M Sakr, S Abdel-Nasser,* ***Mohamed Serry****,* American University in Cairo, Egypt

One of the major drawbacks for successful application of graphene in energy storage and conversion applications is its cone shaped band gap. Therefore, several ongoing researches are currently focusing on the opening of the graphene band gap by doping, patterning and applying electric field on graphene layers [1]. Accordingly, in this work, we study a new composite structure consisting of nanostructured conducting polymer deposited on the surface of graphene-Schottky-diode (Conducting-Polymer/Graphene/Pt/n-Si) for enhanced energy storage and opto-electrical energy conversion applications. Poly (3,4-ethylenedioxythiophene) (PEDOT) was selected as the organic semiconductor material because of its low band gap (1.5−1.7 eV), long-term stability as well as good electrical conductivity. Significant enhancement in the dark current from 99 μA for the bare graphene-Schottky devices to 20 mA for the PEDOT composite structures at −10V bias which corresponds to more than 196 times enhancement in current. The morphology of the composite electrodes (Fig. 1) shows very well dispersed particles of the deposited polymers on the graphene surface. Fig. 2 (a) shows the dark I-V characteristics of the composite electrodes as well as the bare material, which illustrates a distinctive increase in the current behavior for all the PEDOT composite samples with respect to the bare graphene samples. The current response was extensively increased upon the deposition of PEDOT reaching 4.7 mA for the 200 μl PEDOT volume.

5:10pm **PCSI-MoA-39 Applications of Switchable Interfacial Dopants***,* ***Peter Kruse****, A Mohtasebi, T Chowdhury, E Hoque, O Sharif,* McMaster University, Canada

Doping of bulk semiconductors and low-dimensional structures (carbon nanotubes, graphene, etc.) in order to modulate their electronic properties is a well-established concept.[1] However, it is usually permanent. Even in cases where doping of thin films by analytes (e.g. carbon nanotubes by ammonia) is applied in sensors, it is only reversed by physical removal of the dopant molecules, e.g. through heating. On the other hand, molecular switches are also an old concept by now, but practical examples of facile detection of their state with a thin film sensor are less common. We demonstrate the facile doping and de-doping of iron oxide films as well as carbon nanotube networks in contact with different oligoaniline oxidation states as an example of interfacial doping with a switchable dopant, i.e. a molecular switch. The idea that a small local change in carrier concentration (in this case due to a modification of the doping state) results in a large change in resistivity is somewhat reminiscent of (but not identical to) a chemical field effect transistor (in which case the electric field is modulated due to creation of electric charges), in that it also constitutes an active sensor. While for most conventional sensing applications, the removal of the dopants from the film present one challenge and the selectivity to a particular dopant another, even bigger, challenge, our devices keep the dopants in place. The sensing performance is achieved by switching the dopants between active and inactive states. A redox sensor for measuring chlorine concentrations in drinking water [2] is the first member of this new class of sensors, although the concept certainly can be applied to many other systems. Not only are these systems relevant for sensors, but charge transfer in closely coupled redox systems (e.g. oligonanilines and iron oxide) also find applications in corrosion inhibition [3] and smart coatings, another application that we are exploring in our group.

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5:15pm **PCSI-MoA-40 On the Possibility of the Development of Vicinal Superlattices in Quantum Wires on Semiconductor Low - Index Surfaces***, **Victor Petrov,*** Russian Academy of Science, Russian Federation

As is well known, vicinal superlattices (VSLs) are realized in 2D electron systems on semiconductor high-index Miller surfaces. The possibility of existence of such VSLs was predicted theoretically [1,2]; simultaneously and independently they were realized [3]. The existence of SL effects in VSLs is due to the appearance in these systems of a new cristallographic translation period in the plane of quantum wells A >> a_0 (a_0 is the lattice constant). A new translation period A produces minigaps (MGs) in the energetic spectrum of the particles in these systems and, as a result, different SL effects. At the present time, all these VSLs are developed only in 2D systems. At the same time, it is known that superlattice effects should be maximal in quantum wires (QWR) when the SL period A appears along the axis of the QWR.

In this work we suggest a new method of development of VSL in QWR on semiconductor low-index surfaces. For this purpose we suggest to orient the axis of the QWR at the necessary angles to the basic translation vectors on a low-index surface. In this case in the QWR the new basic translation period along the axis of the QWR A > > a_0. Thus, the period A along the surface in the one-dimensional VSL is selected by the orientation of the QWR on the low-index surface. If the QWR is realized in the MOS system with the use of a narrow gate [4] then the orientation of the wire will be determined simply by the appropriate orientation of the gate. The analytic expressions of the new periods A were obtained as a function of the angles which determine orientation of the QWR for the different low-index surfaces GaAs and Si. The positions of MGs in the one-dimensional k-space were determined. It is should be noted that in the region of the particle wave function localization in the QWR there are many crystallographic planes which form a SL energetic spectrum of the particle. Illustrative estimates of the magnitude of the MGs for the QWR of the rectangular cross-section made in the weak coupling approximation demonstrate their dependence on the geometric parameters of the cross-section, on the period A as well as on the crystal potential.

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5:20pm **PCSI-MoA-41 Site-dependent Oxygen Reduction Reaction of N-doped Graphene Nanoclusters***, **Haruyuki Matsuyama**, S Gomi, M Ushirozako, A Akaishi, J Nakamura,* The University of Electro-Communications (UEC-Tokyo), Japan

Nitrogen-doped graphene exhibits high oxygen reduction reaction (ORR) activity [1]. Recently, it has been theoretically revealed that nitrogen atoms prefer to locate near the zigzag edge of graphene [2]. Therefore, many theoretical researchers have focused on the nitrogen atom existing at the graphene edge. In this study, we focus on the role of edge structures of nitrogen-doped graphene on the ORR activity.

We investigated the ORR activity for the hexagonal nitrogen-doped graphene nanoclusters having zigzag or armchair edges, using first-principles calculations within the density functional theory. Electrocatalytic activities were evaluated on the basis of the computational hydrogen electrode model proposed by Nørskov *et al.* [3] In general, the ORR mainly proceeds in two pathways: For the two-electron pathway ($2e^-$), O_2 is reduced to hydrogen peroxide (H_2O_2), and for the direct four-electron pathway ($4e^-$), the final product is water (H_2O). H_2O_2 for the $2e^-$ pathway might erode electrocatalyst materials, leading to low durability. Therefore, we also pay attention to the selectivity for the $4e^-$ pathway.

Figure 1 shows a model of the zigzag graphene nanocluster. Doping sites of nitrogen atoms are indicated in this figure. Figure 2 shows maximum electrode potentials for ORR at each doping site. The maximum potential for the $4e^-$ pathway is higher than that for the $2e^-$ pathway in almost all reaction sites. It is noted that the high selectivity for the $4e^-$ pathway is assured not just at the edge but inside the cluster. The effects of edge structures, cluster sizes, and doping configurations on the ORR activity will be discussed in the presentation.

5:25pm **PCSI-MoA-42 Nanopore Formation with Au Cluster via Ostwald Ripening for Optical Nanobio Sensor***, **SeongSoo Choi**, M Park, C Han, S Oh,* SunMoon University, Republic of Korea*; D Park,* Hallym University, South Korea*; Y Kim,* Sungkyunkwan University, Republic of Korea*; N Park,* Seoul National University, Republic of Korea

There have been tremendous interests about the fabrication of portable optical nano-biosensor due to its potential application of single molecule analysis such as DNA and RNA, and protein. Recently the fabrication of the portable device with an electrical detection technique (MinION by Oxford nanopore technology) was reported, however, the high error rate for DNA analysis were reported and are being hindered its practical application [1]. In this report, we will address the fabrication of optical nanopore by using plasmonic effect. The freestanding ~ 40 nm thick Au films were obtained by using conventional sputter deposition of Au on the SiN films followed by removal of supporting SiN film with a plasma etching technique. The deposited Au films would consist of the mixture of various size Au nanoclusters and nanoparticles. Depending upon the Au cluster size, the melting points would vary due to the cluster shell model. The ~ 100 nm diameter Au aperture was initially fabricated with 30 keV Ga ion focused ion beam on the deposited Au film. Then, the Au pore membrane incorporated with carbon atoms inside the 100 nm diameter Au aperture was formed under electron beam irradiations The Au pore-membrane incorporated with carbon atoms under electron beam irradiations were formed. Initially, the Au atoms (less than 1 nm) on the diffused pore membrane were not able to be detected due to resolution limit of TEM. ~ 1 nm. When the samples were kept under the room environment for several months, the Au nanoclusters were formed on the diffused membrane [2]. During electron beam irradiations, melting of the Au films would be dependent upon the Au nanocluster size, conductivity of the Au films, electrical contacts between the specimen and the sample holder, etc. Under the laboratory environments, the Au clusters on the diffused membrane were formed via Ostwald ripening [2]. The spinodal decoposition, i.e, unstable structural change of the Au structures in the amorphous Au-C membrane system [3] were observed during electron beam irradiations. The Au clusters formed on the Au-C pore membrane can be utilized as an optical nanopore sensor.

+ Author for correspondence: sscphy2010@gmail.com [mailto:sscphy2010@gmail.com]

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5:30pm **PCSI-MoA-43 Tunable-Composition Multi-Component Thin Films using Split-Target Pulsed Laser Deposition**, ***Wayne McGinnis***, *A Hening, T Emery-Adleman,* SPAWAR Systems Center Pacific

A new technique has been developed that uses pulsed laser deposition (PLD) with a two-part (split) ablation target to grow thin layers of a multi-component oxide film with improved control over the resultant film elemental composition. One often heralded advantage of PLD for growth of chemically complex materials is stoichiometric transfer of the target material to the substrate. In some cases, though, target stoichiometry is preserved only under very specific deposition conditions that vary depending on the target material and the substrate temperature. Such conditions are often difficult and time-consuming to determine. The new technique overcomes these difficulties, and has been used to demonstrate the ability to grow mixed-metal oxide films of varied stoichiometry from a single split target.

5:35pm **PCSI-MoA-44 Effective Nitrogen Doping into TiO_2 for Visible Light Response Photocatalysis by Ion Implantation Technique**, ***Tomoko Yoshida***, Osaka City University, Japan; *S Niimi, M Yamamoto, S Yagi,* Nagoya University, Japan

Photocatalytic reactions at the surface of titanium dioxide (TiO_2) under UV light irradiation have been attracting much attention in view of their practical applications to environmental cleaning such as self cleaning of tiles, glasses, and windows. Recently, Asahi *et al.* reported that the doping of nitrogen into TiO_2 contributes to band gap narrowing to provide visible-light response.

In the present study, the thickness-controlled TiO_2 thin films were fabricated by thepulsed laser deposition (PLD) method. These samples functioned as photocatalysts under UV light irradiation and the reaction rate depended on the TiO_2 thickness, i.e., with an increase of thickness, it increased to the maximum, followed by decreasing to be constant. Such variation of the reaction rate was fundamentally explained by the competitive production and annihilation processes of photogenerated electrons and holes in TiO_2 films, and the optimum TiO_2 thickness was estimated to be ca. 10 nm

We also tried to dope nitrogen into the effective depth region (ca. 10 nm) of TiO_2 by an ion implantation technique. The nitrogen doped TiO_2 enhanced photocatalytic activity under visible-light irradiation. XANES and XPS analyses indicated two types of chemical state of nitrogen, one photo-catalytically active N substituting the O sites and the other inactive NOx ($1 \le x \le 2$) species (Fig.1). In the valence band XPS spectrum of the high active sample, the additional electronic states were observed just above the valence band edge of a TiO_2. The electronic state would be originated from the substituting nitrogen and be responsible for the band gap narrowing, i.e., visible light response of TiO_2 photocatalysts.

5:40pm **PCSI-MoA-45 Study on Photodeposition Process of Pt Nanoparticles on TiO_2 Photocatalyst by XAFS Spectroscopy**, ***Yuji Nakano***, *M Akatsuka, M Yamamoto, C Tsukada, S Ogawa, S Yagi,* Nagoya University, Japan; *T Yoshida,* Osaka City University, Japan

TiO_2 is one of the representative photocatalysts used, for example, to purify water and air. In order to enhance the activity of the TiO_2 photocatalyst, Pt nanoparticles are often deposited on the surface[1]. In this study, we aimed to investigate the photodeposition process of Pt nanoparticles on TiO_2 using Pt L_3-edge XAFS spectroscopy focusing on the bonding states of Pt on TiO_2 surface and local structures around Pt atoms.

Before irradiation, the feature of Pt L_3-edge XANES spectrum of the TiO_2 sample adsorbing the Pt precursor was similar to that of PtO_2. The energy position of the main peak of XANES shifted to lower X-ray energy with the photoirradiation time, indicating a decrease in the ratio of Pt^{4+} ions by reduction.

All XANES spectra were reproduced with the linear combination of two XANES spectra of PtO_2 and Pt metal, and the fractions of Pt^{4+} and Pt^0 for all the Pt/TiO_2 samples were directly evaluated. Fig.1 shows irradiation-time dependence of edge jump intensity at 11740 eV and the fraction of Pt^0. The edge jump intensity corresponds to the deposited Pt concentration.

Before photoirradiation, only 20% of Pt^{4+} ions were adsorbed on TiO_2. The Pt^{4+} ions increased to 45% by photo-assisted adsorption after 5 minutes, in which most of the adsorption sites of Pt on the TiO_2 surface would be occupied. Subsequently, the adsorbed Pt^{4+} ions were gradually reduced during the following 5 to 20 minutes of photoirradiation. In the successive period for 20–30 min, the amount of the adsorbed Pt^{4+} ions drastically increased and the reduction of Pt^{4+} to Pt^0 drastically occurred. After that, the fraction of Pt^0 gradually increased by further photoreduction.

Monday Evening, January 16, 2017

PCSI
Room Ballroom South - Session PCSI-MoE
Van der Waals Heterostructures II & New Techniques II

Moderators: Lincoln Lauhon, Northwestern University, Kyle Seyler, University of Washington

7:30pm **PCSI-MoE-1 Controlled Interfaces in 2D Materials*, Arend van der Zande,*** University of Illinois at Urbana Champaign **INVITED**

Interfaces are ubiquitous in material science and technologies. For example, grain boundaries often dominate the mechanical and electrical properties in crystalline materials, while interfaces between dissimilar materials form the fundamental building blocks to diverse technologies, such as building electrical contacts in transistors and PN diodes in solar cells. Interfaces become even more important in 2D materials such as graphene and transition metal dichalcogenides, where the lack of dangling bonds enables material stability down to a single monolayer. In this entirely surface-dominated limit, the usual rules governing 3D interface devices, such as depletion regions, break down.

In this talk, we will discuss our work on engineering in- and out-of-plane 2D materials interfaces, and taking advantage of the outstanding mechanical properties of atomic sheets to build novel devices. We will examine the structure of atomically-thin membranes and the impact of in-plane and out of plane interfaces such as grain boundaries and heterostructures on the mechanical, optical, and electronic properties, and discuss how to utilize interlayer interactions to tailor band alignment and build new optoelectronic devices such as tunable photodiodes. In addition, atomic membranes represent the ultimate limit of mechanical devices. We will discuss our progress on engineering devices utilizing 3D deformations of 2D sheets. Looking to the future, the rapidly expanding family of 2D materials with a diverse set of electronic properties provide a promising palette for discovering emergent phenomena and a motivation for developing overarching design principles for understanding, controlling and manipulating lower dimensional interfaces in 1D, 2D and 3D.

8:00pm **PCSI-MoE-7 Long-lived Spin/Valley Dynamics of Resident Electron and Holes in Gated Monolayer Wse$_2$*, Prasenjit Dey,*** *L Yang, S Crooker,* Los Alamos National Laboratory*; C Robert, G Wang, B Urbaszek, X Marie,* Institut National des Sciences Appliquées, LPCNO

Monolayer transition-metal dichalcogenides (TMDs) such as MoS$_2$, MoSe$_2$, WS$_2$ and WSe$_2$ represent an excellent platform to explore the spin and valley dynamics of electrons, holes, and excitons. Although excitons and charged excitons (trions) are known to exhibit rather short recombination lifetimes of the order of 10 picoseconds, it was recently demonstrated by optical Kerr-rotation spectroscopy that *resident* electrons in electron-doped MoS$_2$ and WS$_2$ monolayers exhibit surprisingly long nanosecond-timescale spin lifetimes and spin coherence [1,2].

These developments have opened up a new route to investigate the dynamics of resident carriers (both electrons and holes) in 2D semiconductors. Here we extend these measurements to single exfoliated flakes of monolayer WSe$_2$ that are electrostatically gated to tune the carrier density (see Figure). We employ both continuous-wave Kerr rotation (CWKR) spectroscopy and also time-resolved Kerr rotation (TRKR) spectroscopy to directly measure the dynamics of spin and valley polarization of resident carriers in both the electron and hole-doped regimes [3]. Both CW and TR- Kerr rotation data as a function of transverse magnetic field and temperature for different electron and hole doping will be discussed.

Author for correspondence: crooker@lanl.gov

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8:15pm **PCSI-MoE-10 Building Complex Semiconductor Nanowires via *in situ* Growth Experiments*, Frances Ross,*** IBM T. J. Watson Research Center **INVITED**

Semiconductor nanostructures can be grown while under observation in a transmission electron microscope by flowing chemical vapor deposition precursor gases over a heated substrate. Video-rate observations, where tens or hundreds of images are obtained per second, provide a unique view of the physics of the self-assembly process that generates the individual nanostructures. Morphology, crystal structure and growth kinetics can be measured, including the response of the growth process to changes in parameters such as pressures and temperature [1]. We have used this technique to examine the epitaxy and self-assembly of Si, Ge, GaAs and GaN nanowires. These nanowires are grown from nanoscale metallic catalytic droplets that act to accelerate growth at the catalyst/nanowire interface (the *vapor-liquid-solid* growth mode), thereby forming an elongated crystal.

We find that the VLS growth mode allows quite complex nanowire-based structures to be grown controllably if we obtain a detailed understanding of the mechanisms at work. We first describe the formation of "nanocrystal-in-nanowire" structures, achieved by supplying metals such as Ni or Mn sequentially to the catalyst during Si nanowire growth [2]. We discuss the range of structures that can be achieved in other materials such as Ge and GaAs. We next consider the opportunities for crystal engineering in III-V nanowires. GaAs, for example, can grow in nanowire form in both the zinc blende crystal structure, which is the equilibrium phase, and the non-equilibrium wurtzite structure, allowing crystal phase heterostructures to be formed. *In situ* microscopy allows the mechanism of this phase selection to be clarified [3]. Finally, we describe nanowires grown into bridges between macroscopically large contacts. Electrical transport through such nanowires can be correlated with their structure and the morphology of the junctions at either end, also measured and controlled *in situ* [4], and electric fields can be used to control nanowire growth directions [5]. This is potentially useful for device integration. We conclude with a perspective on multi-modal experimental probes that may provide the promise of correlating nanowire surface chemistry with structure and properties measured *in situ*.

8:45pm **PCSI-MoE-16 GaN Nanowires as Probes for Scanning Tunneling Microscopy*, Sofie Yngman,*** Lund University, Sweden*; O Scholder,* Lund Univesrity, Sweden*; F Lenrick, M Khalilian, R Timm, L Samuelson, J Ohlsson, A Mikkelsen,* Lund University, Sweden

The high spatial resolution makes scanning tunneling microscopy/spectroscopy (STM/S) an excellent tool for advanced surface characterization, such as local density of states mapping on atomic scales. The most common probes today are metallic (W, Pt/Ir), however, over the years effort has been aimed towards developing probes with particular electronic, optical and mechanical properties[1]. Semiconducting materials, such as doped diamond and InAs nanowires (NWs)[2] have for example been proposed as alternatives.

The electronic, optical and mechanical properties of GaN NWs could make them interesting for both STM/S and Scanning Nearfield Optical Microscopies (SNOM). For the electrical measurements an important potential advantage is if tunneling can be made to occur from a narrow band of states close to the band-edge of the semiconductor. The X-ray optical density of GaN is much lower than W/Pt which significantly simplifies simultaneous STM and synchrotron radiation experiments. Such experiments are difficult with W probes due to the shadowing effect of the probe. Additionally, the large band gap GaN NWs can potentially function as light guides for SNOM applications. Finally, for the mechanical properties, GaN has a hardness which is on par with W and thus constitute a viable candidate in terms of stability and robustness.

We have successfully used GaN NWs based on LED technology[3] as probes in STM/S. We demonstrate atomic resolution imaging on GaAs (110) surfaces (Fig. 1(c)-(d) and STS (not shown). The morphology of the NWs has been tailored for STM by growing them with a sharp tip for measurements (Fig. 1(b)) and high thickness for robustness (Fig. 1(a)). The NWs are *n*-doped and grown by catalyst-free metal organic vapor phase epitaxy using a two-step process. The first growth forms the GaN NW core and the second growth adds a layer of high quality GaN which also builds up the ultra-sharp tip. Several different options for viable probe fabrication based arrays of grown NWs have been evaluated.

Figure 1 *– (a) SEM image of a GaN NW. (b) TEM image of a GaN NW tip apex. (c)-(d) STM image and line scan of a GaAs(110) surface acquired using a GaN NW probe.*

8:50pm **PCSI-MoE-17 TERS: New Method for Nanoscale Characterization of 2D Materials - from Graphene to TMDCs.*, Andrey Krayev,*** *S Bashkirov, V Gavrilyuk, D Evplov, V Zhizhimontov, A Robinson,* AIST-NT Inc.*; M Chaigneau,* Horiba Scientific

Recent advances in tip-enhanced Raman scattering (TERS) instrumentation, availability of commercial highly enhancing probes and development of dedicated TERS imaging modes have brought TERS characterization to the level of an everyday analytical method that can provide important information on structural and electronic properties of different materials at the scale of a few nanometers.

We report the results of TERS characterization of 2 classes of 2D materials: graphene and its derivative and two members of transition metal dichalcolgenides (TMDCs) class- MoS_2 and WS_2. We discovered that the gap mode TERS signal of these 2D materials becomes dramatically enhanced over wrinkles and creases, as well as over nanopatterns imprinted into flakes using a sharp diamond probe.

Resonant Raman spectra of TMDCs contain additional peaks normally forbidden by selection rules. TERS maps of few-layer-flakes of MoS_2 show that the spatial distribution of Raman intensity across the flake varies for different peaks, specifically, the lower energy component of the complex resonant 465cm^{-1} peak is significantly decreased at the edges of the flakes. TERS and tip-enhanced photoluminescence (TEPL) characterization of WS_2 grown on Si/SiO2 show that, similar to the case of MoS_2 flakes, the properties are not uniform across the flake: there exists a narrow, 150-200 nm wide, area along the edges of the flakes with decreased and blue shifted photoluminescence and in the same time enhanced TERS response, both of which indicate decreased charge carrier density in the vicinity of the flake outer edges.

Based on these results, we argue that TERS and TEPL can be an extremely useful tool for nanoscale characterization of the 2D materials.

8:55pm **PCSI-MoE-18 Robust High-Resolution Imaging and Quantitative Force Spectroscopy in Vacuum with Tuned-Oscillator Atomic Force Microscopy**, ***Omur Dagdeviren***, *J Goetzen,* Yale University*; H Hoelscher,* KIT*; E Altman, U Schwarz,* Yale University

Since the first demonstration of atomic resolution in ultrahigh vacuum more than twenty years ago, frequency modulation-based noncontact atomic force microscopy (FM-NC-AFM) has significantly matured and is now routinely applied to study problems that benefit from high-resolution surface imaging. In FM-NC-AFM, control of the tip's vertical position is accomplished by detecting a shift in the cantilever's resonance frequency upon approach to the sample. Consistently ensuring reliable distance control during extended data acquisition periods has nevertheless remained challenging, as most FM-mode-based control schemes employ three feedback loops that may interfere. As a consequence, sample throughput in FM-NC-AFM is often low compared to ambient condition AFM, where the easy-to-implement amplitude-modulation (AM) control scheme is predominantly used. Transfer of the AM methodology to high-resolution measurements in vacuum is, however, difficult as with AM-AFM, instabilities during approach are common. In addition, the lack of viscous air damping and the related significant increase of the cantilever's quality factor generate prolonged settling times, which cause the system's bandwidth to become impractical for many applications. Here we introduce a greatly simplified approach to NC-AFM imaging and quantitative tip-sample interaction force measurement that prevents instabilities while simultaneously enabling data acquisition with customary scan speeds by externally tuning the oscillator's response characteristics [1]. After discussing background and basic measurement principle, examples for its application to a variety of sample systems are provided (see Fig. 1). A major advantage of this operational scheme is that it delivers robust position control in both the attractive and repulsive regimes with only one feedback loop, thereby carrying the potential to boost the method's usability.

PCSI

Room Ballroom South - Session PCSI-TuM

Complex Oxides I/Topological Materials II/Semiconductor Growth I-Extended

Moderators: Andrew Millis, Columbia University, Joanna Millunchick, University of Michigan, Ann Arbor, Can-Li Song, Tsinghua University

8:30am **PCSI-TuM-1 Polar Metals by Geometric Design**, ***Chang-Beom Eom,*** University of Wisconsin-Madison **INVITED**

Polar Metals by Geometric Design

Chang-Beom Eom

Department of Materials Science and Engineering, University of Wisconsin-Madison, Madison, WI 53706, USA

Gauss's law dictates that the net electric field inside a conductor in electrostatic equilibrium is zero by effective charge screening; free carriers within a metal eliminate internal dipoles that may arise owing to asymmetric charge distributions. Quantum physics supports this view, demonstrating that delocalized electrons make a static macroscopic polarization, an ill-defined quantity in metals—it is exceedingly unusual to find a polar metal that exhibits long-range ordered dipoles owing to cooperative atomic displacements aligned from dipolar interactions as in insulating phases. Here we describe the quantum mechanical design and experimental realization of room-temperature polar metals in thinfilm $ANiO_3$ perovskite nickelates using a strategy based on atomicscale control of inversion-preserving (centric) displacements. We predict with *ab initio* calculations that cooperative polar *A* cation displacements are geometrically stabilized with a nonequilibrium amplitude and tilt pattern of the corner-connected NiO6 octahedra—the structural signatures of perovskites—owing to geometric constraints imposed by the underlying substrate. Heteroepitaxial thin-films grown on $LaAlO_3$ (111) substrates. Heteroepitaxial thin-films grown on $LaAlO_3$ (111) substrates fulfil the design principles. We achieve both a conducting polar monoclinic oxide that is inaccessible in compositionally identical films grown on (001) substrates, and observe a hidden, previously unreported, non-equilibrium structure in thin-film geometries [1]. We expect that the geometric stabilization approach will provide novel avenues for realizing new multifunctional materials with unusual coexisting properties.

This work has been done in collaboration with T. H. Kim, D. Puggioni, Y. Yuan, L. Xie, H. Zhou, N. Campbell, P. J. Ryan, Y. Choi, J.-W. Kim, J. R. Patzner, S. Ryu, J. P. Podkaminer, J. Irwin, Y. Ma, C. J. Fennie, M. S. Rzchowski, X. Q. Pan, V. Gopalan, J. M. Rondinelli.

[+] Author for correspondence: ceom@wisc.edu

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9:00am **PCSI-TuM-7 Scavenging of Oxygen from $SrTiO_3$ during Oxide Thin Film Deposition and 2DEG at Oxide Interfaces***, A Posadas, K Kormondy, W Guo, P Ponath, J Geler Kremer,* ***Alexander Demkov,*** The University of Texas

The discovery of a 2DEG at the interface between epitaxial $LaAlO_3$ (LAO) and $SrTiO_3$ (STO) over a decade ago has led to a flurry of research activity exploring the nature and origin of this conductive interface. This 2DEG has sufficient mobility to exhibit SdH oscillationsand much work on developing device applications of this system has been published. Experiment and theory show that the 2DEG at the oxide/oxide interface has many exotic features. It can be paramagnetic, ferromagnetic or even superconducting, with strong Rashba splitting leading to a controllable magnetic moment One explanation involving oxygen vacancies is used for 2DEGs arising in several related interfaces such as amorphous LAO on STO and g -Al_2O_3 on STO. In the vast majority of 2DEGs reported to form at oxide interfaces, the substrate has been TiO_2-terminated STO with only a handful of exceptions.Potential chemical reactions between the arriving metal species during oxide thin film deposition and the substrate have been largely ignored in these explanations for the 2DEG formation although this has recently begun to change. There is growing evidence that many metals steal oxygen from STO even in the presence of relatively high oxygen pressures.

To better understand the effect of metal oxide deposition on a STO surface, we examine the effect of depositing various metals layer by layer on STO in terms of the evolution of the electronic structure and oxidation state of the metal overlayer. We show that the deposition of metals that have a high oxygen affinity on STO, even under an oxygen-rich atmosphere such as in oxide thin film deposition, typically leads to an interfacial layer of oxygen-deficient STO. We analyze the electronic and chemical evolution of metals deposited on STO using in situ XPS and classify metals into three regimes depending on their oxide formation energy and work function. We demonstrate how redox reactions with STO of metals belonging to one of these regimes can be used to produce interfacial 2DEGs that are quite similar to the crystalline LAO on STO system, and that an oxygen-deficient STO layer could even explain the 2DEG in that system.

9:15am **PCSI-TuM-10 Realization of a Vertical Topological p-n Junction in Sb_2Te_3/Bi_2Te_3 Heterostructures***,* ***Gregor Mussler****, M Eschbach, M Lanius, N Demarina, M Luysberg, L Plucinski, D Grützmacher,* Forschungzentrum Jülich, Germany **INVITED**

I will present results on molecular-beam epitaxy (MBE) of the three-dimensional TI materials Bi_2Te_3 and Sb_2Te_3 grown in Si(111). Due to naturally occurring defects, Bi_2Te_3 and Sb_2Te_3 exhibit a high unintentional carrier concentration in the order of ~ 10^{19} cm^{-3}. It turns out that Bi_2Te_3 and Sb_2Te_3 is intrinsically n-type doped, whereas Sb_2Te_3 show p-type behavior. Consequently, a stack of Sb_2Te_3/Bi_2Te_3 poses a p-n junction, where a built-in voltage drags away carriers from its interface, allowing to tune the carrier concentration by varying the thickness of the topmost Sb_2Te_3 layer.

9:45am **PCSI-TuM-16 Surface Structure and Electronic Properties of Epitaxial Topological Crystalline Insulator Films***,* ***Omur Dagdeviren****, C Zhou, K Zou, G Simon, S Albright, S Mandal, M Acosta, X Zhu, S Beigi, F Walker, C Ahn, U Schwarz, E Altman,* Yale University

Topological crystalline insulators (TCI) feature surface electronic states are protected by crystal symmetry. As a representative TCI, the structural and electronic properties of SnTe films grown on $SrTiO_3$(001) were investigated using scanning tunneling microscopy (STM), noncontact atomic force microscopy (NC-AFM), electron and x-ray diffraction, and density functional theory. Initially, SnTe (111) and (001) surfaces formed; however, the (001) surface dominated with increasing film thickness. The film grows domain-by-domain with the [011] direction of SnTe (001) islands rotated up to 7.5° with respect to $SrTiO_3$ [010]. Analysis of the diffraction data reveals a mosaic distribution of SnTe (001) domains. Complementary STM and NC-AFM experiments address the properties of the thicker films in real space. It is found that the growth mechanism induces a variety of defects on different length scales that affect the electronic properties, including: domain boundaries; dislocations at the domain boundaries that serve as periodic nucleation sites for pit growth; screw dislocations; and point defects. These features give rise to variations in the electronic structure of the surface states as evidenced in STM images by standing wave patterns and a non-uniform nanometer scale background superimposed on atomic scale images. Simultaneous force versus and tunneling current versus distance curves indicate that the tip is unusually close to the surface during STM imaging making the surface susceptible to tip-induced modification. The results indicate that both the growth process and the scanning probe tip are candidates to induce symmetry breaking defects in a controlled way to pattern the topological surface states which then eventually enable fabrication of devices.

11:00am **PCSI-TuM-31 Epitaxial Semiconductor – Superconductor Hybrid Materials for Topological Superconductivity**, ***Peter Krogstrup,*** Niels Bohr Institute, Denmark **INVITED**

Semiconductor-metal interfaces are key elements in nanostructured electronics and device architectures. This is in particular true in the field of low dimensional topological superconductivity, where semiconductor nanowires with high spin orbit coupling coupled to a superconducting phase constitute some of the most promising candidates in the search for materials suitable for quantum information technology[1] . I will discuss the synthesis, structural and compositional properties hybrid semiconductor-superconductor nanowire and hybrid materials grown in-situ by Molecular Beam Epitaxy [2] . Because these materials give a hard superconducting gap proximitized in the semiconductor, they serve as excellent platform for studying Andreev bound states and Majorana bound states, which opens for new application possibilities in the field. I will present on the synthesis of various types of hybrid semi-super materials and discuss the challenges and material requirements needed for realizing and eventually manipulating topological protected quantum states.

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11:30am **PCSI-TuM-37 One-dimensional Electronic Transport in Epitaxial-Al/InAs Quantum Well Heterostructures**, ***JoonSue Lee***, *B Shojaei, M Pendharkar, A McFadden, C Palmstrom, Y Kim,* University of California, Santa Barbara; *M Kjaergaard, C Marcus,* Niels Bohr Institute, Denmark

One-dimensional (1D) electronic transport as well as induced superconductivity in a semiconductor is a crucial ingredient to realize topological superconductivity. Our approach employs two-dimensional (2D) semiconductors (InAs quantum wells), which are advantageous for fabricating complex nano-structures consisting of electrically confined 1D channels and superconductors. To achieve transparent superconductor/semiconductor contacts, the InAs quantum wells are cleanly interfaced with epitaxial Al by molecular beam epitaxy. Gate-tunable supercurrent is observed in an S-N-S geometry with a top gate, and it persists in the presence of in-plane magnetic field up to ~800 mT.

We study 1D electronic transport in shallow InAs quantum wells with a thin top potential barrier (10 nm $In_{0.75}Ga_{0.25}As$), after removing Al layer on top, using quantum point contacts and gate-defined quasi-1D channels. Conductance through a quantum point contact is quantized in units of the conductance quantum ($2e^2/h$), and half-integer values of the conductance quantum, due to Zeeman spin splitting, appear as perpendicular magnetic field is applied. We also observe an evolution of 0.5 conductance quantum as the lateral potential confinement of a quantum point contact becomes highly asymmetric. Conductance through gate-defined quasi-1D channel shows quantization only in the quantum Hall regime with large perpendicular magnetic field. Weak localization from magneto-conductance measurements at various gate-voltages, reveals a systematic change of the coherence length of the InAs channel. Our studies of the 1D electronic transport as well as the induced superconductivity in epitaxial superconductor/2D semiconductor systems could realize large-scale nano-structures utilizing multiple Marjorana fermiones for quantum computing applications

11:35am **PCSI-TuM-38 Theoretical Investigations for the Stability and Electronic Structures of Two-dimensional Group-IV Ternary Alloy Monolayers**, ***Toru Akiyama***, *G Yoshimura, K Nakamura, T Ito,* Mie University, Japan

Two-dimensional (2D) nanostructures in the honeycomb lattice have currently been paid much attentions due to their peculiar electronic properties. Furthermore, Si, Ge, and Sn monolayers (silicene, germanene, and stanene, respectively) are expected to be potential alternatives to graphene for electronic devices [1-3]. In contrast to flat 2D monolayers consisting of sp^2 hybridization such as graphene, silicene, germanene, and stanene form a mixture of sp^2 and sp^3 hybridization, resulting in the buckled hexagonal configuration. Recent theoretical calculations within density functional theory (DFT) have suggested that these materials possess a linear band dispersion with Dirac cone at the *K* point regardless of the buckled atomic configuration [4]. Moreover, it has been suggested that monolayer SiGe with buckled configuration also has a linear band dispersion similar to graphene [5]. However, there are few systematic studies for the atomic structure and electronic properties of group-IV alloy monolayers from theoretical viewpoints. In our previous study, we have systematically investigated the structural stability and electronic properties of group-IV binary alloy monolayers, such as monolayer Si_xGe_{1-x}, Ge_xSn_{1-x}, and Si_xSn_{1-x} on the basis of electronic structure calculations within the DFT [6]. In this study, we extend our study to ternary alloy semiconductor monolayers.

Our DFT calculations for $Si_xGe_ySn_{1-x-y}$ monolayers demonstrate that the buckled configuration is stabilized over the entire composition range. The calculated excess energy of $Si_xGe_ySn_{1-x-y}$ monolayers (~0.11 eV/atom) is found to be comparable to that of bulk phase of ~0.16 eV/atom, indicating that the miscibility of ternary alloy monolayers is similar to that of bulk phase. The analysis of band structures reveals that an almost linear band dispersion with Dirac cone at the *K* point similar to graphene appears in $Si_xGe_ySn_{1-x-y}$ over the wide range of Si and Ge compostions, while a small energy gap within 0.17 eV is formed at the *K* point for $Si_{0.5}Ge_{0.125}Sn_{0.375}$. These results thus suggest that the composition control is of importance in tailoring the electronic properties of group-IV ternary alloy monolayers. Furthermore, effects of carbon incorporation on the atomic structures and electronic properties of group-IV monolayers are clarified.

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[6] T. Akiyama *et al.*, Jpn. J. Appl. Phys. **55**, 04EP01 (2016).

11:40am **PCSI-TuM-39 A Simple Interpretation for Heteroepitaxial Growth Mode in Terms of Surface and Interface**, ***Tomonori Ito***, *T Akiyama, K Nakamura,* Mie University, Japan

It is well known that hetero-epitaxial systems exhibit various growth behaviors depending on the lattice mismatch including three dimensional island growth (3D-coherent) and two dimensional growth with misfit dislocation formation (2D-MD). Despite a constant lattice mismatch of InAs on GaAs, the 3D-coherent is found on (001) while the 2D-MD appears on (110) and (111)A. Moreover, it is found that insertion of buffer-layer in the InAs/GaAs(110) changes its growth mode from the 2D-MD to the 3D-coherent. Although many studies have been done to investigate the 3D-coherent on the InAs/GaAs(001) [1], there have been very few studies for systematic interpretation for the growth mode depending on orientations. In this study, the growth mode of the InAs/GaAs system is simply interpreted by using our phenomenological macroscopic theory in terms of surface and interface with the aid of microscopic theory such as ab initio and empirical interatomic potential calculations.

In our macroscopic theory, free energy F (eV/Å^2) for the 2D-coherent, the 3D-coherent and the 2D-MD is described as a function of layer thickness h as follows [2].

$F=\gamma(1+\beta)+1/2M(1-\alpha)\varepsilon^2(1-l_0/l)h+E_d/l$,

where γ, β, M, α, ε, l_0, l, andE_d denote the surface energy, the effective increase in surface energy of the epitaxial layer due to 3D island formation, the effective elastic constant, the effective decrease in strain energy due to 3D island formation, the intrinsic strain of the system, the average MD spacing, the MD spacing at which strain is completely relaxed, and the formation energy of the MD, respectively. Using eq. (1), the boundary between the 2D-MD and the 3D-coherent is described as $\beta/\alpha=1/(2\gamma)(E_d/l_0)$. Using E_d obtained by ab initio and empirical potential calculations, the growth mode boundaries for the InAs/GaAs is shown in Fig. 1 as functions of β/α and γ. Employing β/α~0.2 and γ~0.05(eV/Å^2), the 2D-MD is favourable in the (110) and the (111)A, while the (001) exhibits the 3D-coherent. This depends on the values of E_d, i.e., the smaller the E_d, the more favourable the 2D-MD. Moreover, decrease in γdue to lattice relaxation with the buffer-layer insertion tends to favour the 3D-coherent found in the (110). Consequently, the growth mode on the InAs/GaAs can be qualitatively interpreted by considering $\gamma$and E_d.

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11:45am **PCSI-TuM-40 Surface Mediated Formation of Horizontal ErSb Nanowires**, ***Nathaniel Wilson***, *S Kraemer, C Palmstrøm,* University of California, Santa Barbara

ErSb, and related Rare Earth-Group V materials, are semi-metallic in nature and compatible with III-V semiconductors structures, forming sharp stable epitaxial interfaces. Unfortunately overgrowth of III-V material is hampered due to the difference in symmetry between ErSb [001] (4-fold) and GaSb [001] (2-fold) resulting in symmetry defects preventing the use of ErSb as a buried contact. One proposed method of circumventing this problem is to use ErSb horizontal nanowires as a buried contact while allowing percolative GaSb growth to occur between the nanowires to maintain crystal orientation. ErSb is known to form a variety of nanostructures in GaSb depending on the ratio of Ga to Er flux during deposition. [1] Understanding the growth mechanisms behind the formation of these different nanoparticles is an important step towards their use as buried contacts, and to achieve nanowire formation in other material systems.

We investigate the growth of horizontal nanowires in the ErSb/GaSb material system, and observe a growth process involving large GaSb macrosteps as the mechanism behind the transition from vertical nanowires to horizontal nanowires.

We also observe a previously unseen low temperature growth mode resulting in horizontal nanowire formation under a much wider range of flux conditions. This new growth mode does not use the embedded growth observed at higher temperatures and may allow for horizontal nanowire formation without the presence of macrosteps, as well as the formation of significantly smaller nanoparticles which may be useful for accessing nanoparticle dimensions that result in electron confinement.

12:00pm **PCSI-TuM-43 Effect of Ga-Dangling Bonds at the GaSb/GaAs Interface of GaSb TPV Cells Grown on GaAs Substrates by IMF Technique***, **Emma Renteria**, A Mansoori, S Addamane, A Soudachanh, G Balakrishnan,* University of New Mexico

The growth of metamorphic GaSb epitaxial layers on GaAs substrates has become of significant interest in the areas of mid to long wave infra-red (IR) optoelectronic devices. In the case of thermophotovoltaics (TPVs), GaAs substrates are an attractive alternative to GaSb substrates on account of their semi-insulating nature, relatively lower cost, and ability to scale up to large wafer sizes. Unfortunately, the mismatched growth of GaSb epitaxial layers on GaAs substrates results in significant threading dislocations in the GaSb epitaxial layer due to the 7.78% lattice mismatch between the two binary semiconductors. However, the threading dislocation density (TDD) on the GaSb epitaxial layer can be reduced by inducing arrays of 90° interfacial misfit dislocations (IMF) at the GaSb/GaAs interface [1]. This technique reduces the TDD in the GaSb epitaxial layer to the low 10^8 defects/cm^2, which has been sufficient to demonstrate a wide range of devices. However, for TPVs, the residual threading dislocations on the GaSb epitaxial layer severely affects the performance of the GaSb diodes under illumination. Although we are continuously working on optimizing the growth technique to further reduce the TDD, the 90° IMF are made of Ga-dangling bonds localized along the GaSb/GaAs interface which also affect the electronic properties of the devices [2]. These Ga-dangling bonds can act as trap carriers and further affect the performance of metamorphic GaSb TPVs. We have grown and processed a p-n GaSb TPV cell on GaAs substrates. To study the effect of the Ga-dangling bonds on the performance of the cell, we placed the n-type contacts above the IMF interface for some cells and below the IMF for other cells. The presentation will provide extensive characterization data including J-V characteristics of solar cells under dark and illumination.

12:05pm **PCSI-TuM-44 Surface Recombination in Sb-based Infrared Detectors Obtained by Release and Transfer of Membranes***, **Marziyeh Zamiri**,* University of New Mexico*; B Klein,* Sandia National Laboratory*; V Dahiya, F Cavallo, S Krishna,* University of New Mexico

We have recently isolated Sb-based type II superlattice (T2SL) in the form of free-standing membranes. The tremendous potential of these new structural elements has been demonstrated through fabrication and characterization of infrared (IR) detectors on T2SLs transferred to Si substrates. Here we investigate the effect of surface recombination on the dark current density of IR detectors obtained by release and transfer of membranes. Specifically, we perform a theoretical and experimental study to isolate the contribution of rough sidewalls on the device characteristics.

For this purpose we fabricate and characterize IR detectors on InAs/GaSb T2SLs transferred to bulk Si using two different techniques. Briefly, a 1.6 µm p-i-n T2SL is epitaxially grown onto a 60 nm $Al_{0.4}Ga_{0.6}Sb$ sacrificial layers on a GaSb substrate. Upon selective removal of the $Al_{0.4}Ga_{0.6}Sb$ layer *via* chemical etching, the 25 × 25 µm^2 membrane becomes freestanding, and it can be transferred to the alternative host. In one case, both the top surface and the sidewalls of the membrane are coated with a hard-baked polymer film (*i.e.*, photoresist), and therefore they are unexposed to the chemical etchant. Scanning electron microscopy of the membrane bonded to bulk Si shows that the structure of the T2SL is not altered during release. In the other case, the photoresist is isolating only the top surface of the T2SL, thereby resulting in a significant roughening of the sidewalls. The poor selectivity of the etching solution between GaSb and the $Al_{0.4}Ga_{0.6}Sb$ sacrificial layer is responsible of this structural change in the transferred membrane. Rough sidewalls are expected to enhance surface recombination in the T2SL and therefore increase the dark current density of an IR detector. We quantify this effect by characterizing IR detectors fabricated on the two mesas. A comparative analysis of the dark current density measured for the two devices signify the effect of having exposed sidewalls during membrane release. These experimental results are consistent with theoretical calculations which show a relative enhancement of surface recombination at increasing roughness of the membrane sidewalls.

+ Author for correspondence: marziyeh.zamiri@gmail.com

PCSI
Room Ballroom South - Session PCSI-TuE
Majorana Fermions in Atomic Structures

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

7:30pm **PCSI-TuE-1 From Majorana Fermions to Parafermions in Nanowires and Atomic Chains***, **Daniel Loss**,* University of Basel, Switzerland **INVITED**

I will present recent results on Majorana fermions and parafermions which can emerge in one nanowires and atomic chains in the presence of spin orbit interaction or spatially periodic magnetic fields, in RKKY systems forming intrinsic spin helices, and in the presence of superconductivity. I will present candidate materials such as semiconducting Rashba nanowires, ^{13}C nanotubes, and atomic magnetic chains. In contrast to Majorana fermions, parafermions emerge only in the presence of strong electron-electron interactions and have a more powerful braid statistics enabling entanglement and CNOT gates.

8:00pm **PCSI-TuE-7 Probing Atomic Structure and Majorana Wavefunctions inMono-Atomic Fe-chains on Superconducting Pb-Surface***, **Rémy Pawlak**, M Kisiel, J Klinovaja, T Meier, S Kawai, T Glatzel, D Loss, E Meyer,* University of Basel, Switzerland **INVITED**

Motivated by the striking promise of quantum computation, Majorana bound states (MBSs) [1] in solid-state systems [2-3] have attracted wide attention in recent years [4-6]. In particular, the wave-function localization of MBSs is a key feature and crucial for their future implementation as topological qubits [2-3]. Here, we investigate the spatial and electronic characteristics of topological superconducting chains of iron atoms on the surface of Pb(110) by combining scanning tunneling microscopy (STM) and atomic force microscopy (AFM) at low temperature. We demonstrate that the Fe chains are mono-atomic, structured in a linear fashion, and exhibit zero-bias conductance peaks at their ends which we interpret as signature for a Majorana bound state. Spatially resolved conductance maps of the atomic chains reveal that the MBSs are well localized at the chain ends (< 25 nm), with two localization lengths as predicted by theory [7-8]. Our observation lendsstrong support to use MBSs in Fe chains as qubits for quantum computing devices.

+ Author for correspondence: remy.pawlak@unibas.ch

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8:30pm **PCSI-TuE-13 Majoroana Fermions in Atomic Chains: Spin and Charge Signatures***, **Ali Yazdani**,* Princeton University **INVITED**

I will review the platform for realization of topological superconductivity and Majorana fermions in chains of magnetic atoms on the surface of a superconductor. I will describe high resolution studies of spatial mapping of spectroscopic signature of Majorana fermions in spectroscopic experiments with the STM. These will include experiments at lowest possible temperature with the STM, with superconducting tips, as well as those using spin-polarized STM techniques. In each case Majoranas are predicted to leave a distinct signature than other in gap states of a superconductor, which can be diagnosed experimentally.

Author for correspondence: Yazdani@princeton.edu

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PCSI

Room Ballroom South - Session PCSI-WeM

Spintronics II/Van der Waals Heterostructures II/Semiconductor Interfaces/Complex Oxides II

Moderators: Aaron Arehart, The Ohio State University, Michael Flatte, University of Iowa, Masataka Higashiwaki, National Institute of Information and Communications Technology, Chakrapani Varanasi, ARO

8:30am **PCSI-WeM-1 Current Switching of a Single Ferromagnetic Layer***,* ***Chia-Ling Chien,*** Johns Hopkins University **INVITED**

Spin Hall effect (SHE) switching allows current switching of a single ferromagnetic (FM) layer in contact with a heavy metal (HM), where the pure spin current from the HM exerts a spin orbit torque to switch the adjacent FM layer. However, this highly attractive pure current switching scheme cannot occur unless a magnetic field is also applied along the current direction, thus greatly diminishing its prowess. In this work, we describe the essential role of the necessary magnetic field, which not only breaks geometrical symmetry and but also causes asymmetrical domain wall motion that accomplishes switching. More importantly, we demonstrate a new method of pure current switching by exploiting HMs with opposite spin Hall angles, different Dzyaloshinskii-Moriya interaction constants and competing pure spin current. We describe the intricate physics that accomplishes pure current switching of a single ferromagnetic layer without external field, built-in exchange bias or asymmetrical structure.

9:00am **PCSI-WeM-7 Epitaxial Heusler Superlattices with Perpendicular Magnetization***,* ***Tobias Brown-Heft****, A McFadden, J Logan, C Palmstrom,* University of California, Santa Barbara

Magnetic tunnel junctions for use in system-on-chip memory require ferromagnetic electrodes with four key ingredients. First, single crystal thin film contacts must grow epitaxially on a variety of substrates to facilitate uniform performance across large arrays of devices. Second, perpendicular magnetic anisotropy (PMA) is desired to reduce spin transfer torque critical current, which reduces Joule losses for electrically switched devices. Perpendicular contacts also possess higher magnetic thermal stability as compared with in-plane magnetized contacts, which serves to preserve the magnetic state for technologically useful timescales. Third, Fermi level spin polarization must be high to enhance the tunnel magnetoresistance ratio and thereby improve state discrimination during read operations. Fourth, the contact must have low Gilbert damping, which further decreases spin transfer torque critical current.

Recently, J.G. Azadani *et al.* utilized theory calculations to argue that superlattices composed of alternating layers of certain full-Heusler compounds produce materials with all four of the properties mentioned above [1]. Specifically, epitaxial Co_2MnAl – Fe_2MnAl (CMA-FMA) superlattices are predicted to be half-metallic with 100% spin polarization, possess dominant PMA, and are composed of low Z elements with low damping coefficients. Furthermore, the spin polarization and PMA depend strongly on the superlattice periodicity, which is on the order of a single unit cell.

In this work, we utilize molecular beam epitaxy with computer controlled source shutters to grow CMA-FMA superlattices of varying periodicity on both GaAs(001) and MgO(001) substrates. High resolution x-ray diffraction is used to verify epitaxial growth. SQUID magnetometry and anomalous Hall effect are used to probe the magnetic and electronic properties of the films. We show that CMA-FMA films with a periodicity of 1.5 unit cells grown on GaAs(001) have lattice parameter $a \approx c = 5.98$Å, and exhibit dominant PMA below 200K. Similar films grown on MgO(001) are epitaxial with $a = 5.74$Å and $c = 5.80$Å, and work is in progress to find conditions giving strong perpendicular behavior. Future work includes spin-resolved photoemission and point contact Andreev reflection spectroscopy to probe the spin polarization of the films.

$^+$ Author for correspondence: cpalmstrom@ece.ucsb.edu

[1] J.G. Azadani, *Jour. of App. Phys.*, *119*(4), 43904 (2016)

9:05am **PCSI-WeM-8 Interface-dependent Spin Transfer Torque at Ferromagnetic Topological-Insulator Contacts***,* ***Sarmita Majumder,*** University of Texas, Austin

In previous work, we have shown large magnetoresistances at room temperature (RT) for three Ferromagnet/Topological Insulator (FM/TI) devices (Fe/Bi_2Te_3-based devices with and without an evaporated SiO_2 oxide, and an Fe/Bi_2Se_3-based device without evaporated oxide) [1]. The observed magnetoresistance was substantially larger than previously reported for the same system at RT [2] and at low temperatures [3, 4], and was particularly enhanced when an evaporated SiO_2 layer was introduced between the Fe and Bi_2Te_3, and when Bi_2Se_3 was used instead of Bi_2Te_3. We have speculated that the Fe deposition directly onto the TI might form an Fe-rich FeTI compound [5] which might have been prevented in the case when an evaporated oxide was present between Fe and Bi_2Te_3.

In this presentation, we will show large interface-dependent magnetoresistances in these devices due to spin polarization of the Fe bar via electron injection and extraction from the TI to the Fe (STT) at 2 K. The required switching current for STT in our case is comparable to the previous results in [6] for Cr-TI/TI contacts. Moreover, to support our speculation regarding the interfacial dependencies, we have performed cross-sectional transmission electron microscopy (XTEM) at the FM/TI interfaces. Cross-sectional samples were prepared using focussed Ga-ion beam milling. Fig. 2 shows XTEM images from (a) Fe/Bi_2Se_3, and (b) $Fe/SiO_2/Bi_2Te_3$ interfaces. The Fe/Bi_2Se_3 interface shows an extra crystalline layer at the interface with a slightly larger half period of 0.53 nm compared to the Bi_2Se_3 fringes (1.02 nm/2 = 0.50 nm). Energy dispersive X-ray spectroscopy (EDX) profiling using scanning transmission electron microscopy (STEM) imaging across the interface confirmed the inclusion of Se into Fe. Fig. 1(b) shows an abrupt interface between the crystalline Bi_2Te_3 and evaporated SiO_2.

9:10am **PCSI-WeM-9 Annealing Effects on Interfacial Electronic Structure in Epitaxial $Co_2MnSi/MgO/CoFe$ Magnetic Tunnel Junctions***,* ***Anthony McFadden****, T Brown-Heft, C Palmstrom,* University of California, Santa Barbara

We investigate the effects of post-growth annealing in ultrahigh vacuum on the temperature dependent transport properties and tunneling magnetoresistance (TMR) in single crystal $CoFe/MgO/Co_2MnSi$ magnetic tunnel junctions (MTJ's) grown by molecular beam epitaxy. Full-Heusler $Co_2MnSi(001)$ layers were grown at elevated temperature on Cr buffered MgO(001) substrates while MgO tunnel barriers and CoFe top electrodes were grown at room temperature and annealed post-growth. MTJ's with areas varying from $2.5x5\mu m^2$ to $12.5x25\mu m^2$ were fabricated using optical lithography. The MTJ structures were determined to be epitaxial and single crystalline before annealing as assessed by *in-situ* reflection high energy electron diffraction (RHEED). While they crystal quality of the top CoFe layer was observed by RHEED to improve somewhat upon annealing, we find that the transport properties of fabricated devices are altered dramatically. Samples annealed above 250°C show an expected monotonic increase in tunneling magnetoresistance (TMR) with decreasing temperature while the omission of the annealing step results in devices with an unexpected maximum TMR at temperature near 30K while TMR declines for lower temperatures. Differential conductance vs. voltage measurements performed at 2K show the presence of electronic structure near zero bias which vanishes upon annealing and which suppresses conductance when the magenetic layers are in a parallel orientation while enhancing conductance when in the antiparallel configuration. The anomalous decline of TMR with decreasing temperature in unannealed MTJ's is explained by the presence of this interfacial electronic structure combined with the thermal distribution of tunneling electrons about the Fermi energy

9:15am **PCSI-WeM-10 Valley Excitons in van der Waals Heterostructures***,* ***Kyle Seyler****, P Rivera, D Zhong,* University of Washington*; J Schaibley,* University of Arizona*; X Linpeng, B Huang, E Schmidgall,* University of Washington*; R Cheng,* Carnegie Mellon University*; H Yu,* University of Hong Kong*; M McGuire, J Yan, D Mandrus,* Oak Ridge National Laboratory*; W Yao,* University of Hong Kong*; D Xiao,* Carnegie Mellon University*; K Fu, X Xu,* University of Washington **INVITED**

Two-dimensional materials have recently developed into a powerful platform from which to explore the science of surfaces and interfaces. Of particular excitement is their use as versatile building blocks for more advanced van der Waals heterostructures. Here we present our latest experimental progress in understanding the interfacial effects on excitons in two types of van der Waals heterostructures. We first discuss the interlayer excitons formed at the interface between two different monolayer semiconductors, $MoSe_2$ and WSe_2. Through photoluminescence measurements, we reveal that these excitons possess valley pseudospin properties like their intralayer counterparts, but with enhanced lifetime and intriguing relaxation dynamics. We then introduce a new van der Waals heterostructure between monolayer WSe_2 and an ultrathin ferromagnetic semiconductor, CrI_3. Strong interfacial magnetic interactions have a dramatic effect on the WSe_2 exciton valley properties. We also demonstrate that basic optical studies on this type of heterostructure can provide rich information on the spin interactions in layered magnets.

9:45am **PCSI-WeM-16 Influence of the Dielectric Environment on Exciton Properties in 2D Semiconductors: Insights from High Magnetic Fields***, **Andreas Stier**,* Los Alamos National Laboratory*; N Wilson, G Clark, X Xu,* University of Washington*; S Crooker,* Los Alamos National Laboratory

Excitons in atomically thin 2D semiconductors such as monolayer MoS_2 or WSe_2 necessarily lie close to a surface, and therefore their properties such as size and binding energy (E_B) are expected to be strongly influenced by the surrounding dielectric environment.

However, studies exploring this role are both scarce and challenging, in part because the most readily accessible exciton property, its optical transition energy, is largely unaffected by the surrounding dielectric medium. This is because any reduction in E_B is accompanied by an equal reduction of the free-particle bandgap, resulting in a nearly unchanged exciton transition energy. Therefore, it is desirable to identify alternative optical probes of some other exciton parameter that is directly impacted by the surrounding dielectric medium.

Here we show that the exciton size can be directly measured via the small diamagnetic shift of the exciton transition energy in pulsed magnetic fields to 65 Tesla [1]. Utilizing a new measurement technique (Fig. 1(a)), in which we transfer exfoliated WSe_2 flakes over the core of a single mode optical fiber, we tune the surrounding dielectric environment by encapsulating the flakes with different materials and perform circularly-polarized low-temperature magneto-absorption studies [2]. As determined from the systematic increase of the diamagnetic shift of the exciton with increasing dielectric screening of the environment (Fig. 1(b)), we find a systematic increase of the A exciton size in monolayer WSe_2 from 1.2 nm to 1.6 nm.

The increase in exciton size and concurrent reduction in the binding energy are compared with the leading theoretical (Keldysh) model. Within this model, we find E_B systematically varying from 200 - 450 meV for our examined samples and extrapolate to freestanding WSe_2 where we find $E_B \approx$ 500 meV.

9:50am **PCSI-WeM-17 Electronic Properties and Defects in Germanane***, **Thaddeus Asel**, E Yanchenko, S Jiang, K Krymowski, W Windl, J Goldberger, L Brillson,* The Ohio State University

We have used a combination of surface science techniques to study the electronic properties and defects in germanane, a chemically functionalized two dimensional (2D) material. With the advent of graphene there has been a focus on 2D materials due to their unique properties, and the ability to further manipulate them both chemically and mechanically. Similar to graphene and MoS_2, germanane is a 2D material with a direct band gap that can be manipulated by terminating with different ligands, making it an exciting candidate for optoelectronic applications. Germanane is synthesized by deintercalating $CaGe_2$ in an acid to result in a particular termination [1]. We applied depth-resolved cathodoluminescence spectroscopy (DRCLS)[2] to measure the electronic transitions including the band gap in hydrogen terminated germanane (GeH), methyl-terminated germanane ($GeCH_3$), dimethylether terminated germanane ($GeCH_2OCH_3$), and allyl-terminated germanane ($GeCH_2CH{=}CH_2$). Using surface photovoltage spectroscopy (SPS) and DRCLS we have directly observed defects in "bulk" germanane.

A key feature of germanane is that terminating the germanium lattice with different ligands can affect the size of the direct band gap. The combination of the effects due to ligand size and electronegativity. The electronegativity of the ligand is believed to determine the extent of electron density withdrawal from the germanium scaffold, which weakens Ge-Ge bonding and reduces the band gap. Large ligand size can introduce strain and as a result also reduce the band gap energy. We used DRCLS to examine this relationship. The electronegativity of each ligand decreases from $–CH_2OCH_3$ > -H > $-CH_3$ > $-CH_2CH{=}CH_2$. DRCLS finds the band gap energies increase from CH_2OCH_3 (1.47 eV) > $-CH_2CH{=}CH_2$ (1.50 eV) > -H (1.52 eV) > $-CH_3$ (1.62 eV). These values follow the trend in electronegativity with the exception of the allyl termination, which can be explained using strain as it is the largest ligand.

We used SPS and DRCLS to observe sub band gap optical states in $GeCH_3$. SPS shows E_C - 0.85 eV and E_V+1.05 eV. DRCLS shows complementary transtions due to gap states at 0.82, 0.96, 1.02, and 1.35 eV. Investigating $GeCH_3$ samples that have been deintercalated for one week and three weeks the 1.02 eV feature disappears in the sample that had been deintercalated for three weeks. This can be tentatively attributed to the removal of residual CaI_2 from interlayer spacing of the $GeCH_3$ layers. This demonstrates that defects can be identified and eliminated. through systematic chemical processing. This work supported by NSF MRSEC under award number DMR-1420451.

9:55am **PCSI-WeM-18 Electrostatic Doping and Hybrid Carriers in Graphene on a Polar $SrTiO_3$ (111) Surface: Theoretical Investigation***, D Shin, **Alexander Demkov**,* The University of Texas

Figure 1. (a) Band structure of graphene on STO (111). A dashed line represents the Fermi level which is set to zero. Probability distribution calculated within the energy window (± 0.03 eV) corresponding to the band crossing point (b) and charge density corresponding to the Fermi level ©. It shows the charge density of graphene sheet and the surface of STO (111).

Graphene is a two-dimensional carbon sheet with a honeycomb lattice structure. It is a zero-gap-semiconductor that has a linear energy dispersion near the Fermi level [[file:///C:/Users/Alexander/Documents/ALEX/Papers/Abstracts/2016/PCSI-44_Abstract_grphene.doc#_ENREF_1], [file:///C:/Users/Alexander/Documents/ALEX/Papers/Abstracts/2016/PCSI-44_Abstract_grphene.doc#_ENREF_2]].Doping graphene layers presents a difficult practical and fundamental problem. We consider theoretically, the possibility of electrostatic doping of graphene by the intrinsic field of a polar substrate. Density functional theory calculations are carried out for a graphene sheet placed on the (111)-oriented perovskite $SrTiO_3$ surface. We find that the Fermi surface moves well below the Dirac point of graphene, resulting simultaneously in a fast conducting channel in graphene, and a slow, large effective mass channel in the oxide surface. Electrostatic gating may allow one to explore peculiar states that, through the "no-crossing" reminiscent of polaritons, would represent a hybrid carrier that exists simultaneously in both materials. In Fig. 1 we show the near edge electronic structure and corresponding charge distribution of the system. Importantly, in addition to the field doping, we identify a more "obvious" mechanism of doping through the contact potential difference, which may have wider applications in the doping of two-dimensional materials.

[+] Author for correspondence: demkov@physics.utexas.edu

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11:00am **PCSI-WeM-31 Dielectric Related Issues in GaN Based MIS HEMTs***, **Gaudenzio Meneghesso**,* University of Padova, DEI, Italy*; D Bisi, I Rossetto, M Ruzzarin, C De Santi, M Meneghini, E Zanoni,* University of Padova - DEI, Italy **INVITED**

Over the last few years GaN has emerged as an excellent material for the fabrication of high-voltage devices (high electron mobility transistors, HEMTs) for application in the power conversion systems. Thanks to the low on-state resistance (<100 mW for a 20 A transistor [1]) and the low leakage (<1-10 μA at 650 V [2]) these devices are currently targeting the 650 V market segment. One of the most promising solutions for normally-off operation is the combined use of a normally-on GaN HEMT and a low-voltage silicon MOSFET in cascode configuration [3], [4]. A metal-insulator-semiconductor (MIS) HEMT can be used to this aim. This approach guarantees low gate leakage current levels and a high intrinsic robustness. However, in a MIS-HEMT the dielectric represents a critical element, that is subject to a relevant electric field: under off-state conditions, the field peaks at the edge of the gate (or field plate) on the drain side, while under positive gate bias conditions the field on the dielectric is more uniform, since the 2-dimensional electron gas (2DEG) is formed under the gate.

Several dielectrics can be used for the fabrication of MIS-HEMTs including SiN[5], Al_2O_3[6], SiO_2[7], HfO_2[8], and TiO_2[9]. In most of the cases these dielectrics are deposited by chemical vapor deposition (CVD, as in the case of SiN) or by atomic layer deposition (ALD, as in the case of Al_2O_3).

This paper reviews the most relevant dielectric-related trapping mechanisms in GaN-based transistors. Metal-insulator-semiconductor (MIS) devices with partially-recessed gate have been submitted to pulsed and constant voltage stress, with the aim of evaluating the impact of charge trapping processes on the dynamic properties of the devices and on the negative-bias threshold instabilities (NBTI) induced by negative gate bias. Three different dielectrics were considered for this investigation: SiN deposited by rapid thermal chemical vapour deposition (RTCVD), SiN deposited by plasma enhanced atomic layer deposition (PE-ALD), and Al2O3 deposited by atomic layer deposition (ALD). The results obtained within this paper are critically compared to previous literature reports, to provide a more complete view of the state-of-the-art.

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11:30am **PCSI-WeM-37 Device Physics Modeling of Metal-Semiconductor Interfaces from an Induced Gap State Perspective***, **John Wager**, K Kuhn,* Oregon State University

Induced gap state (IGS) modeling attempts to explain the electronic properties of metal, semiconductor, or insulator surfaces or interfaces in terms of intrinsic behavior associated with quantum mechanically induced evanescent states arising from the abrupt termination of a bulk material at a surface or interface [1]. Although IGS modeling pertains to a wide variety of surfaces and interfaces, this presentation will focus primarily on one specific case – the metal-semiconductor (MS) interface – in order to provide a tutorial introduction to the topic of IGS modeling.

Figure 1. Equivalent circuit of a MS interface for (a) an ideal (ignoring interface states) macroscopic dipole, (b) a non-ideal (including interface states) microscopic dipole, and © a non-ideal (including interface states) macroscopic dipole.

A very unusual but powerful aspect of IGS modeling is its persistent use of equivalent circuits to elucidate surface and interface electronic behavior. For example, Figure 1 shows three equivalent circuits that are useful for assessing an MS interface. For an ideal situation in which interface states are ignored, Figure 1a reveals that the surface potential, ψ_{Sm}, is simply equal to the MS work function difference, $\Phi_S - \Phi_M$. This idealized case is described as involving a macroscopic dipole since charge separation between the sheet of charge at the MS interface and the charge centroid associated with the semiconductor space charge region is of macroscopic (rather than atomic) dimensions. In contrast, Figure 1c shows that when interface states are accounted for, the true surface potential, ψ_S, is degraded from what it would be in the absense of interface states, i.e., ψ_{Sm}, by a microscopic (atomic dimensions) dipole voltage due to interface states, i.e., Δ_{MS}. Evaluation of Δ_{MS} requires using Figure 1b to determine how much the charge neutrality level misalignment voltage, $\Phi_{CNLS} - \Phi_M$, drops across the microscopic dipole interface capacitance, C_i.

The origin of the eqivalent circuits shown in Figure 1 will be clarified in the presentation via a discussion of the electrostatics of MS interface formation.

$^+$ Author for correspondence: jfw@ece.orst.edu

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11:35am **PCSI-WeM-38 Investigation of ZnO/PbS Nanocrystal Interfaces for Photonic Device Applications***, **Diogenes Placencia**,* Naval Research Laboratory*; I Sellers,* University of Oklahoma*; J Boercker, J Tischler,* Naval Research Laboratory

Research into lead sulfide (PbS) nanocrystal devices has garnered much attention recently due to their notable performance as photovoltaic devices and short wave infrared photodetectors, among other applications.[1,2] Common within such devices is the use of metal oxide thin-films (e.g., ZnO, ITO, NiO, etc.) that act as charge-selective contacts. Therefore, characterization of the interfacial properties between metal oxides and PbS nanocrystals is crucial to the overall development of these technologies. In this contribution, we present our investigations into the properties that dominate operational efficiency of the ZnO/PbS heterojunction. Through a series of varying oxide pre-treatments (e.g., plasma cleaning, small-molecule surface modifications, and wet-chemical etching), we investigate how the state of the surface affects band-edge offsets (via Ultraviolet Photoemission Spectroscopy), changes in the surface chemistry at the interface (through X-ray Photoemission Spectroscopy), and overall structural changes (utilizing Scanning Probe Microscopy). Additionally, we provide insight into how these pre-treatments affect overall device performance in the standard inverted device geometry.

$^+$ Author for correspondence: d.placencia@nrl.navy.mil

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11:40am **PCSI-WeM-39 Defect Density Reduction in Core layer of ZnTe Electro-Optical Waveguide by Low Lattice Mismatched Interfaces***, **Wei-Che Sun**,* Waseda University, Japan*; T Nakasu, K Odaka,* Waseda University*; M Kobayashi,* Waseda University, Japan*; T Asahi,* JX Nippon Mining & Metals Corp.

ZnMgTe(Cladding)/ZnTe(Core) thin film waveguide has been proposed to form a practical Electro-optical (EO) device due to the high EO coefficient of ZnTe (r_{41}= 4.5 pm/V) [1]. For low loss ZnMgTe/ZnTe waveguide, large refractive index difference between layers can be achieved by adding Mg content (Mg %). However, high Mg% results in lattice mismatch enlargement (lattice mismatch between ZnTe and MgTe is 4.1%), and misfit dislocations at interfaces would befall and degrade the crystal quality. In previous study, waveguide with Mg 20%, 0.6 μm cladding layer was found to have high-performance [2]. However, large in-plane lattice mismatch (0.8%) between ZnMgTe and core layers, and high defect density in core layer at the interface region was observed (4×10^9 /cm^2). Therefore, low Mg % interlayers were introduced to create a series of low lattice mismatch interfaces and circumvent the effect of the large lattice mismatch (two-step index waveguide). In this study, two kinds of structures were considered to realize a low loss two-step index waveguide. One structure was designed to insert 0.1 μm low Mg% interlayers, and cladding layer thickness and Mg % were kept about 0.6 μm and 20%, respectively (sample 1). The other structure was designed to have the cladding layer 0.3 μm with Mg 20% and Mg 10% 0.45-μm-thick interlayer (sample 2).

By cross-sectional transmission electron microscope observation, both samples had lower defect densities (2×10^8 /cm^2 for sample 1; 2×10^9 /cm^2 for sample 2) than the single-step index waveguide in core layer at the interface region. It indicates that extra interfaces with lower lattice mismatches were successfully helped to improve crystallographic properties. The interlayer worked efficiently even if thickness was only about 0.1 μm thick. With the reduction in defect density of the ZnTe layer, the EO property of the device is expected to be improved. However, the propagation loss was not improved by the introduction of the low Mg % interlayers when the average Mg % of ZnMgTe layers was in sufficient. By carefully control of the average Mg %, ZnTe waveguide with a series of low lattice mismatches interfaces could have better crystal quality without dropping the optical confinement.

11:45am **PCSI-WeM-40 Charge Transfer and Lattice Strain at Oxide Interfaces: Emergent Mottness, Multiferroicity and Antisite Defects***, **Andrew Millis**,* Columbia University **INVITED**

Interfaces separating transition metal oxide materials of different functionalities have the potential to host novel and potentially behavior. Understanding how to design interfaces that optimize desired properties while minimizing the potential for undersireable effects is an important research goal. In this talk I highlight the important roles of substrate-induced strain and across-interface charge transfer in controlling the properties of transition metal oxide-based superlattices. Charge transfer is controlled by the relative electronegatives of the transition metal ions while strain is controlled by the substrate. I give examples of how charge transfer and strain may lead to desirable properties including emergent Mott insulating behavior [1] and multiferroicity [2] as well as undesirable properties including antisite defects [3]. Strengths and weaknesses of calculational methods are outlined [4]. This work was performed in collaboration with Hanghui Chen and supported by DOE ER-046160 and NSF-DMR-1120296.

12:15pm **PCSI-WeM-46 Large Piezoelectric Characteristics of $KNbO_3$ Nanorods***, **SeolHee Oh**,* Ewha Womans University, Republic of Korea*; B Yun, J Jung,* Inha University, Republic of Korea*; W Jo,* Ewha Womans University, Republic of Korea

Piezoelectric nanomaterials have been receiving a great deal of attention because its applicable features to an energy conversion devices using mechanical-electrical-thermal coupling. $KNbO_3$ (KNO), potassium niobate, is one of the promising lead-free piezoelectric materials due to its high Curie temperature and large piezoelectric constants for nanoscale energy harvesting devices [1,2]. In this study, the piezoelectric properties of KNO nanorods (NRs) with respect to their intrinsic structural properties were studied via piezoresponse force microscopy. High-quality KNO NRs with orthorhombic as well as monoclinic structures were synthesized by using a hydrothermal method. It is notable that the stable monoclinic phase is only observed in nanoscale structure. The effective value of piezoelectric constant, d_{eff}, is 83.5(1) pm/V for monoclinic KNO NRs, which is 1.6 times larger than that of the orthorhombic KNO NRs (54.2(1) pm/V). It is caused by unconstrained rotational polarization of monoclinic KNO NRs, whereas polarizations of orthorhombic KNO NRs are constrained along the direction which is differ from maximum piezoresponse axis. In addition to, approximately 6% piezoelectric enhancement compared to as-grown KNO NRs was observed as a result of the alignment of the polarization of KNO NRs by applying bias on monoclinic and orthorhombic KNO NRs.

12:20pm **PCSI-WeM-47 Strain Engineering and Interfacial Effects on the Photovoltaic Response in Epitaxial Complex Oxides***, **Adrian Podpirka**, A Bennett-Jackson, D Imbrenda, Z Gu,* Drexel University*; V Fridkin,* Drexel University/Shubnikov Inst. for Crystallography

Ferroelectric oxide perovskites are promising for use in photovoltaic solar energy conversion because carrier separation can occur even in the absence of a *p-n* junction, photovoltage can exceed the band gap, and power conversion efficiencies greater than the band gap-specific limit can be attained.[1] While ferroelectric devices exhibit efficiencies as high as ≈8%,[2] the influences of strain and of space charge near the ferroelectric-metal interface on photovoltaic properties are only beginning to be understood. [3] Using epitaxial $BaTiO_3$ films produced by pulsed laser deposition as a model system, we report here on investigation of the effects of strain profiles and interfacial band offsets on the photovoltaic response. Work supported by the US Army Research Office under W911NF-14-1-0500 and the SunShot Program of the US Department of Energy under DE-SC000144664.

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12:25pm **PCSI-WeM-48 Symmetry Breaking in Abnormally Elongated $PbVO_3$ Thin Films Epitaxially Grown by Pulsed Laser Ablation***, **SeolHee Oh,*** Ewha Womans University, Republic of Korea*; C Roh, J Lee,* Gwangju Institute of Science and Technology (GIST), Republic of Korea*; W Jo,* Ewha Womans University, Republic of Korea

An intriguing polar magnetic $PbVO_3$ (PVO) has a VO_5 square-pyramidal structure rather than VO_6 octahedron due to extreme tetragonal distortion, which leads the 2-dimensional antiferromagnetic ordering and large pyroelectric polarization by 152 $\mu C/cm^2$. In this study, we fabricated epitaxial PVO thin films on $LaAlO_3$ (LAO) (001) and $SrTiO_3$ (STO) (001) substrates by pulsed laser deposition with off-stoichiometric condition [1]. Structural properties of the epitaxial PVO thin films with respect to mechanical strain induced by lattice mismatch with substrates were investigated by X-ray diffraction, high-resolution transmission electron microscopy, Raman scattering spectroscopy. As a result, abnormal lattice elongation of the PVO thin films along c-axis and consequent octahedral distortion were observed. In addition, the experimental characterizations of linear and nonlinear optical properties for the PVO thin films were performed through spectroscopic ellipsometry and second harmonic generation (SHG), respectively. Symmetry breaking along c-axis in PVO thin films were demonstrated by using SHG signal with nonlinear susceptibility and Fresnel's formula fitting.

PCSI
Room Ballroom South - Session PCSI-WeA
Semiconductor Growth III/Wide Gap/Oxide Interfaces/Low-D Structures

Moderators: Chang-Beom Eom, University of Wisconsin-Madison, Stefan Fölsch, Paul-Drude-Institut für Festkörperelektronik, Gaudenzio Meneghesso, University of Padova - DEI, Markus Wohlgenannt, University of Iowa

2:00pm **PCSI-WeA-1 The Application of Bismuth as a Surfactant During the Growth of Strain-balanced InAs/InAsSb Superlattices***, **Shane Johnson**, P Webster,* Arizona State University **INVITED**

Recent investigations of the optoelectronic properties of MBE grown strain-balanced type–II InAs/InAsSb superlattices indicate that they have the minority carrier lifetimes and absorption properties necessary for high performance infrared photodetectors [1,2]. The optical performance of this material system can be enhanced by optimizing the constituent layer thicknesses and the Sb mole fraction [2], and through the utilization of bismuth as a surfactant during growth. The presence of a Bi surface layer reduces the incorporation of surface Sb into the InAs/InAsSb superlattice structure and enhances the photoluminescence intensity for dilute Bi fluxes (Bi/In ratio ~ 1%) [3]. As a surfactant, Bi can be applied during the growth of the entire superlattice structure or only during the growth of the constituent InAs layers as a means to moderate the unintentional incorporation of Sb into the InAs material. The figure shows photoluminescence from strain-balanced InAs/InAsSb superlattices grown at 430 ºC using Bi/In flux ratios ranging from 0 to 3%. The inset provides the integrated photoluminescence intensity versus Bi/In flux ratio (%). The peak efficiency occurs at a Bi/In flux ratio around 1% for 430 ºC growth temperatures. These results and the examination of the unintentional incorporation of Sb into the InAs layers will be presented.

2:30pm **PCSI-WeA-7 Atomic Scale Study of Isovalent Bi Atoms in the (110) InP Surface***, **Christian Krammel**,* Eindhoven University of Technology, Netherlands*; F Davis-Tilley, M Roy, P Maksym,* University of Leicester, UK*; L Zhang, P Wang, K Wang, Y Li, S Wang,* Chinese Academy of Sciences, China*; P Koenraad,* Eindhoven University of Technology, Netherlands

Recent advances in semiconductor growth technology have led to the development of highly mismatched III-V semiconductors, such as dilute nitrides and bismides. This novel material class has attracted much attention from both a fundamental and application-oriented point of view [1,2]. Compared to the well-studied dilute nitrides, little is known about dilute bismides at the atomic length scale, which are in many ways complementary to dilute nitrides [3,4]. We address this issue in state of the art Bi:InP by cross-sectional scanning tunneling microscopy (X-STM) [5].

Bi atoms up to the second monolayer below the (110) InP surface are identified with the help of a geometrical hard sphere model [6] and complementary density functional theory (DFT) calculations. It is found that the contrast of Bi atoms in and directly beneath the (110) surfaces is mainly related to local strain effects of the large Bi atoms on the InP matrix. Besides these structural effects, the influence of Bi impurities on the local electronic structure is addressed in dI/dU point spectra. Here, specific Bi related resonances in the valence band of Bi atoms in the first three surface layers are discussed with respect to theoretical expectations. Bi:InP shows compared to other Bi doped III-Vs an unusual sub band gap photo luminescence. In this light, the short-range ordering of Bi atoms is addressed in Bi doped InP quantum wells and films. The X-STM measurements revealed an enhanced tendency for the formation of first nearest neighbor Bi pairs. At higher Bi contents additional Bi clustering is observed. Bi:InP/InP quantum wells show in contrast to dilute nitrides characteristic segregation patterns.

$^+$ Author for correspondence: c.m.krammel@tue.nl

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2:45pm **PCSI-WeA-10 Current State-of-the-Art of Gallium Oxide Power Device Technology***, **Masataka Higashiwaki**, M Wong, K Konishi,* National Institute of Information and Communications Technology, Japan*; K Sasaki, K Goto,* Tamura Corporation, Japan*; R Togashi, H Murakami, Y Kumagai,* Tokyo University of Agriculture and Technology, Japan*; B Monemar,* Linköping University, Sweden*; A Kuramata, S Yamakoshi,* Tamura Corporation, Japan **INVITED**

Recently, gallium oxide (Ga$_2$O$_3$) has emerged as a new competitor to SiC and GaN in the race toward next-generation power devices by virtue of the excellent material properties and the relative ease of mass wafer production. Following a short introduction of material properties and features of Ga$_2$O$_3$, this presentation will review our recent development progress in device processing and characterization of Ga$_2$O$_3$ metal-oxide-semiconductor field-effect transistors (MOSFETs) and Schottky barrier diodes (SBDs).

Ga$_2$O$_3$ MOSFETs were fabricated with unintentionally-doped (UID) Ga$_2$O$_3$ epitaxial layers grown on semi-insulating Fe-doped β-Ga$_2$O$_3$ (010) substrates by ozone molecular beam epitaxy [1]. Selective-area Si-ion implantation doping of the UID Ga$_2$O$_3$ epitaxial layer formed the device channel and ohmic contacts [2], while the high resistivity of UID Ga$_2$O$_3$ was utilized for planar device isolation without mesa etching. SiO$_2$-passivated depletion-mode MOSFETs with a gate-connected field plate (FP) demonstrated a high off-state breakdown voltage (V_{br}) of 755 V, a large drain current on/off ratio of over nine orders of magnitude, DC-RF dispersion-free output characteristics, and stable high temperature operation against thermal stress at 300°C.

We also fabricated and characterized Pt/Ga$_2$O$_3$ FP-SBDs on n$^-$-Ga$_2$O$_3$ drift layers grown on n$^+$-Ga$_2$O$_3$ (001) substrates [3], owing to the success of halide vapor phase epitaxy for high-speed growth of high-quality Ga$_2$O$_3$ thin films [4, 5]. The illustrative device with a net donor concentration of 1.8×10^{16} cm^{-3} exhibited a specific on-resistance of 5.1 mΩ·cm^2 and an ideality factor of 1.05 at room temperature. Successful FP engineering resulted in a high V_{br} of 1076 V. Note that this was the first demonstration of V_{br} of over 1 kV in any Ga$_2$O$_3$ power devices.

In summary, the FP-MOSFETs and FP-SBDs revealed excellent device characteristics and demonstrated great potential of Ga$_2$O$_3$ devices for power electronics applications.

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$^+$ Author for correspondence: mhigashi@nict.go.jp

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3:15pm **PCSI-WeA-16 CO$_2$ Reduction with H$_2$O over Ga$_2$O$_3$ Photocatalysts Prepared at Various Calcination Temperatures***, **Masato Akatsuka**,* Nagoya University, Japan

Gallium oxide (Ga$_2$O$_3$) photocatalysts can reduce CO$_2$ with H$_2$Oto produce CO, although the reaction rate of CO production is very low. It has been reported that the loading of Ag on Ga$_2$O$_3$ promoted CO production [1], on the other hand, improvement of Ga$_2$O$_3$ structure should be also essential. In our previous work [2], Ga$_2$O$_3$ loaded Al$_2$O$_3$ samples (Ga$_2$O$_3$/ Al$_2$O$_3$) were prepared to change coordination structures around Ga atoms, and we succeeded to enhance CO production rate. Recently, we found that the photocatalytic activity of Ga$_2$O$_3$ depended on the calcination temperature for a Ga$_2$O$_3$ precursor in the preparation stage. Therefore, in this study, we will discuss the reason why the CO production was enhanced by controlling calcination temperature.

Ga$_2$O$_3$ samples were prepared by calcination of Ga(NO$_3$)$_3$·8H$_2$O powder in the air at given temperatures (673 - 1173 K) for 4 h. We carried out photocatalytic CO$_2$ reduction with H$_2$O over the Ga$_2$O$_3$ samples. Fig.1 shows CO production rate for each Ga$_2$O$_3$ sample. Ga$_2$O$_3$ prepared by calcination at 823 K (Ga$_2$O$_3$(823 K)) showed a specifically high activity for CO production, although the H$_2$ production rate for this sample was comparable with those for Ga$_2$O$_3$ (673, 773, 873 K). It was found that the H$_2$ production rate increases with the surface area of the sample.

In XRD measurement of Ga$_2$O$_3$(823 K), very weak and broad diffraction peaks were observed, suggesting the formation of low crystallinity β-Ga$_2$O$_3$. Taking into account that a low crystallinity photocatalyst has many defects to promote the recombination of excited electron-hole pairs, high CO production activity for Ga_2O_3(823 K) would be resulted from an improvement of CO_2 adsorption process rather than electrons and holes diffusion process. Therefore We performed FT-IR measurements for chemisorbed species on Ga_2O_3 samples after introduction of CO_2. It was revealed that adsorbed species on Ga_2O_3(823 K) are different from those on other Ga_2O_3 samples. The FT-IR spectrum of Ga_2O_3(823 K) indicated preferential formation of CO_2 species interacting with water adsorbed on Ga_2O_3 surface.

3:20pm **PCSI-WeA-17 ZrO_2 as a High-k Gate Dielectric for Enhancement-mode AlGaN/GaN MOS HEMTs***,* ***Charles Eddy, Jr.****, V Wheeler,* U.S. Naval Research Laboratory*; D Shahin,* University of Maryland*; T Anderson, M Tadjer, A Koehler, K Hobart,* U.S. Naval Research Laboratory*; A Christou,* University of Maryland*; F Kub,* U.S. Naval Research Laboratory

Advanced applications of AlGaN/GaN high-electron-mobility transistors (HEMTs) in high-power RF and power switching are driving the need for an insulated gate technology. We present here basic and early applied studies of the use of zirconium oxide (ZrO_2) as a high-k, high breakdown gate dielectric for reduced gate leakage and a fully-recessed barrier structure for enhancement-mode operation of AlGaN/GaN HEMTs. We include the study of GaN surface preparations for dielectric deposition, surface/interface characterization and device operation wherein a world record threshold voltage of +3.99V is achieved.

An optimum GaN surface preparation involving a piranha etch followed by a thermal oxidation of the surface has previously been shown [1] to result in smooth, clean GaN surfaces that exhibit the best electrical performance when ALD high-k dielectrics are deposited thereon. This same preparation is applied to ALD ZrO_2 dielectrics. ZrO_2 films were deposited by atomic layer deposition (ALD) using two different metal precursors [zirconium (IV) tert-butoxide (ZTB) and tetrakis(dimethylamido)zirconium(IV) (TDMAZ)] and water. For the former we also assessed both water and ozone as the oxygen precursor. ZrO_2 films grown by ALD with ZTB were found to be slightly oxygen rich whether ozone or water were used as the oxygen source. However, films grown with ZTB and ozone did have carbon contamination. Films grown with TDMAZ and water were found to be stoichiometric and free of carbon.

Films grown with ZTB and water on optimally prepared surfaces again shown the best electrical performance for the dielectric-semiconductor interface in terms of smoothness, low leakage in forward and reverse bias ($< 10^{-5}$ A cm^{-2}) and low hysteresis. Unlike in previous studies with ALD deposited Al_2O_3 and HfO_2, where total trapped charge was in the mid-10^{11} to low 10^{12} cm^{-2} range, ZrO_2 films show considerably higher trapped charge densities in the high 10^{12} to mid-10^{13} cm^{-2} range. The nature of this charge is uncertain at this time but believed to be due to excess oxygen in ZTB deposited films and is directly responsible for a 1.5 – 2 V positive shift in threshold voltage.

$^{+}$ Author for correspondence: chip.eddy@nrl.navy.mil

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3:25pm **PCSI-WeA-18 Defects and Electrical Characteristics of Pt-based Ohmic and Schottky Contacts to ZnO Nanowires***,* ***Jon Cox****, G Foster, A Jarjour,* The Ohio State University*; H Von Wenkstern, M Grundmann,* Universität Leipzig Institut für Experimentelle Physik II, Germany*; L Brillson,* The Ohio State University

Zinc oxide has emerged as a promising wide bandgap material (3.35eV at 300K) for use in next-generation nanoelectronics, with important piezoelectric, gas sensing, and optoelectronic (UV) properties. We report the *in-situ* fabrication of both Ohmic and Schottky contacts to single ZnO nanowires prepared by pulsed laser deposition (PLD) and carbothermal vapor phase transport, using only Pt metal and Ga-ion surface modification.

In bulk ZnO, defects have been shown to strongly affect the behavior of metal contacts, by modifying band bending and allowing trap-assisted tunneling transport through the metal-ZnO Schottky barrier [1].

A Ga focused ion beam (FIB) was operated at 30 keV to implant NW surfaces before metallization for creation of Ohmic contacts, and at 5 keV to gently mill the outer annulus and reduce defect concentrations at the surface, promoting formation of Schottky contacts. Electron beam induced deposition (EBID) was used to pattern Pt metal contacts to the wires, and current-voltage characteristics were measured. Depth-resolved cathodoluminescence spectroscopy (DRCLS) was used to measure native point defects at the nanowire surface, into the bulk, and under 30nm Pt contacts. Depth profiles of DRCL spectra at and under Ga-implanted Ohmic contacts reveals interfacial segregation of copper on zinc site defects (Cu_{Zn}, 2.34eV) and oxygen vacancies (V_O, 2.54eV). Ohmic contact resistivity was also found to decrease with increasing 30 keV Ga-implantation dose. A depth profile of DRCL spectra at the interface of a Ga-milled area and 30nm Pt contact demonstrates that milling of the NW surface decreases concentration of Cu_{Zn} by an order of magnitude, promoting the formation of Schottky contacts. A Schottky contact with 2 orders of magnitude rectification was fabricated to the thin end of a tapered NW, whose diameter increases linearly from 400nm to 1µm at the other end. Investigation of defect dependence on NW diameter also demonstrated a 2x linear increase in Cu_{Zn} from 500nm to 1µm diameter. To cause pinch-off, the depletion width must be comparable to the NW diameter [2]. Thus, thinner wires are easier to pinch-off and have a lower inherent concentration of surface defects, promoting easier formation of Schottky contacts.

The interfacial physics of contacts to NW's is influenced by the diameter of the NW and its defect profile at the interface. Through the control of defects in these NW's by Ga-ion surface modification, Ohmic and Schottky contacts can be fabricated *in*-situ using a single metal. The authors gratefully acknowledge support from National Science Foundation Grant No. DMR-1305193 (Charles Ying and Haiyan Wang).

4:30pm **PCSI-WeA-31 Investigation of Schottky Contacts and Traps in β-Ga_2O_3***,* ***Aaron Arehart****, S Ringel, E Farzana, Z Zhang,* The Ohio State University*; E Ahmadi, Y Oshima, J Speck,* University of California, Santa Barbara **INVITED**

Beta-phase gallium oxide (β-Ga_2O_3) is an ultra-wide bandgap (UWBG) semiconductor that is promising for a broad range of applications including power electronics and chemical sensing, but the understanding of this material is still in its infancy. β-Ga_2O_3 is attracting particular interest due to its large, direct bandgap of ~ 4.8 eV, the availability of *n*-type doping, the ability to create heterostructures, and the availability of native substrates to support homoepitaxial growth. Additionally, several groups have reported promising initial results with high breakdown voltage transistors demonstrating the promise of this material [1-3]. However, there has been little research so far to understand the source and concentration of defects or their impact on device behavior so far [4]. Additionally, the properties of Schottky contact metals are not well explored, but is essential for metal semiconductor field effect transistors (MESFET) and similar devices. This presentation will focus on characterization of defects in β-Ga_2O_3 (Fig. 1), exploration of Schottky barrier heights for Ni, Au, Pt, and Pd metals (Fig. 2) using internal photoemission, capacitance-voltage, and current-voltage-temperature (I-V-T) measurements, and the carrier transport in the Schottky contacts using I-V-T.

$^{+}$ Author for correspondence: arehart.5@osu.edu

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5:00pm **PCSI-WeA-37 Defect Distribution and Electronic Properties of the IrO_x/ZnO Interface***,* ***Geoffrey Foster****,* The Ohio State University*; G Mackessy,* Columbus School for Girls*; A Hyland, M Allen,* University of Canterbury, New Zealand*; L Brillson,* The Ohio State University

We used depth-resolved cathodoluminescence spectroscopy (DRCLS) to measure the spatial distribution of native point defects at Zn- and O-polar ZnO interfaces with iridium oxide (IrO_x) and their impact on Schottky barrier formation. Oxidized metal, such as IrO_x and PtO_x, have sparked interest in their high work functions allowing them to be used as both Ohmic and Schottky contacts[1]. These oxidized metal layers produce Schottky contacts with the ZnO. These diodes have rectification of 8.6 and 5.5 orders of magnitude, respectively, with barrier heights of 0.89 eV and 0.67 eV. For the same RF sputter of a 32 nm IrO_x layer, on ZnO, sample on both Zn-polar and O-polar ZnO, incident electron beams with energies E_B = 1 -5 keV generated electron-hole (e-h) pairs that recombined to exhibit DRCLS spectra past the IrO_x layer, with 3.35 eV intrinsic band gap transitions in ZnO, and 2.01 eV and 2.08 eV V_{Zn} transitions in the Zn-polar and O-polar ZnO respectively. V_{Zn} acts as a compensating defect, acting to increase the depletion width at the IrO_x/ZnO interface creating the Schottky diode [2]. DRCLS enabled us to profile the V_{Zn} density across the IrO_x/ZnO interface on a near nm scale as defined by Monte Carlo simulations of electron-hole (e-h) pair creation rate vs. depth. This defect depth precision revealed interfaces with V_{Zn} profiles in the ZnO that varied with the Zn-Polar and O-polar ZnO orientations. The depth profiles show a clear difference in the density of V_{Zn} in each sample with nearly a 1.5 times increase in V_{Zn} density from th e O-polar to the Zn-polar sample.

The variation of the V_{Zn} between each is significant since it explains the higher barrier height in the Zn-polar ZnO. This increased barrier height from growing oxidized metals on semiconductor films could have implications since these high work function metals could be used as Ohmic contacts on p-type semiconductors. The authors gratefully acknowledge support from National Science Foundation Grant No. DMR-1305193 (Charles Ying and HaiyanWang).

*Author for correspondence: foster.887@buckeyelamil.osu.edu

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5:05pm **PCSI-WeA-38 Ultrasound Treatment Influece on the Si-SiO_2 Interface Defects Structure***, **Daniel Kropman**, T Laas,* Tallinn University, Estonia*; A Medvids,* Riga Technical University

The effect of ultrasonic treatment (UST) on the defect structure of the Si–SiO_2 system by means of electron spin resonance (ESR), metallography, MOS capacitance technique and secondary ions mass-spectroscopy is presented. The non-monotonous dependence of the point defect densities on the US wave intensity has been observed. The US frequency influence on the ESR signal intensity of the defect centres depended on the defects type and may be caused by vibrational energy dissipation which are a function of defect centre’s type. The density of point defects and absorbed impurities at the Si–SiO_2 interface can be reduced by appropriate choise of UST.

Before UST a signal with g=1.9996 (Pa centers) connected with vacancy complexes is observed. After UST appears another signal with g=2.0055 (broken bonds of Si atoms).Investigation of the dependence of the spin density on the US frequency of the UST in Si-SiO_2 samples with [lll] and [100] crystallographic orientation was carried out. It has been shown that the influence of the US frequency and the sample orientation on the ESR signal intensity varies for different centres. The frequency and orientation dep endence of the ESR signal with g=l.9996 and the lack of this dependence for the centres with g=2.0055 show that the vibrational energy dissipation depend on the type of defect centres and their orientation. Defect density grows with an increase of the US intensity or changes nonmonotonously depending on the oxides thickness.In the samples with thick oxide there is a maximum in the dependence of the charge carriers life time on the US wave amplitude, while in samples with thin oxide -a minimum. This shows that the structural defects form electrically active centres and their density can be varied by UST.

5:10pm **PCSI-WeA-39 The Effects of B and Ga Co-doped ZnO Electron Transporting Layer on the Properties of n-ZnO /p- GaN UV Photodetector***, J Huang, **Linjun Wang**, K Tang, Y Shen, F Gu,* Shanghai University, China

Recently, ZnO has attracted much attention in short wavelength optoelectronic devices and sensors [1-2] due to its direct wide optical bandgap (3.37eV) and high exciton binding energy (60meV). Also ZnO is intrinsically an n-type semiconductor and can easily be a heterojunction with other p-type materials, such as p-Si, p-NiO, p-SiC, p-GaN as well as some p-type organic-polymers. Based on the very good characteristics of ZnO mentioned above, it is very popular to be chosen as electron selective layer in ultraviolet (UV) photodetectors (PDs) [3-4].

B and Ga co-doped ZnO (BGZO), as a transparent conduction oxide electrode, has many good physical properties, such as high electrical conductivity, excellent optical transparency and thermal stability, which would replace the traditional ITO or FTO due to its low cost and easy process [5]. Herein, we prepared BGZO with different thicknesses as an electron transporting layer of the ZnO /GaN heterojunction and the ultraviolet photoresponse characteristics of the devices were investigated. From the results, we find that the PDs with BGZO coating showed higher responsivity.

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5:15pm **PCSI-WeA-40 2D Silica and Aluminosilicate Bilayers on Pd(111): From Incommensurate to Commensurate Crystalline***, **Jin-Hao Jhang**, C Zhou, G Hutchings, E Altman,* Yale University

Zeolite silicate frameworks are essential in facilitating numerous catalytic reactions. Although zeolites have been used for decades, it is still a long-term challenge to understand how surface properties of zeolites promote catalytic reactions. Recently, two-dimensional (2D) van der Waals silica and aluminosilicate bilayers have been successfully prepared on metal substrates, e.g. Pd(100) [1], Pt(111) [2], and Ru(0001) [3,4]. This achievement creates a new pathway for investigating zeolites using surface science approaches.

Both silica and aluminosilicate bilayers can grow in crystalline and amorphous forms. On Pt(111) only amorphous silica bilayer can be formed likely due to the relatively large lattice mismatch with the crystalline form, whereas on Ru(0001) both crystalline and amorphous bilayers are seen due to a low lattice strain. However, the structural information of the bilayer -growth transition between crystalline and amorphous phases is still lacking. Pd(111) thus becomes a suitable substrate to gain the information because of the degree of the lattice mismatch: Pt(111) = 4.6% > Pd(111) = 3.7% > Ru(0001) = 2%. We report structural studies of silica and aluminosilicate bilayers on Pd(111) via low energy electron diffraction and scanning tunneling microscopy, complemented by density functional theory (DFT) calculations. Our results reveal that silica bilayers grow in an incommensurate crystalline form on Pd(111) which is found neither on Pt(111) nor Ru(0001) and is in contrast to Pd(100) where a commensurate form is observed. It puts the maximum biaxial tensile strain that can be imparted on the bilayer to less than 3.7%. The aluminosilicate bilayer was successfully prepared by replacing 25% of the Si with Al, and importantly, it grows commensurately on Pd(111). The DFT calculations reveal that the longer Al-O bonds reduce the strain energy by decreasing the mismatch to 1.9% as well as by softening it; thereby explaining the transition from incommensurate to commensurate forms. Overall, this work clearly provides an insight into the possibility of manipulating the structure of a 2D material.

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5:20pm **PCSI-WeA-41 Electron-phonon Coupling Dynamics for Tunable Bandgap of Transition Metal Dichalcogenide Atomic Layers***, **Quinton Rice**, T Neupane, D Jayakodige, B Tabibi, F Seo,* Hampton University

The atomic layers of 2-dimensional transition metal dichalcogenides (TMDCs, MX_2; M=Mo or W; X=S, Se, or Te) are of great interest in the areas of optoelectronic and photonic applications due to the bandgap conversion from direct for monolayer and indirect for bilayer or multilayer; unique properties of valley orbital, spin, and optical helicity; and compositional tuning of exciton bandgaps in visible and near-infrared region. In this work, the average acoustic phonon energy involved in the electron-phonon interaction as well the coupling strength between electrons and phonons is analyzed using the O’Donnell and Chen relation for the temperature-dependent bandgap of TMDCs. The analysis shows that as the temperature is increased the exciton band energy is decreased. When the electron-phonon coupling strength is large (small) the tunability of exciton bandgap is wide (narrow) for a constant acoustic phonon energy. Weak electron-phonon coupling (S=2) leads to a linear decrease in the bandgap energy for temperature above ~85 K but strong coupling (S=30) above ~60 K. The bandgap was changed from 2 eV to 0.5 eV for both weakly and strongly coupled electrons, however, for a constant electron-phonon coupling strength, large (small) acoustic phonon energy results in narrow (wide) tunability of the bandgap. The ability to control the exciton bandgap through the electron-phonon interaction and average acoustic phonon energy at various temperatures leads to tunable optoelectronic and photonic devices based on 2-dimensional TMDCs. Acknowledgement: This work at HU is supported by ARO W911NF-15-1-0535, NSF HRD-1137747, and NASA NNX15AQ03A.

5:25pm **PCSI-WeA-42 Nonlinear Absorption Characteristics of Monolayer and Bilayer/Multilayer of TMDC***, **Tikaram Neupane**, Q Rice, D Jayakodige, B Tabibi, F Seo,* Hampton University

The nonlinear absorption properties of TMDC depends on the changes of band gap where monolayer of TMDC has a direct bandgap and the bilayer and multilayer have an indirect band gap. The bandgap of the monolayer is wider than that of bilayer and multilayer. This absorption process is described by Jablonski diagrams which may include two-step absorption with one-photon for each step, two-photon absorption to the real final state through a virtual intermediate state. In the one-photon excitation, the electric dipole transition |i> to |f> is allowed due to other parities between two states. Hence the saturable (negative) absorption (SA) is observed due to the higher ground-state absorption cross-section than the excited-state absorption cross-section, $\sigma_g > \sigma_e$. But in the two-photon excitation, the electric dipole transitions |i> to |n| and |n> to |f> are allowed due to same parities between the initial and final states via intermediate virtual state. Therefore, the reverse saturable (positive) absorption (RSA) is dominant due to the higher value of the excited-state absorption cross-section than the ground-state absorption cross-section. The band gap changes due to the number of layers and temperature switches RSA to SA or vice versa. The atomic layers with SA are utilized for laser Q-switch and mode-locker, while the atomic layers with RSA are utilized for optical power limiter. Acknowledgement: This work at HU is supported by ARO W911NF-15-1-0535, NSF HRD-1137747, and NASA NNX15AQ03A.

5:30pm **PCSI-WeA-43 Graphene Moiré Pattern Ultra-High Resolution Atomic Force Microscopy***, B Kim, **Gerald Pascual**, K Lee,* Park Systems Corporation

The ultra-high resolution of AFM was demonstrated in a Graphene/hexagonal Boron Nitride (hBN) sample evaluation conducted by AFM. The sample consisted of hBN substrate overlaid with a Graphene layer and was scanned under ambient air. The purpose of the evaluation was to assess the AFM ability to characterize the topography of the moiré pattern that was created when one layer was set on top of the other and offset by rotation. Using non-contact AFM mode and a standard AFM probe tip, the AFM was able to successfully image the moiré pattern super lattice constant of the sample in scans as large as 500 x 500 nm (Figure (a)). In the higher magnification image of Figure (b) taken at a scan size of 60 x 60 nm provides the clear evidence that not only are the super lattice constants of the moiré pattern about 15 nm [1] in width, but that the spacing between each striation on the moiré pattern is roughly 4-5 nm in length. Observations of such striations in Graphene/hBN systems have been previously reported [2]. This latter distance is in line with the expected tip radius curvature values for the AFM tip used to acquire all four sets of data.

5:35pm **PCSI-WeA-44 Nucleation of Cu_2Te Layer by a Closed Space Sublimation Method Toward the Growth of Te Based Chalcopyrite***, **Youhei Sakurakawa**, A Uruno, M Kobayashi,* Waseda University, Japan

The two-step closed space sublimation (CSS) growth of high quality $AgGaTe_2$ layer was successfully achieved by the formation of the Ag_2Te layer as a first step. This $AgGaTe_2$ layer was successfully applied to the solar cells. $CuGaTe_2$ has been focused on because of the lower material cost than $AgGaTe_2$. Based on the success of $AgGaTe_2/Ag_2Te$, $CuGaTe_2/Cu_2Te$ was proposed and the growth of Cu_2Te by the CSS method was attempted in this study. It has been confirmed that the surface morphology was widely varied depending on the growth parameter in case of the Ag_2Te layer growth. The realization of the membrane-filter structure for the Ag_2Te layer was the key for the formation of high quality $AgGaTe_2$ layer. In this study, Cu_2Te layer was formed on various substrate materials and surface orientations using various source materials. Judging from the phase diagram of Cu-Te, Cu-Te compounds would exhibit various structures depending on the temperature and the mole ratio, hence the surface structure of the layer could be drastically controlled. The substrate surface chemistry (dangling bond density, polarity, and so on) would also affect the formation process of Cu-Te compounds.

Cu_2Te layers were grown using 3N Cu_2Te powder or 3N CuTe powder. The substrate temperature during the layer growth was varied from 590 °C to 700 °C. The substrates used were Si(001), Si(111) and Al_2O_3(0001). The surface structure of the obtained layer was characterized using scanning electron microscope (SEM) . The crystallographic property of the layer was mainly analyzed by the ϑ-2ϑ profile of the x-ray diffraction.

Figure 1 shows the SEM image of the layer grown on Si (001) at 590 °C. Plateaus and cells surrounding them were observed. This surface structure was probably associated with the peritectoid reaction of Cu and Te [3]. The size of plateau and their spacing were sub-micrometer scale, and such structures would be useful for fabricating various nano-structures. The size and the shape of the plateau revealed to be affected by the substrate temperature and the surface orientation of the substrate. The nucleation of the $CuGaTe_2$ layer on this surface structure would be also reported.

5:40pm **PCSI-WeA-45 Gallium Nanoparticles Based Heterostructures for Full Color Thermally Stable Plasmonic and Photonic Platforms***, **Maria Losurdo**,* Cnr-Nanotec, Institute of Nanotechnology, Italy*; A Suvorova,* The University of Western Australia*; K Hingerl,* Johannes Kepler University Linz*; J Humlicek,* Masaryk University, CEITEC, Brno,*; A Brown,* Duke University

Gallium, Ga, a group-III metal, is of fundamental interest due to its polymorphism, unusual phase transition behaviors and optical properties. In recent years, substrate-supported Ga nanoparticle ensembles have been shown to be efficacious for plasmonics applications in the full NIR-VIS-UV spectral range [1]. Although bulk Ga is liquid under ambient conditions, new solid phases have been observed when Ga is confined at the nanoscale. Herein, we discuss structural, thermal and optical properties of Ga nanoparticles (Ga NPs) creating heterostructures with silicon, silicon carbide, graphene, and sapphire. We show that at the nanoscale the support plays a fundamental role in determining Ga nanoparticle phases. Specifically, we demonstrate the stable coexistence in sapphire/Ga NPs and SiC/Ga NPs of the Ga solid g-phase core and a liquid shell. The driving forces for the nucleation of the g- phase are a combination of surface energies, the Laplace pressure in the nanoparticles and its epitaxial relationship to the substrate. Amorphous, deformable substrates, like glass and graphene as well as chemically reactive substrates, such as Si, inhibit solid phase nucleation. Sapphire and SiC, which are rigid and non-reactive with Ga, creates a semi-coherent lattice nucleating a g-phase solid core when the nanoparticles are above 50 nm. The solid-liquid phase coexistence is stable from 180K to 800K [2]. We present extensive correlations between structural, using HRTEM and TERS, and optical characterisations using ellipsometry and magneto-spectroscopy, from the infrared to visible and ultraviolet range, to describe phenomena arising from coupling wavelength-resolved light into the various heterostructures. Therefore, impacts of the stable solid-liquid phase coexistence and of superheating and supercooling in core-shell NPs on plasmonics are discussed.

The study is extended also to a variety of Ga-based bimetallic nanoparticles to provide a general framework for understanding how nanoscale confinement, metals interfacial and surface energies, and crystalline relationships to the support (graphene, semiconductor, or insulator) enable and stabilize the coexistence of unexpected phases providing criteria for choosing heterostructure type to control nanoparticle optical behavior and interfacial charge transfer.

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$^+$ Author for correspondence: maria.losurdo@cnr.it

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Thursday Morning, January 19, 2017

PCSI

Room Ballroom South - Session PCSI-ThM

Grande Finale

Moderator: Chris Palmstrom, University of California, Santa Barbara

8:30am **PCSI-ThM-1 Spin-Dependent Processes in Organic Solar Cells: Recombination at Bulk Heterojunctions***, **Martin Brandt**,* Walter Schottky Institut, Technische Universität München, Germany*; A Kupijai,* Walter Schottky Institute/Technische Universität München, Germany*; K Behringer, F Schaeble, N Galfe, M Stutzmann,* Walter Schottky Institut, Technische Universität München, Germany **INVITED**

Spin selection rules govern electronic transport and can therefore be used to identify important transport processes. Electrically detected magnetic resonancd provides an extensive toolbox for this purpose with its recently developed techniques based, e.g., on spin locking and electron double resonance. It is partucularly informative when spin pairs are studied, where the constituents can be easily distinguished spectroscopically.

In this talk, studies of the domnant spin-dependent processes in organic solar cells are summarized using bulk heterojunctions of PCBM and P3HT or PCDTBT. At low temperatures, we identify the recombination of bipolar polaron pairs as the dominant processes and determine the time constants characteristic for this recombination. With increasing temperatures, the negative PCBM polaron becomes invisible. At room temperature, we find the spin-dependent transport in P3HT/PCBM to be governed by a recombination process involving two spin species in P3HT, the positive polaron and a hitherto unreported, possibly defect-related state. We introduce electrically detected magnetic resonance as a method, briefly review its range of applications and discuss the results obtained on our organic devices as a function of temperature and bias voltage.

9:00am **PCSI-ThM-7 Exciton Spin Dynamics in Hybrid Organic-inorganic Perovskites***, P Odenthal, W Talmadge, N Gundlach, R Wang, C Zhang, D Sun,* University of Utah*; Z Yu,* Washington State University*; Z Vardeny, **Yan Li**,* University of Utah **INVITED**

The hybrid organic-inorganic perovskites have emerged as a new class of semiconductors which make excellent solar cells with an efficiency over 20%. They are also highly promising semiconductors for the field of spintronics due to their large and tunable spin-orbit coupling, spin dependent optical selection rules, and predicted electrically tunable Rashba spin splitting. I will present our latest study of exciton spin dynamics on the solution processed polycrystalline $CH_3NH_3PbCl_xI_{3-x}$. With time-resolved Faraday rotation (TRFR) and optical Hanle measurements, we demonstrate the optical orientation and quantum beating of excitons in the perovskites, which confirms the spin-dependent optical transitions. The energy dependence of the Faraday rotation follows the exciton absorption band at low temperatures, confirming its excitonic origin. The TRFR in zero field reveals unexpected long spin lifetimes exceeding 1 ns at 4K, given that Pb and I exhibit large spin-orbit coupling, and usually lead to fast spin relaxation. Application of a transverse magnetic field causes quantum beating at two distinct frequencies, and the approximate linear relationships give two g-factors, which we tentatively assign to electrons and holes as $g_e = 2.63$, and $g_h = -0.33$. Temperature dependence and power dependence of the spin lifetimes reveal some clues to the spin relaxation mechanisms.

9:30am **PCSI-ThM-13 Group IV-SiGeSn Core/Shell Nanowires***, **Simone Assali**, A Attiaoui, O Moutanabbir,* École Polytechnique de Montréal, Canada **INVITED**

Sn-containing Si and Ge alloys in an emerging family of semiconductors with the potential to impact group IV materials-based devices. Indeed, the ability to independently engineer both lattice parameter and band gap holds premise to develop enhanced or novel photonic and electronic devices. The ability to incorporate Sn atoms into silicon and germanium at concentrations about one order of magnitude higher than the equilibrium solubility is at the core of these emerging class of semiconductors. Combining the unique properties of SiGeSn with the flexibility in design and fabrication offered by nanowires creates a wealth of opportunities to implement innovative devices. With this perspective, in this presentation we will address the epitaxial growth and stability of these metastable semiconductors with focus on core-shell nanowires. We will discuss their optical and electronic properties based on theoretical and experimental investigation. Strategies to integrate these nanowires in fabrication of optoelectronic devices will also be presented.

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