PCSI
Room Keauhou II - Session PCSI-SuA
2D Surfaces I

Moderator: Emanuel Tutuc, University of Texas at Austin

3:45pm **PCSI-SuA-1 Generating Valley Current and Magnetoelectricity in MoS$_2$***, Jieun Lee,* Ajou University, Korea **INVITED**

Atomically thin crystals, such as monolayer transition metal dichalcogenides (TMDs), provide a new platform to investigate the electrons in low dimensional solid state systems. In these materials, two inequivalent energy band extrema occur at the edges of the Brillouin zone, known as valleys, which serve as a binary degree of freedom of electrons similar like spins [1]. The unique control of valley pseudospins by optical and electrical means are not only fundamentally interesting, but may also find applications in valley-based electronics and optoelectronics [2,3].

In this talk, we discuss methods to manipulate the valley polarization in 2D TMD materials. First, we describe the observation of the valley Hall effect in monolayer molybdenum disulfide (MoS$_2$), in which the valley current is generated transverse to the charge current. We use optical techniques to directly image the valley polarization accumulated at the edges of MoS$_2$ channel with spatial resolution [4]. We will also discuss the possibility to tune the valley Hall conductivity by controlling the crystal's inversion symmetry in bilayer. Second, we apply strain to monolayer MoS$_2$ to break the crystal's 3-fold rotational symmetry which leads to the generation of valley magnetoelectricity [5]. The observed valley magnetization switches the sign when the in-plane bias direction flips and the magnitude scales with the amount of channel current. We discuss the dependence of the observed magnetization on bias, gate, strain direction, and external magnetic fields.

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4:15pm **PCSI-SuA-7 Diffusion of Silver and Nickel into Few-Layer MoS$_2$ and Its Effect on Contact Resistance***, **Timothy Walter**, A Domask, M Abraham,* The Pennsylvania State University*; B Kabius,* Materials Research Institute*; K Cooley, S Mohney,* The Pennsylvania State University

MoS$_2$ is attractive for a variety of nanoelectronic devices due to its ability to maintain desirable semiconducting properties at the single layer limit [1]. Understanding the behavior of metal/MoS$_2$ interfaces is important for developing low-resistance contacts for scaled transistors and other emerging applications of MoS$_2$. Our recently published work on Ag/MoS$_2$ contacts shows that after annealing in Ar at 250 and 300 °C, the contact resistance R_C is reduced from 0.8–3.5 kΩ·μm to 0.2–0.7 kΩ·μm, likely due to the incorporation of Ag donors between layers of MoS$_2$ [2]. This result is very good relative to the state-of-the-art. More recently, we have verified using transmission electron microscopy and electron energy loss spectroscopy that Ag diffuses into MoS$_2$ at low levels.

Now we have discovered that Ni also diffuses into MoS$_2$ — without altering its structure — after annealing in Ar at a temperature as low as 200 °C. Therefore, we fabricated Ni-based contacts to MoS$_2$ and characterized them before and after annealing. However, annealing caused an increase in R_C in every Ni-contacted device. As deposited, R_C varied from 2.5–8.0 kΩ·μm, but it increased by 50% after annealing at 200 °C, and increased by 650% after annealing at 300 °C. While Ag acts as a donor when intercalated in MoS$_2$ [3], Ni might not. Our further efforts towards understanding the effects of diffusion of Ag, Ni, and possibly other transition metals into MoS$_2$ may ultimately guide us in achieving even lower contact resistances.

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[2] M. Abraham and S. E. Mohney, J. Appl. Phys. **122**, 115306 (2017).

[3] D. M. Guzman *et al*., J. Appl. Phys. **121**, 055703(2017).

4:20pm **PCSI-SuA-8 Ultra-thin van der Waals Heterostructure: How Thin can a Diode be?***, **Mahfujur Rahaman**, A Mukharjee,* Chemnitz University of Technology, Germany*; S Gemming,* Institute for Ion beam Physics and Materials Research, Germany*; D Zahn,* Chemnitz University of Technology, Germany

With the advent of atomically thin van der Waals materials, it is now possible to combine p and n doped 2D semiconductors to realize p-n junctions at their ultimate thickness. [1-3] Due to the lack of a depletion width in atomically thin van der Waals materials, however they are conceptually different compared to conventional diode. [4]Here, we demonstrated strong rectification behaviour for a p-n junction made of bilayer n-type MoS$_2$ and ultrathin (10 nm) p-type GaSe with a rectification ratio of 10^4. The threshold voltage is determined to be 0.57 V. The I – V characteristics under illumination using below band gap excitation reveals a marked photovoltaic effect suggesting efficient exciton dissociation due to the presence of an electric field at the interface. The below band gap excitation also suggests the presence of accessible states in the forbidden gap of MoS$_2$. To validate our experimental observations we also performed DFT calculations on such heterostructure. Our theoretical findings indicate that the electronic band structure of bilayer MoS$_2$ is modified by the interaction with GaSe. This interaction creates accessible states in the forbidden gap of MoS$_2$ and may explain the below band gap excitation and the rectification behaviour of the p-n junction.

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3. Ross, J. S.; Klement, P.; Jones, A. M.; Ghimire, N. J.; Yan, J.; Mandrus, D. G.; Taniguchi, T.; Watanabe, K.; Kitamura, K.; Yao, W.; Cobden, D. H.; Xu, X.; *Nat Nano* **2014,***9* (4), 268-272.

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4:25pm **PCSI-SuA-9 Surface Modification of SiC by Plasma Oxidation to Form Graphene/SiC Structure with Low Pit Density***, **Kenta Arima**, R Ito, O Minami, K Hosoo, Y Sano, K Kawai,* Osaka University, Japan

The sublimation of Si atoms from a SiC surface by annealing in UHV is a familiar method for the epitaxial growth of graphene. However, a problem is the pitted morphology of the graphene/SiC(0001) structure after simple annealing above 1100°C in UHV. It is well known that, prior to graphene growth above 1100°C, a buffer layer is formed at around 1000°C. The pitted morphology is probably caused by the insufficient amount of liberated carbon atoms on the SiC surface to form a uniform buffer layer because the rapid sublimation of Si atoms occurs on an area not covered by a buffer layer, causing the formation of pits. Thus, the control of the carbon concentration at the monolayer level on an initial SiC surface is important.

We have found a new chemical route to achieve this, which is the plasma oxidation of a SiC surface near room temperature followed by HF etching. This is referred to as the plasma-assisted process hereafter. We took the change in O1s XPS spectra caused by the plasma-assisted process. It indicated that the initial untreated SiC surface is terminated by OH species, which are the origin of the hydrophilic property of the surface. In contrast, after the plasma-assisted process, a shoulder peak corresponding to C-O bonds appeared in the O1s spectrum. Taken together with the C1s spectrum, we consider that a mixture of C-C and C-O bonds exists, which agrees with the slightly hydrophobic property of the treated SiC surface. We speculate that carbon species composed of C-C and C-O bonds accumulated at the SiO$_2$/SiC interface during plasma oxidation near room temperature. When the SiO$_2$ layer was stripped off by subsequent HF etching, additional carbon species with a thickness of 1-2 monolayers appeared on the SiC surface. When this surface was annealed at 1100°C for 30 min in UHV, a graphene/SiC structure with a low pit density was obtained, which is completely different from the structure on the untreated SiC surface. This is probably because the additional carbon species produced by the plasma-assisted process contribute to the formation of a uniform buffer layer, which suppresses random Si sublimation at elevated temperatures of above 1000°C.

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PCSI
Room Keauhou II - Session PCSI-SuE
Coherent Effects in 0D Systems

Moderator: Erik Bakkers, Eindhoven University of Technology

7:30pm **PCSI-SuE-1 Rational Design of Coordination Complexes for Quantum Information***, **Danna Freedman**,* Northwestern University**INVITED**

Careful synthetic design of molecules and coordination materials enables the construction of systems with precise control over electronic spin location and nuclear spin distance. Harnessing the tools of synthetic chemistry we can address simple questions such as the relationship between electronic spin coherence time and nuclear spin proximity. We can progress from asking those questions to constructing materials where candidate qubits or quantum sensors are precisely positioned with atomic level reproducibility. Conferring a high level of precision to the location and orientation of quantum objects is a vital prerequisite for the design of quantum sensors and quantum information processing systems. This talk will focus on fundamental questions that can be addressed by coordination chemistry.

8:00pm **PCSI-SuE-7 Detecting Low-Intensity Light at the Interface of Chromophores and Diamond***, **Nicholas Harmon**, M Flatté,* University of Iowa

Long spin coherence times of nitrogen vacancy (NV) center spins in diamond under ambient conditions have made these systems attractive candidates for quantum information processing. Substantial progress has been accomplished in using NV centers as nanoscale magnetometers. Aside from zero-field splitting, the spin-orbit interaction in conjunction with an electric field also induces spin splitting of the m_s = ±1 states. The dependence of the NV ground state on electric field suggests these centers are also useful as electric field sensors.

We develop a theory in which the optical output of an NV center is used to determine the presence of an electric field. Beyond this utility, we also present a nanoscale model of few photon detection accomplished when a chromophore lies at the interface of a NV center in diamond. Photons incident upon the chromophore induce a conformational change which includes a sizable charge polarization and electric dipole moment (>10 D). Using the formalism of positive operator values measurements (POVMs), we predict the existence of the photo-excited electric dipole field and, by extension, the incident photon given a measured readout state (photoemission) from the NV center. We find that an applied magnetic field plays a non-trivial role that can reduce the error rate. We describe a scheme by which the time of the incident photon can be resolved. Finally we investigate the role of multiple, coupled NV centers interfaced with multiple chromophores in offering spatial resolution to the detection.

8:15pm **PCSI-SuE-10 A New Approach to Magnetic Resonance at Heterointerfaces: Spin Dependent Charge Pumping in 4H-SiC MOSFETs***, **Patrick Lenahan**, M Anders,* The Pennsylvania State University*; A Lelis,* U.S. Army Research Laboratory **INVITED**

Although 4H SiC MOSFETs have great promise in high power and high temperature applications, their great promise is limited by the presence of a defective silicon carbide- silicon dioxide interface region. We have utilized a new electron paramagnetic resonance (EPR) approach to explore the defect structure at these SiC- oxide interfaces in fully processed transistors: multi-field and RF frequency spin dependent charge pumping.

Conventional electron paramagnetic resonance (EPR) offers unrivalled analytical power for the identification of point defects in semiconductors and insulators. Unfortunately, the sensitivity of conventional EPR measurements is, at best, about ten billion total defects. This sensitivity is inadequate for measurements in most devices of technological significance. A second limitation of conventional EPR in device physics studies is that it is sensitive to all paramagnetic defects within structure under study. EPR detection via electrically detected magnetic resonance (EDMR) can overcome both of these limitations. It provides a sensitivity typically at least ten million times higher than that of conventional EPR and is also exclusively sensitive to defect centers which impact the electronic behavior of the devices.

EDMR studies nearly always utilize spin dependent recombination (SDR). SDR is quite sensitive to deep level defects but, in studies of heterointerfaces such as the SiC/SiO_2 boundary, defects throughout the entire interface bandgap can be important. In this study, we utilize a new EDMR approach to investigate the silicon carbide silicon dioxide interface: multi-magnetic field and RF frequency spin dependent charge pumping (SDCP).

SDCP allows quite sensitive EDMR measurements of interface defects with levels throughout nearly the entire interface bandgap. The SDCP sensitivity is very nearly magnetic field and frequency independent and is typically more sensitive than SDR. The enhanced sensitivity as well as the field and frequency independence allows us to make measurements at resonance frequencies as high as 16 GHz and as low as 85 MHz. The multi-field and frequency measurements yield information about the relative contributions of hyperfine and spin orbit interactions and thereby aid in defect identification. In this presentation I will briefly review the physics involved in SDCP and discuss the defects which we observe via SDCP. In addition, I will briefly outline the close connection between the low frequency SDCP and a near zero field non- resonant response in the charge pumping currents. The near zero field response may one day provide a remarkably simple tool for the study of interface defect structure.

PCSI

Room Keauhou II - Session PCSI-MoM

New 2D Materials/Magnetic Interfaces/Organics/New Techniques I

Moderators: James Chelikowsky, University of Texas, Austin, Scott Crooker, Los Alamos National Laboratory, Georg Schmidt, Martin-Luther-Universität Halle-Wittenberg, Shigeki Kawai, University of Basel

8:30am **PCSI-MoM-1 First-Principles Assisted Design of Molecular Scale Graphane Analogues***, **Wolfgang Windl**, O Restrepo, K Krymowski, L Brillson, J Goldberger,* The Ohio State University **INVITED**

Graphene's success has shown that it is not only possible to create stable, single-atom thick sheets of a crystalline material, but that these materials can have electronic properties that are fundamentally different than the parent. Recent work at The Ohio State University has shown that unique single-layer 2D materials based on group-IV elements and especially germanium can be synthesized, stabilized by appropriate ligands [1]. In this talk, we will discuss density-functional theory predictions of structure, properties, defects and transport in such graphane analogues, as well as their experimental realization and validation. Examples discussed include electronic and conduction properties [2] and their strain- [3] and ligand-tunability (Fig. 1) [4,5], as well as point defects and oxidation mechanisms and their experimental observation. Figure 1 Band structure of silicane with H (left) and CH3 (right) ligands, calculated with HSE06 hybrid potentials [5].

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9:00am **PCSI-MoM-7 Graphene-like Nanoribbons Periodically Embedded with Four- and Eight-membered Rings***, **Meizhuang Liu**, D Zhong,* Sun Yat-Sen University, China

Graphene nanoribbons, defined as nanometer-wide strips of graphene, have attracted extensive attention as promising building blocks for nanoelectronics and spintronics. The electronic properties of nanoribbons can be modulated at nanoscale by controlling the edge structure and width [1], chemical doping [2] and formation of heterojunctions. Embedding non-hexagonal rings is considered a promising strategy to tailor the electronic properties of carbon-based nanomaterials. However, non-hexagonal rings are energetically unstable compared to the hexagonal counterparts, making it challenging to embed non-hexagonal rings in a controllable manner. Here, we report an on-surface synthesis of graphene-like nanoribbons with periodically embedded four- and eight-membered rings. The scanning tunnelling microscopy and atomic force microscopy study revealed that four- and eight-membered rings are formed between adjacent perylene backbones with a planar configuration. The nonhexagonal rings as a topological modification markedly change the electronic properties of the nanoribbons. The highest occupied and lowest unoccupied ribbon states are mainly distributed around the eight- and four-membered rings, respectively. The realization of graphene-like nanoribbons comprising non-hexagonal rings demonstrates a controllable route to fabricate non-hexagonal rings in nanoribbons and makes it possible to unveil their unique properties induced by non-hexagonal rings.

9:05am **PCSI-MoM-8 Hexagonal Boron Nitride on Single-Crystal Epitaxial Graphene and SiC(0001) Substrates by Plasma-Enhanced CBE Deposition***, **Daniel Pennachio**, N Wilson, E Young, T Brown-Heft,* University of California, Santa Barbara*; K Daniels, R Myers-Ward, D Gaskill, C Eddy, Jr.,* U.S. Naval Research Laboratory*; C Palmstrøm, A McFadden,* University of California, Santa Barbara

A unique high temperature, plasma assisted chemical beam epitaxial (CBE) deposition of hexagonal boron nitride (h-BN) is explored as a versatile method to grow thin films on large-area single crystal substrates in an effort to produce wafer-scale, epitaxial h-BN. Epitaxial graphene on SiC(0001) and reconstructed SiC(0001) surfaces are examined as candidate substrates for this growth method as single-crystal alternatives to transition metal foils typically used as h-BN substrates. Borazine dosing with the addition of RF nitrogen plasma exposure and substrate temperatures up to 1450°C, achieved with a custom modified manipulator,produced films with with increased crystallinity and reduced polyaminoborane particulates on epitaxial graphene substrates. Samples were transferred *in-vacua* for X-ray photoelectron spectroscopy (XPS) to examine stoichiometry and chemical environment of the sub-to-few monolayer BN films. Films grown with nitrogen plasma exhibited 10% higher nitrogen incorporation relative to those without plasma, showing active nitrogen is beneficial in maintaining stoichiometry at these growth temperatures in ultra-high vacuum. Use of plasma aids single-phase growth as indicated by the absence of shoulder peaks in B 1s and N 1s XPS spectra (Fig. 1). Crystallinity and orientation of nuclei was examined by *in-vacuo* and *in-situ* scanning probe microscopy.

Growth of single-phase, stoichiometric h-BN was also achieved on SiC(0001) substrates, *In-situ* reflection high-energy electron diffraction during h-BN deposition shows nucleation differs between the Si-rich (3x3) and the C-rich (6√3×6√3)*R*30° SiC surface reconstructions: the (3x3) reconstruction quickly transitioned to a (1x1) reconstruction upon precursor dosing, but the C-rich reconstruction persists. Instead of triangular nuclei seen on graphene surfaces, h-BN growth on reconstructed SiC surfaces followed the stepped morphology of the SiC surface.

9:10am **PCSI-MoM-9 Data Mining for More Than a Thousand Layered Materials, Hundreds of One-dimensional Materials and Lattice-commensurate Heterostructures***, **Gowoon Cheon**, K Duerloo, A Sendek, C Porter, Y Chen, E Reed,* Stanford University

Layered materials held together by weak interactions including van der Waals forces, such as graphite, have attracted interest for both technological applications and fundamental physics in their layered form and as an isolated single-layer. Only a few dozen single-layer van der Waals solids have been subject to considerable research focus, although there are likely to be many more and which could have superior properties. To identify a broad spectrum of layered materials, we present a novel data mining algorithm that determines the dimensionality of weakly bonded subcomponents based on the atomic positions of bulk, 3D crystal structures. By applying this algorithm to the Materials Project[2] database of over 50,000 inorganic crystals, we identify 1173 two-dimensional layered materials and 487 materials that consist of weakly bonded one-dimensional molecular chains. This is an order of magnitude increase in the number of identified materials, with most materials not known as two- or one-dimensional materials. Moreover, we discover 98 weakly bonded heterostructures of two-dimensional and one-dimensional subcomponents that are found within bulk materials, opening new possibilities for much-studied assembly of van der Waals heterostructures. [1]

Chemical families of materials, band gaps and point groups for the materials identified in this work are presented. Point group and piezoelectricity in layered materials are also evaluated in single-layer forms. 325 of these materials are expected to have piezoelectric monolayers with a variety of forms of the piezoelectric tensor. This work significantly extends the scope of potential low-dimensional weakly bonded solids to be investigated.

9:15am **PCSI-MoM-10 Thermal Hall Effect and Topological Edge Modes of Magnons***, **Shuichi Murakami**, A Okamoto,* Tokyo Institute of Technology, Japan **INVITED**

In electronic systems, various interesting phenomena such as spin Hall effect and topological insulators originate from Berry curvature of Bloch wavefunctions. We theoretically study analogous phenomena for magnons (spin waves). We propose that the dipolar interaction gives rise to nonzero Berry curvature [1-5]. In a thin-film ferromagnet, the Berry curvature is nonzero only when the magnetic field is out-of-plane. This Berry curvature gives rise to thermal Hall effect of magnons, and to a shift of wavepackets in reflection or refraction. Furthermore, in analogy to the quantum Hall effect for electrons, we can design topological magnon band structure. By introducing artificial spatial periodicity into the magnet, for example by fabricating nanostructures with two different magnets in a periodic structure or by making a periodic array of nanomagnets, we theoretically propose emergence of topological edge modes, analogous to those in electronic quantum Hall effect [6-7]. The edge modes are chiral, and propagate along the edge of the magnet in one way. We call this a topological magnonic crystal.

If the time allows, we also discuss our recent results on various Edelstein effects, which can be used for generating angular momenta in crystals without inversion symmetry [8, 9].

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9:45am **PCSI-MoM-16 Strong Zero-Field Topological Hall Effect in B20-FeGe Thin Film and Oxide Bilayer Skyrmion Systems***, **Fengyuan Yang**, J Gallagher, K Meng, J Brangham, H Wang, B Esser, D McComb,* The Ohio State University

Magnetic skyrmions have attracted significant interests in recent years due to their intriguing magnetic interactions and potential for magnetic storage applications. B20 phase materials enable magnetic skyrmions due to the bulk spin-orbit coupling (SOC) and non-centrosymmetric structure. One major effort in this emerging field is the stabilization of skyrmions at room temperature and zero magnetic field. We grow high quality FeGe epitaxial films of 100, 65, and 36 nm thicknesses on Si(111) by UHV off-axis sputtering [1]. The Hall resistivity hysteresis loops show three regions of distinct features: 1) a linear background at large fields (> 2 T) due to the ordinary Hall effect, 2) a magnetic reversal behavior at intermediate fields that follows the magnetization hysteresis loop due to the anomalous Hall effect, and 3) a hysteresis loop within ±3000 Oe due to the topological Hall effect (THE). The THE signals were extracted by subtracting out the anomalous and ordinary Hall effect. The THE reaches near 1,000 nOhm cm at 250 K, the highest reported to date. In particular, a large remanent topological Hall resistivity (77% of the maximum THE signal) was observed at zero magnetic field and 5 K. This substantial topological Hall effect at zero field shows a robust skyrmion phase without the need of an external magnetic field. In addition, a class of skyrmion materials has recently emerged in oxide bilayers due to strong interfacial Rashba SOC that could enable skyrmions of 10 nm. We grow $SrRuO_3/SrIrO_3$ epitaxial bilayers which exhibit high crystalline ordering and dominant topological Hall effect (see Fig. 2). Remarkably, we observe dominant THE in a single 2 nm thick $SrRuO_3$ layer, demonstrating that the skyrmions can be stabilized in single FM oxide thin films.

This work was primarily supported by the U.S. DOE under Grant No. DE-SC0001304 and in part by NSF under Grant No. DMR-1507274 and No. DMR-1420451.

10:00am **PCSI-MoM-19 Surface Termination Layer Dependence in Heusler Superlattices***, **Tobias Brown-Heft**, A McFadden, J Logan,* University of California, Santa Barbara*; C Guillemard,* University of Lorraine, France*; P Le Fevre, F Bertran,* Synchrotron SOLEIL, France*; S Andrieu,* University of Lorraine, France*; C Palmstrom,* University of California, Santa Barbara

Heusler atomic superlattices were recently predicted to combine both perpendicular magnetic anisotropy and half-metallicity in a single material [1]. Until now, these two properties have been optimized in separate material systems (e.g. CoFeB [2] and Co_2MnSi [3]). In Heusler superlattices, the magnetic anisotropy arises from strain and electronic structure at each sublayer interface, while half-metallicity arises from Fermi-level tuning via alloying effects.

Single-crystal atomic superlattices with periodicity of one to three unit cells (5.8 Å to 17.4 Å) have been successfully grown by molecular beam epitaxy. Superlattices consisting of B2 ordered full-Heusler Co_2MnAl and Fe_2MnAl were grown on GaAs (001), MgO (001), and Cr (001)/MgO (001). Films are fully strained to each substrate up to at least 20 nm film thickness. Electron energy loss spectroscopy confirmed well-defined Heusler layers as seen in Fig. 1. Superlattices grown on GaAs (001) with aluminum excess over 20% experienced an out-of-plane spin reorientation transition for temperatures below 200 K. Spin polarization at the bulk X point was measured via synchrotron-based spin resolved photoemission spectroscopy on samples grown *in-situ* in an attached MBE chamber. Surface spin polarization was found to depend strongly on surface termination. Pure Fe_2MnAl and superlattices terminated with Fe_2MnAl had 25% spin polarization. Pure Co_2MnAl had 65% spin polarization. Superlattice terminated with Co_2MnAl had the highest spin polarization of 95% (Fig. 2), with the Fermi level at the bottom of the Slater-Pauling gap, suggesting that the superlattice does provide some Fermi level tuning. Magnetic tunnel junction and magnetotransport behavior will also be discussed.

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10:05am **PCSI-MoM-20 Measurement of Band-alignments in Semiconducting Half-Heusler Heterojunctions Grown by MBE***, **Sean Harrington**, A Rice, A McFadden, D Pennachio, C Palmstrom,* University of California, Santa Barbara

Half-Heusler (h-H) compounds are an exciting class of intermetallics due to their diverse electrical and magnetic properties, including semiconducting [1], half metallic [2], thermoelectric, and topologically insulating [3]. With a crystal structure and lattice parameters similar to III-V compound semiconductors, the possibility of h-H/III-V semiconductor heterostructures with unique properties is achievable. Integration of epitaxial h-H compounds with existing III-V technologies requires a deeper understanding of their interface. Most experimental studies of h-H compounds have been limited to bulk polycrystalline samples, which cannot be used for measurements of interface properties. CoTiSb has been extensively studied in the bulk and recently in molecular beam epitaxy (MBE) grown films where record high carrier mobilities were demonstrated [4] and the valence band offsets measured with lattice matched III-Vs [5]. However, the conduction band offsets expected from density functional theory vary immensely depending on the band gap obtained. Heyd, Scuseria, Ernzerhof functionals predict a bandgap of 1.45 eV [5], while the generalized gradient approximation gives 1.0 eV [1]. Electron transport across and confined to these interfaces can give great insight into these values.

In this presentation, the heterointerfaces formed between the semiconducting h-H compound CoTiSb and the III-V compounds, InAlAs and InGaAs, are investigated through vertical transport measurements. In addition, the heterointerface formed between CoTiSb and another semiconducting h-H, NiTiSn is investigated. Lattice-matched $In_{0.52}Al_{0.48}As$ and $In_{0.53}Ga_{0.47}As$ layers were epitaxially grown on InP (001) substrates in a dedicated III-V MBE system. The epitaxial CoTiSb and NiTiSn layers were grown in a separate dedicated MBE system. A variety of heterojunctions between CoTiSb and the III-Vs were designed and grown. Heterointerfaces between CoTiSb (intrinsically n-type) and n-InGaAs, p-InGaAs, n-InAlAs, and p-InAlAs were investigated. Temperature-dependent vertical transport I-V and C-V measurements of the n-n and n-p structures were performed for etched mesas of a variety of sizes. In addition, the valence-band discontinuity and interdiffusion in an abrupt CoTiSb/NiTiSn heterojunction were determined using XPS. Vertical and in-plane transport were performed to probe the band alignment. Finally, by alloying Fe with CoTiSb, p–type CoTiSb is achievable. CoTiSb based p-n homojunctions were formed and the electrical properties measured.

10:10am **PCSI-MoM-21 Magnetoresistance, Metallic Conductivity and Magnetic Properties of Sr and Co Modified Polycrystalline $BiFeO_3$***, Z Zhang, **Azizur Rahman**,* University of Science and Technology of China, China

Sr^{2+} and Co^{3+} co-doping in an antiferromagnetic insulator $BiFeO_3$ (BFO), results the occurrence of room temperature conductivity and magnetoresistance and enhances the magnetic properties. Here we reported for a very first time the occurrence of magnetoresistance (MR%) up to 35% in polycrystalline BFO system with dopants of Sr and Co at room temperature. Bi^{3+} in A site of BFO substituted by Sr^{2+} results in the presentation of holes carrier and further changes its conductivity. The enhancement in MR% is observed with the increasing magnetic field and temperature. XPS results reveal that cobalt modification in Sr-doped BFO controls the formation of oxygen vacancies. Co substitution in Sr doped BFO also significantly enhances the magnetism, i.e. the values of saturation and remnant magnetization are 5 emu/g and 1.1 emu/g, respectively.

Figure (a) The room temperature metallic conductivity, (b) the magnetic field dependent MR% for 5% Cobalt doping in 15% Sr doped BFO and © MR% for 8% Cobalt doping in 15% Sr doped BFO at 7T .

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10:15am **PCSI-MoM-22 Interface Magnetization Transition via Minority Spin Injection at Multiferroic Oxide Interface*, Gunter Luepke,*** College of William & Mary

Electric-field control of magnetism is a key issue for future development of low-power spintronics and magnetic random access memories. In multiferroic tunnel junctions the magnetoelectric (ME) coupling enables an electric field to manipulate the interfacial magnetization through switching of the ferroelectric (FE) polarization resulting in a four-state resistance and large tunneling electroresistance effect. Here we selectively probe the interface magnetization of the n-type $BaTiO_3/La_{0.7}Sr_{0.3}MnO_3$ (BTO/LSMO) heterojunction and discover a new interface ME effect [1]. The injection of minority spins at the interface causes a sudden, reversible transition of the spin alignment of interfacial Mn ions from ferromagnetic (FM) to antiferromagnetic (AFM) exchange coupled (Fig. 1), while the bulk magnetization remains unchanged. We attribute the emergent interfacial AFM interactions to weakening of the double-exchange mechanism caused by the strong Hund's rule coupling between injected minority spins and local magnetic moments. The effect is robust and may serve as a viable route for electronic and spintronic applications.

11:30am **PCSI-MoM-37 A Single-molecule View of the Structure and Energetics at Interfaces in Dilute Heterojunction Organic Solar Cells*, Erik Mårsell,*** University of British Columbia, Canada, Uppsala University, Sweden*; B Yuan, K Cochrane, M DeJong, D Jones,* University of British Columbia, Canada*; M Riede,* University of Oxford, England*; S Burke,* University of British Columbia, Canada

Organic photovoltaics offers a path to lightweight, flexible, and low-cost solar cells, but suffers from low power conversion efficiencies. This is partly because of a tradeoff between open circuit voltage and generation efficiency of free charge carriers. The active region in an organic solar cell typically consists of a blend layer of roughly equal amounts of donor and acceptor molecules, where the interface facilitates dissociation of the strongly bound exciton into separated charges. Recently, it was shown that reducing the donor concentration in bulk heterojunction solar cells to 5–10% can improve the open circuit voltage by more than 100 mV, resulting in an improved power conversion efficiency in these systems [1]. Questions however remain about the energetics of the interface and how it correlates with light absorption and exciton dissociation in these almost single-component solar cells.

To study the heterojunction interface in detail, we use a combination of low-temperature scanning probe microscopy techniques applied to model systems of such dilute heterojunctions. The model systems consist of single impurity molecules on multilayer C60 films deposited *in situ* in an ultrahigh vacuum chamber. This gives us access to a controlled system where we can study the interface with sub-molecular spatial resolution. As model impurity molecules, we choose zinc phthalocyanine (ZnPc) functionalized with different amounts of fluorine, as these molecules are structurally similar but display different energy level alignments [2].

The physical structure of the system is measured using atomic force microscopy with a CO-functionalized tip for submolecular resolution. The electronic structure is instead measured using pixel-by-pixel scanning tunnelling spectroscopy (STS), as shown in Fig. 1. We show how the different impurity molecules affect the energy levels of the surrounding C60 molecules.

11:35am **PCSI-MoM-38 A Comparison of the Electronic Structure of Single Crystal Hybrid and Inkjet Printed Nanocrystalline Inorganic Perovskite Films*, Andrew John Yost,*** *T Komesu,* University of Nebraska-Lincoln*; C Ilie,* State University of New York- Oswego*; F Guzman,* California State University-San Bernardino*; B Swanson, I Evans,* State University of New York- Oswego*; P Costa, J Teeter, M Shekhirev, N Benker,* University of Nebraska-Lincoln*; S Sikich,* Doane College*; A Enders,* Universitat Bayreuth, Germany*; P Dowben, A Sinitskii,* University of Nebraska-Lincoln

Halide based perovskite solar cells (HPSCs) have recently drawn plenty of attention due to their low cost, extraordinary power conversion efficiency, and long carrier lifetimes and diffusion lengths. Unfortunately organic based HPSCs have a few drawbacks including being sensitive to heat, moisture, and radiation induced degradation [1]. An alternative approach is the use of inorganic based HPSC materials as a way of circumventing some of the drawbacks.

$CsPbBr_3$ quantum dot (QD) inks have been used in an inkjet printer to print photoactive-perovskite QD films. We discuss how these perovskite QDs differ from the single crystal hybrid perovskite $MAPbBr_3$ (MA= methyl-ammonium). The current-voltage I(V) and capacitance-voltage C(V) transport measurements indicate that the photocarrier drift lifetime, t, can exceed 10 msec. for the $CsPbBr_3$ quantum dot printed perovskites films, as shown in Figure 1. The single crystal hybrid perovskite $MAPbBr_3$ exhibit significant mobilities, m, leading to a significant diffusion carrier length equal to the product of mt [2], but suffer from lead segregation to the surface [3]. The successful printing of photoactive-perovskite QD films of $CsPbBr_3$, indicates that the rapid prototyping of various perovskite inks and multilayers is realizable.

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[2] D. Shi, *et al., Science* 2015, **347**, 519-522

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11:40am **PCSI-MoM-39 CREM of Photo Induced Charge Separation Mechanisms across Controlled Molecular Spacers*, Hagai Cohen,*** Weizmann Institute, Israel

Thin dielectric spacers are commonly used for the enhancement and real-time control over charge separation mechanisms in various devices. Interesting features in this matter are proposed by self-assembled molecular layers (SAMs), with which fine tuning of the spacer thickness, interfacial binding and intrinsic properties is typically available. On the other hand, the structural and composition integrity of molecular spacers frequently presents critical issues and a challenging demand for simultaneous detection of electrical and structural characteristics.

Specifically for the latter characterization challenge, a promising answer is proposed by the CREM (chemically resolved electrical measurements) technique.[1-3] Based on x-ray photoelectron spectroscopy (XPS), CREM has already demonstrated unique capabilities with which detailed understanding of charge transport processes in heterostructures could be achieved. Within a single experiment, CREM would usually provide the system's composition and its real-time modifications under external stimuli; a measure of the internal fields and band offsets; charge transport data, trapping characteristics and more; all extracted with no top contact and, frequently, at remarkably high sensitivities.

The present work focuses on the transport of hot, photoexcited, charges across organic spacers. Samples consist of molecular layers self-assembled on gold, on top of which CdSe nanoparticles are deposited. Under light illumination, electron-hole pairs are created at the CdSe particles and their transport to the gold through the mediating linker is investigated. The competing mechanisms of electron vs hole transport are found to vary in magnitude as a function of spacer thickness and conjugation degree. In addition, the emergence of defect states and their (sometimes surprising) impact on structural and electrical characteristics are revealed. Deeper insight is proposed by our theoretical study and complementary techniques. Remarkably, the entire set of SAMs can thus be put on a common ruler that governs leading factors in the transport problem.

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11:45am **PCSI-MoM-40 Synthesis and Field Effect Transistor of Covalent Organic Framework Thin Films*, Dong Wang,*** Chinese Academy of Sciences, China

2D Covalent organic frameworks (COFs), a class of porous, crystalline materials, are organic analogue of 2D inorganic materials and have drawn remarkable research interests. Layered 2D COFs feature the planar π-conjugated system and well-ordered columnar stacking arrangement, which are expected to exhibit anisotropic electrical properties. Π-Stacking columns of COFs have been demonstrated to exhibit high carrier mobility, and great potential applications in electronics. Inspired by the exceptional high mobility in graphene planes, it is of great interest to sight the intrinsic carrier mobility in π-conjugated backbone of 2D COFs. However, the further understanding of the electric property of 2D COFs faces great challenges. Firstly, the insolubility of COF powders in most of solvents makes it difficult for device or electrode fabrication. Secondly, the randomly oriented microcrystals in COF powders conceals the intrinsic charge transport behaviour. Therefore, it is of highly demand to fabricate COF films with well-defined structures. We demonstrate that it is possible to fabricate COF thin film for regular field effect transistor characterization. Both planar and vertical FET based COF thin film will be presented.

[1] B. Sun, C. H. Zhu, Y. Liu, C. Wang, L.J. Wan, D. Wang, Chem. Mater. 29, 4367 (2017).

[2] B. Sun, J. Li, W. L. Dong, M.L. Wu, D. Wang, J. Phys. Chem. C 120, 14706 (2016)

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Figure 1. Device structure and Typical transfer characteristics for the COF based OFET device

11:50am **PCSI-MoM-41 Surface Structure and Activity of Immobilized Protein G Mutants***, E Harrison, Y Wang,* ***David Castner,*** University of Washington

Controlling how proteins are immobilized is essential for optimizing the performance of *in vitro* protein-binding devices. Comprehensive analysis of surface immobilized proteins provides the level of detail about the immobilization process and the structure of the immobilized biomolecules needed to develop optimized these devices. In particular, surface analysis methods such as XPS, ToF-SIMS, SFG, NEXAFS, SPR and QCM-D, when combined with Monte Carlo (MC) and molecular dynamics (MD) computation methods provide a powerful method for obtaining information about the attachment, type, orientation, conformation and spatial distribution of surface immobilized proteins. The focus of this work was to control and characterize the orientation of Protein G B1, an immunoglobulin (IgG) antibody-binding domain of Protein G, on well-defined surfaces as well as measure the effect of Protein G B1 orientation on IgG antibody binding.

A MC algorithm was developed to predict the most likely orientations of wild type (WT) Protein G B1 onto a hydrophobic surface. The MC simulations predicted that WT Protein G B1 is adsorbed onto a hydrophobic surface in two different side-on orientations. This prediction was consistent with SFG vibrational spectroscopy results. QCM-D experiments showed that WT Protein G B1 absorbed onto polystyrene retained its IgG antibody-binding activity. Additional MD simulations provided further detail about the structure of WT Protein G B1 on hydrophobic surfaces.

To systematically vary the orientation of Protein G B1, five different cysteine mutants were immobilized onto maleimide oligo(ethylene glycol) (MEG) covered flat and nanoparticle gold surfaces. The amount of Protein G B1 immobilized along with its IgG binding activity was measured with XPS and QCM-D. The surface sensitivity of ToF-SIMS was used to distinguish between the different Protein G B1 mutant orientations by monitoring the changes in intensity of characteristic amino acid mass fragments from different locations in the Protein G B1 structure. ToF-SIMS results showed that the Protein G B1 orientation can be flipped by changing the location of the Cys from the C-termius to the N- terminus, which has implications for IgG binding since the binding site for IgG is located near the C-terminus of Protein G B1. QCM-D measurements show that when a monolayer of Protein G is immobilized with the C-terminus facing outward it can bind a monolayer of IgG. Conversely, QCM-D measurements show that when a monolayer of Protein G B1 is immobilized with the N-terminus facing outward it binds very little IgG (~x30 decrease in binding capacity).

11:55am **PCSI-MoM-42 Neutron Scattering Studies of Bio-Interfaces: From Model Systems to Living Cells***,* ***Jaroslaw Majewski,*** Los Alamos National Laboratory

The non-destructive nature of neutron scattering coupled with its isotopic sensitivity and penetrability has made it an ideal tool to study model biological interfaces at different complex environments. In this presentation I will discuss methods to create and characterize the model bio-interfaces (from lipid membranes to cell cultures) which can mimic many of the critical attributes of living systems. I will demonstrate that neutron scattering methods can be used to characterize the structure, composition, and organization of these objects and their response to external stimuli like pH, temperature and flow shear.

12:00pm **PCSI-MoM-43 Optical Pump-probe Scanning Tunneling Microscopy-Present and Future***,* ***Hidemi Shigekawa,*** University of Tsukuba, Japan **INVITED**

Since the invention of scanning tunneling microscopy (STM) in 1982. the addition of high time-resolution to STM has been one of the most challenging issues, and various time-resolved STMs have been considered [1, 2]. The most successful approach among them is to combine STM with electric and optical pump-probe techniques [2-4]. In the optical pump-probe STM (OPP-STM) which we have been developing [3], the sample surface below STM tip is excited by a train of pulse pairs, similarly to the case of the original OPP method, however, instead of measuring, for example, the change in the reflectivity of probe pulses, tunneling current is measured as a function of delay time. There are two ways to probe dynamics. One is the use of absorption bleaching mechanism like the original OPP method. When tunneling current induced by the probe pulse depends on the delay time due to absorption bleaching, the change in the total tunneling current measured by OPP-STM provides the information on the carrier dynamics. With the use of circularly polarized light for excitation and probing, spin dynamics can be detected [5,6]. When tunnel current depends on the change in the material conductivity, like photo-stimulated phase transition, its dynamics also can be probed. A new technique is to use THz pulses. Although it is difficult to apply a high bias voltage between the STM tip and sample in general, the tip-enhanced electric field obtained by ultrashort THz pulse enables it, and taking a snapshot of ultrafast dynamics becomes possible [7-9]. Control of the carrier envelope phases in pump and probe pulses paves the way for the development of new time-resolved analyses. Details will be discussed at the conference with recent results and the prospects for future researches.

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12:30pm **PCSI-MoM-49 New Visualization Method by Two-dimensional Imaging of Transmitted Hydrogen on Stainless Steel***,* ***Naoya Miyauchi,*** National Institute for Materials Science, Japan*; T Iwasawa,* Toho University, Japan*; Y Murase,* National Institute for Materials Science, Japan*; S Takagi,* Toho University, Japan*; A Itakura,* National Institute for Materials Science, Japan

The behavior of hydrogen in metals should be made clear to understand the mechanisms of hydrogen embrittlement and storage. To understand these phenomena, various hydrogen diffusion models have been proposed. We have observed the behavior of hydrogen in metals by visualizing sequentially spatial distributions of permeated hydrogen on the surface of stainless steel membrane.

The distributions of surface hydrogen were obtained using ions emitted by the method of desorption induced by electronic transitions (DIET) process with the scanning electron microscope (SEM)[1]. The experimental setup is shown in Fig. 1. The two-dimensional pulse counting system is synchronized with the scanning electron beam. The sample is SUS304 stainless steel, which has austenite structure with martensite dislocations caused by cold working. The diameters of austenite grains are about 100 µm. The thickness of membrane is 200 µm. The back side of SUS membrane was exposed to hydrogen (2.5×10^5 Pa) and the permeated hydrogen on the opposite observation side was observed by DIET method.

Fig. 2(a) and (b) are the secondary electron image and the permeated hydrogen map which is obtained by accumulating DIET ions at 473 K, respectively. A comparison of two kinds of image suggested that the hydrogen permeation depends on the grain structure.

There is also a difference in the distribution of hydrogen in one grain, which is a difference in crystal orientation.

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12:35pm **PCSI-MoM-50 Environmental Charge Compensation - Near Ambient Pressure XPS as a Tool for Surface Chemical Analysis of Insulators without Charging Effects***, **Thomas Schulmeyer**, S Bahr,* SPECS TII Inc.

For many decades XPS (or ESCA) has been the well-accepted standard method for non-destructive chemical analysis of solid surfaces. To fulfill this task existing ESCA tools combine reliable quantitative chemical analysis with comfortable sample handling concepts, integrated into fully automated compact designs. Generically insulators will positively charge in XPS due to the irradiation with X-rays and the emission of photoelectrons. Without compensation this effect leads to strong continuous shifts and asymmetric line shapes of the emission lines in the spectra. To perform an exact characterization and quantification of strongly insulating materials different concepts of charge compensation or neutralization have been developed over the last decades. A short overview is given starting from low energy electrons offered from so-called "flood guns" or other sources, via compensation by a combination of electrons and ions to rare methods like illumination with visible light during the analysis and compensation by the produced electron-hole pairs. The opportunities and challenges of the different methods are compared. The development of XPS method towards environmental or (near) ambient pressure working conditions has revolutionized this method regarding applications. In-situ and in-operando measurements in pressure of up to and above 25mbar are easily possible, even with laboratory based systems and using EnviroESCA even in a standard analytical tool. During the last months, measurements on insulators have shown, that they can be measured with exception in surrounding pressures of a couple of mbar without any charging. This new technique of charge neutralization is neamed Environmental Charge Compensation (ECC). This presentation summarizes results of measurements on insulating polymer samples, showing the resulting spectroscopic resolution for C1s and O1s emission lines. A comparison for PET and PTFE to other neutralization techniques is given. In addition measurements on bulk insulators from polymeric materials, ceramics, food samples, aqueous solutions, stones, soil and even zeolites are shown, that cannot easily be obtained in UHV based XPS systems. Furthermore the effect is described in detail, including the influence of pressure and gas composition on the charge neutralization. An outlook is presented towards completely new resulting fields of application of XPS, when combined with ECC.

12:40pm **PCSI-MoM-51 Opto-Valleytronic Spin Injection in Monolayer MoS_2/Few-Layer Graphene Hybrid Spin Valves***, **Yunqiu (Kelly) Luo**, J Xu, T Zhu, G Wu, E McCormick, W Zhan,* The Ohio State University*; M Neupane,* U.S. Army Research Laboratory*; R Kawakami,* The Ohio State University

Two dimensional (2D) materials provide a unique platform for spintronics and valleytronics due to the ability to combine vastly different functionalities into one vertically-stacked heterostructure, where the strengths of each of the constituent materials can compensate for the weaknesses of the others. Graphene has been demonstrated to be an exceptional material for spin transport at room temperature, however it lacks a coupling of the spin and optical degrees of freedom [1]. In contrast, spin/valley polarization can be efficiently generated in monolayer transition metal dichalcogenides (TMD) such as MoS_2 via absorption of circularly-polarized photons, but lateral spin or valley transport has not been realized at room temperature [2]. In this talk, we fabricate monolayer MoS_2/multilayer graphene hybrid spin valves and demonstrate, for the first time, the opto-valleytronic spin injection across TMD/graphene interface [3]. We observe that the magnitude and direction of spin polarization is controlled by both helicity and photon energy. In addition, Hanle spin precession measurements confirm optical spin injection, spin transport, and electrical detection up to room temperature. Finally, analysis by a one-dimensional drift-diffusion model quantifies the optically injected spin current and the spin transport parameters. Our results demonstrate a 2D spintronic/valleytronic system that achieves optical spin injection and lateral spin transport at room temperature in a single device, which paves the way for multifunctional 2D spintronic devices for memory and logic applications.

PCSI

Room Keauhou II - Session PCSI-MoA

Wide Bandgap/Organic Spintronics/New Approaches to Epitaxy I/Nanowires and Nanostructures

Moderators: Leonard Brillson, Ohio State University, Danna Freedman, Northwestern University, Fengyuan Yang, The Ohio State University, Erik Lind, Lund University

2:00pm **PCSI-MoA-1 Use of Electrografted Aryldiazonium Salts to Control the Surface Conductivity and Reactivity of ZnO**, ***Alexandra McNeill,*** University of Canterbury, New Zealand*; K Bell,* MacDiarmid Institute for Advanced Materials and Nanotechnology*; R Gazoni, R Reeves, A Downard, M Allen,* University of Canterbury, New Zealand

Zinc oxide (ZnO) is a transparent, earth-abundant, wide band-gap semiconductor with high surface sensitivity and reactivity that must be controlled for use in electronic applications, in particular transparent thin film transistors and UV photodetectors. In ambient conditions, the ZnO surface is terminated by hydroxyl groups that cause the conduction and valence bands to bend downwards, creating an electron accumulation layer that renders the surface highly susceptible to unwanted atmospheric adsorbates [1]. The surface hydroxyl termination can be deliberately replaced with covalently bonded organic functional groups. In doing so, the surface band bending and surface conductivity can be directly manipulated. In this work, nitro- and trifluoromethyl-phenyl multilayered films have been attached to ZnO by electrografting from aryldiazonium salt solutions. Synchrotron X-ray photoemission spectroscopy confirms that both surface modifiers remove the native downward band bending, with the nitro-phenyl termination producing a large upwards band bending consistent with an electron-depleted surface. It was also observed that X-ray-induced reduction of the nitro-terminated film serves to further increase the upward band bending, which is an unexpected and as yet unexplained phenomenon. Diazonium salt chemistry has been rarely used to modify ZnO, yet this work indicates that it is a highly promising surface modification strategy for controlling the surface conductivity and reactivity of this technologically-important transparent semiconductor.

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2:15pm **PCSI-MoA-4 Influence of Interface State and Band Bending on In and N Polar InN from Angle-resolved XPS***, T Honda,* ***Yusuke Nakajima,*** Kogakuin University, Japan

Indium nitride (InN) has a smallest bandgap and a largest mobility among III-V nitride semiconductors[1]. However, the epitaxially grown InN layer contains a surface-charge-accumulation-layer, in which the Fermi-level is pinning at an energy position sufficiently higher than the conduction band minimum, resulting in a degradation of device performance[2]. The surface-charge-accumulation-layer induces a band bending and subsequent influences on the electrical properties in the surface region [3]. In this paper, surface band bending in In and N polar InN films was observed using angle-resolved X-ray photoelectron spectroscopy (AR-XPS) to discuss the surface states.

In and N polar InN layers were grown on (0001)GaN templates and free-standing $(000\underline{1})$GaN by RF-MBE. AR-XPS (JEOL, JPS9000) spectra were observed using a Mg K_α line (1253.6 eV) as an excitation source. The binding energies in the spectra were corrected using the C1s core level emission peak. The background intensities based on a white noise were considered. The observation was performed at RT. Before the observation, the surface oxides on the samples were removed using a HCl solution. The AR-XPS spectra near the valence band maximum at detection angles of 0 and 40 degrees are shown in Fig. 1 (a) and (b). Both figures are normalizing the spectrum. Both spectra are similar to those in a previous report[4], but slightly changed each other. Difference in between the spectra is shown in inset. The observed angle is defined as the tilt angle from the normal direction of the detector and is related to the average excitation depth in XPS. The result shows that the band bending is downward on the surface. Here, “downward” means that some holes in a bulk region move to its surface states [2]. The XPS spectra around the valence bands (VBs) of In- and N-polar InN layers are shown in Fig. 1 (c) (d). The tailing states are observed around the VBs, which will be due to the surface states occupied by electrons

2:20pm **PCSI-MoA-5 Influence of Al_2O_3/ $In_{0.76}Si_{0.24}O_{0.99}C_{0.01}$ Interface on Reliability for Oxide Thin Film Transistor***,* ***Kazunori Kurishima,*** Meiji University, National Institute for Materials Science, Japan*; T Nabatame,* National Institute for Materials Science, Japan*; T Onaya,* Meiji University, National Institute for Materials Science*; T Kizu, K Tsukagoshi, A Ohi, N Ikeda, T Chikyow,* National Institute for Materials Science, Japan*; A Ogura,* Meiji University, Japan

Recently, influence of dipole and fixed charge of SiO_2/Al_2O_3 interface on threshold voltage (V_{th}) control has been reported in back-gate-type Indium oxide (InO_x)-based thin film transistors (TFTs) with SiO_2/Al_2O_3 dilecetrics[1]. Previously, effect of In-Si-O film as a new InO_x-based channel material on stability of transistor properties was demonstrated [2] . Here, we pay attention to characteristics at interface between the Al_2O_3 dielectric and $In_{0.76}Si_{0.24}O_{0.99}C_{0.01}$ (ISOC) channel of ISOC TFT with Al_2O_3 dileletric. In this paper, we focus on the reliability of bottom-gate-type ISOC TFT with Al_2O_3 dileletric.

The bottom-gate-type ISOC TFTs were fabricated as follows. At first, Pt gate electrode was patterned on Si/SiO_2 substrate using photolithographic process. Next, a 30-nm-thick Al_2O_3 film was deposited on Pt gate electrode by ALD at 300 °C using TMA precursor and H_2O gas and was annealed at 300 °C in O_2. A 10-nm-thick ISOC film was subsequently deposited on Al_2O_3 film by sputtering using SiC and In_2O_3 targets and was annealed at 300 °C in air. The Au (100 nm)/Ti (10 nm) source/drain electrodes were patterned on ISOC film and was finally annealed at 250 °C in O_3.

Fig. 1 shows typical I_d-V_g properties of the TFT with Al_2O_3 dielectric. The V_{th}, on/off current ration and filed-effect-mobility value of Al_2O_3/ISOC TFT were -0.3 V, 6.4×10^8 and 15.2 cm^2/Vs, respectively. The lower subthreshold swing (SS) of 88.5 mV/decade was obtained. Negative gate bias stress was applied to examine stability of transistor properties of Al_2O_3/ISOC TFT. The change of V_{th} (ΔV_{th}) increased with increasing the V_g-V_{th} (Fig. 2 (a)). The ΔV_{th} in Al_2O_3/ISOC TFT was -4.6 V at a stress time of 3 h when V_g-V_{th} was applied -10 V. This suggested that the ISOC channel body was depleted, and the holes near the Al_2O_3/ISOC interface were trapped by deep donor-like trap states, which were oxygen-vacancy-related defect states, as shown in Fig. 2(b) [3].

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2:25pm **PCSI-MoA-6 Thermodynamic Analysis of 3Ga-H Surface Reaction Process for GaN(0001)***,* ***Kazuki Sekiguchi,*** *H Shirakawa, K Chokawa, M Araidai,* Nagoya University, Japan*; Y Kangawa, K Kakimoto,* Kyushu University*; K Shiraishi,* Nagoya University, Japan

Clarification of the growth mechanism during GaN MOVPE is crucial for the practical realization of GaN power devices, with which significant energy savings can be achieved. In our previous study, we analyzed the TMG decomposition process based on a calculation of the formation free energy and the activation energy [1]. It has been reported that TMG loses methyl groups one by one which react with H_2 and finally decomposes into GaH in the vapor phase. We concluded that the main reaction gases on the surface of the substrate are GaH and NH_3, which are the gallium and nitrogen sources, respectively. So, we have been investigating the behavior of GaH and NH_3 on the surface of GaN. According to a previous study [2], the reconstructed surface is a 3Ga-H surface, which means the hydrogen terminates 3 out of the 4 top Ga, under the growth conditions of our previous study [1]. Therefore, in this study, we clarify the reactions of GaH and NH_3 and the growth process on a 3Ga-H surface.

In the analysis of the reactions given by GaH and NH_3 at a 3Ga-H surface, we calculated the formation energy of the various surface reactions such as the adsorption reactions of NH_3, NH_2, GaH, and so on. As a result, on a 3Ga-H surface, GaH decomposition occurs, and Ga atom is adsorbed while H2 is desorbed in the vapor phase. Only this reaction can occur at 1300 K, which is the substrate temperature. With this reaction, the surface of the substrate changes from Fig.1 (a) to (b). Moreover, this reaction is repeated. Therefore, at a 3Ga-H surface, GaH decomposes into Ga and H atoms, and the Ga atoms are adsorbed one after another as shown in the following figure; Fig.1 (a) à (b) à (c) à (d). Finally, all 3 H atoms on the surface are desorbed in the vapor phase and 3 Ga atoms are adsorbed onto the GaN surface, forming a Ga-rich layer. This is also considered to correspond to the formation of Ga droplets.

2:30pm **PCSI-MoA-7 Effects of Incorporating Si into Al_2O_3 Gate Oxides in GaN-MOSFETs**, ***Eiji Kojima**, K Chokawa, H Shirakawa, M Araidai, K Shiraishi, K Shiozaki, T Kachi,* Nagoya University, Japan

There has been a growing interest in gallium nitride (GaN) as a material for next-generation power conversion devices. In order to realize GaN-MOSFETs, it is important to determine the most suitable gate oxide. Among the various materials for gate oxides, Al_2O_3 is one of the best owing to its relatively large conduction band offset (CBO) for GaN. However, the CBO of Al_2O_3 is smaller than that of SiO_2, which means the leakage current of GaN devices with Al_2O_3 gate oxides are higher than those with SiO_2 gate oxides. Leakage current can lead to instability of the threshold voltage. Kikuta et al. have reported that $Al_{1-x}Si_xO_3$ mixed oxides deposited by plasma-enhanced atomic layer deposition might achieve high reliability MOSFET devices with reduced leakage current.[1] In this study, we investigated the effect of incorporating Si at oxygen vacancies in Al_2O_3. We calculated the atomic and electronic structures of oxygen vacancies in amorphous $Al_{1-x}Si_xO_y$ using first-principles calculations.

The calculations were performed using the VASP code[2], which is based on density-functional theory with the Perdew-Burke-Ernzerhof (PBE) generalized gradient approximation.[3] We prepared amorphous Al_2O_3 with 120 atoms and constructed $Al_{0.8}Si_{0.2}O_3$, $Al_{0.46}Si_{0.54}O_3$ and $Al_{0.23}Si_{0.77}O_3$ models. Next, we removed an oxygen atom and calculated the atomic and electronic structures. In Al_2O_3, we found the well-known oxygen vacancy structures. However, a new Si-Si bond was formed in $Al_{0.8}Si_{0.2}O_3$, $Al_{0.46}Si_{0.54}O_3$ and $Al_{0.23}Si_{0.77}O_3$. As a result, no deep defect levels were formed in the bandgap with the $Al_{1-x}Si_xO_3$ mixed oxides, although deep defect levels originating from oxygen vacancies were formed in amorphous Al_2O_3 (Fig. 1 (a)-(d)). These results indicate that gate leakage would be reduced in MOSFETs with $Al_{1-x}Si_xO_y$ mixed oxides. Thus, $Al_{1-x}Si_xO_3$ is one of the best candidates for GaN-MOSFETs.

2:35pm **PCSI-MoA-8 Native Point Defect Measurement, Processing, and Identification Near Ga_2O_3 Surfaces**, *H Gao, G Foster,* The Ohio State University*; H Von Wenckstern,* University of Leipzig, Germany*; M Grundmann,* Universität Leipzig Institut für Experimentelle Physik II, Germany*; M Higashiwaki,* National Institute of Information and Communications Technology, Japan*; **Leonard Brillson**, H Zhao,* The Ohio State University

Ga_2O_3 research has expanded rapidly due to its wide band gap enabling very high breakdown fields and n-type doping ranging from intrinsic to degenerate, both features which lead to numerous solid state electronics applications. However, it is not yet known what defects form to compensate free carriers, reduce their mobilities, and limit their densities. We used a combination of depth - resolved cathodoluminescence spectroscopy (DRCLS), surface photovoltage spectroscopy (SPS), and remote oxygen plasma (ROP) processing to measure and begin to identify native point defects within the outer tens of nanometers of Ga_2O_3 grown by pulsed laser deposition (PLD), low pressure chemical vapor deposition (LPCVD), and edge- defined film- fed growth (EFG). All three growth methods exhibit common optical features corresponding to transitions into and out of multiple deep level defect states within the Ga_2O_3 band gap. (Fig.1.) DRCLS permits measurements of defect states from the free semiconductor surface into the bulk with depth resolution of tens of nanometers or less [1]. (Fig.2.) This capability permits us to measure how near-surface chemical processing changes DRCLS features, initially, how ROP filling of oxygen vacancies (V_O) reduces specific V_O-related deep level features, as found for other oxide semiconductors [2,3]. ROP processing produces clear reductions in specific defect features corresponding to V_O-related features, largest near the surface and extending more than 40 nm below. (Fig. 3) SPS features determine deep level energies corresponding to DRCLS transitions. (Fig. 4.) These SPS energies complement DRCLS transition energies and correlate with defect energies predicted theoretically for V_O in different lattice configurations (VDW) [4] and with energy levels extracted experimentally from deep level transient and optical spectroscopies DLTS and DLOS (SAR), respectively [5]. (Fig.5.)

These results indicate that oxygen vacancies in Ga_2O_3 form multiple defect levels in the range of 2.5 – 3.5 eV above the valence band maximum (E_V). More near-surface processing and characterization methods are available to probe the defect nature of other deep level features now observed. The combined near-surface detection and processing of Ga_2O_3 opens a new avenue for identifying and controlling native point defects in this and other semiconductors too. Supported by NSF Grants No. DMR-1305193 and DMR-1755479 with thanks to Tamura Corp.

2:40pm **PCSI-MoA-9 Geometry Effects in Spin Pumping through Thin Organic Films**, ***Georg Schmidt**,* Martin-Luther-Universität Halle-Wittenberg, Germany **INVITED**

We have investigated spin pumping from yttrium iron garnet (YIG) into Pt through ultrathin organic films (C_{60}, DH_4T) by measuring the damping in ferromagnetic resonance (FMR) by spin pumping and the DC inverse spin-Hall effect (ISHE) in the Pt. With increasing thickness d_0 of the organic the damping drops monotonically from a maximum for zero interlayer thickness to zero for 10 nm or more. The ISHE, however, changes in a non-monotonic way. Maximum ISHE is observed for $d_0=0$. For d_0 of 1 or 2 nm the ISHE drops to less than 50% (Fig. 1). Further increase leads to a reversal of this trend for both organic materials and only after a second maximum is reached a drop to zero is observed which is approx. exponential with interlayer thickness. The origin of this effect can be found in the growth mode of the organic layers. In very thin films the organic molecules grow as islands which can ideally be regarded as half spheres. Magnitude and direction of the ISHE depend on the absolute directions of pumped spins and spin current and their relative orientation. The spin current enters through the bottom of the islands but exits perpendicular to the organic/Pt interface. Only the spin current through the top of the island causes a maximum signal (Fig. 2) while currents flowing almost in plane barely contribute. They either do not cause any ISHE or they cause an ISHE-voltage perpendicular to the measurement direction. With increasing thickness the islands coalesce to a closed layer and all spin currents again pass the interface perpendicular to the layer. The original effect is then restored, except for a decrease by spin flip in the organic film. Simulations and transmission electron microscopy show that this model fully describes our findings. The results are important because they show that especially for spin pumping through very thin films the morphology is extremely important and many different layer thicknesses need to be investigated to get a coherent picture. Due to the purely geometrical origin the effect is universal for all conducting interlayer materials.

3:10pm **PCSI-MoA-15 Controlling Anisotropy in Organic-Based Magnets for Microwave Electronics and Quantum Magnonics**, ***Michael Chilcote**, M Harberts, Y Lu, I Froning, H Yu,* The Ohio State University*; B Fuhrmann,* IZM, Martin-Luther-Universität Halle-Wittenberg*; K Lehmann,* Institute für Physik, Martin-Luther-Universität Halle-Wittenberg*; A Franson,* The Ohio State University*; N Zhu, H Tang,* Yale University*; G Schmidt,* Martin-Luther-Universität Halle-Wittenberg, Germany*; E Johnston-Halperin,* The Ohio State University

Progress in the field of organic electronics has yielded significant advances in the development and application of organic light emitting diodes, organic photovoltaics, and organic field effect transistors. The success of these device applications suggests that further expansion of the field to include magnetic functionality may be promising. At the same time, the emergence of optimized thin film growth of and successful encapsulation strategies for organic magnets allows for long term stability of high quality magnets under ambient conditions. Organic-based magnets of the form $M[Acceptor]_x$ (M = transition metal, $x \approx 2$) exhibit room temperature magnetic ordering and provide the opportunity to tailor magnetic properties through the careful selection of the transition metal ions and organic ligands. However, despite the promise of these systems, important outstanding questions remain. For example, while these materials are typically considered to be globally disordered structurally, the canonical magnet of this materials class, vanadium tetracyanoethylene ($V[TCNE]_x$), exhibits robust magnetism, has a single-peaked, ultra-narrow magnetic resonance feature (approximately 1 G at 10 GHz), and has been shown to have a Curie temperature as high as 600 K.

We present work that illustrates strategies to control the anisotropy in this material system through growth morphology or temperature-dependent structural changes. We present the facile synthesis of a new class of organic-based magnetic nanostructures consisting of nanowires of $V[TCNE]_x$. These nanowires exhibit uniaxial magnetic anisotropy in direct contrast to the isotropic in-plane response of typical thin-films. Furthermore, the magnetic anisotropy persists to the point of re-coalescence of the nanowires into a thin film, suggesting that dipole fields arising from shape anisotropy do not play a dominant role, instead pointing to interface-templated structural ordering as the origin of this anisotropy. Moreover, isolated films of $V[TCNE]_x$ analogs show a temperature-dependent switch in the easy axis, pointing towards the presence of an additional contribution to the uniaxial anisotropy. These results introduce a new degree of freedom for organic-based magnetism, allowing for the engineering of magnetic anisotropy in materials that exhibits both robust room-temperature magnetic order and the benefits typically found in other organic materials. Together with recent demonstration of encapsulation technologies and demonstrated functional microwave devices that exhibit high quality factors across a frequency range, these results suggest future promising applications in microwave electronics and quantum magnonics.

3:15pm **PCSI-MoA-16 Controlling the Self-Assembly and Optoelectronic Properties of Porphyrin Nanostructures***, **James Batteas**, A Wan, T Reyes, M Elinski, M Buzbee,* Texas A&M University*; C Drain,* Hunter College of CUNY

Porphyrins are highly conjugated macrocyclic organic compounds which, due to their rich photophysical properties, have found numerous applications in areas ranging from catalysis, to optoelectronics, to photodynamic cancer therapies.[1,2] To tune their described structural and electronic properties, self-organizing porphyrins into hierarchical structures is often desirable.[3] Here, utilizing simply electrostatic interactions via the acidification of tetra(*p*-carboxyphenyl)porphyrin (TCPP) using hydrochloric acid, we have created porphyrin nanostructures, whose structural and optical properties are found to be pH dependent. From combinations of UV-visible absorption spectroscopy and atomic force microscopy (AFM) we have observed that after the carboxylate groups of TCPP were protonated (at ca. pH 5), the porphyrins form J-aggregate nanoplatelets. These structures further evolve, and by lowering pH to ca. pH 2, nanotubes ranging from ca. 30 - 300 nm in diameter with aspect ratios of > 400:1 are formed, with the absorption spectrum of the porphyrin nanotubes showing a collapse of the Q bands, revealing that protonation of the central nitrogens on the porphyrin macrocycle has occurred. Both in solution and on surfaces, these structures can be formed and cycled between, simply by changing solution pH. The porphyrin nanotubes have been observed by cryo-TEM to exhibit a highly organized lattice, and elemental mapping, as well as X-ray photoelectron spectroscopy (XPS) shows that chloride is intercalated within the porphyrin nanotubes at low pH, but not in the mid-pH range platelet structures. Photoconductivity of the porphyrin nanofibers was measured by four point probe and two-terminal current voltage (I-V) measurements and show the material to be semi-conducting in nature. As in solution, the structures on the surface can be tuned from platelet to nanofiber structures, simply by local pH changes, and using capillary condensation around an AFM tip, we can pattern these structures spatially on the surface.

4:30pm **PCSI-MoA-31 Tailoring Semiconductor Growth with Light***, **Kirstin Alberi**,* National Renewable Energy Laboratory **INVITED**

The development of new semiconductor materials, heterostructures and interfaces critically relies on our ability to direct their synthesis. Vapor phase epitaxy methods generally allow crystal growth to be controlled to a high degree through parameters such as substrate temperature, atomic or molecular fluxes and substrate properties (crystallographic orientation, atomic step density, etc). Yet, these parameters alone may not always provide sufficient degrees of freedom to regulate the resulting material phase, compositional profiles and defect populations. Here we examine the mechanisms by which photons can affect semiconductor growth processes and may thus be used as an independent, externally controlled growth parameter. Many of the changes are driven by the influence of excess free carriers on adatom incorporation and desorption processes or a change in the electron potential at the growth surface. We discuss our recent work on how light can be used to address two specific growth challenges: 1) the incorporation of large Bi atoms into GaAs [1] and 2) the formation of heterovalent GaAs/ZnSe interfaces [2]. Based on our understanding of photo-assisted growth mechanisms, we also highlight other areas where light may provide additional control over end material properties.

[1] D.A. Beaton, A. Mascarenhas and K.Alberi, *J. Appl. Phys*., **118**, 235701 (2015)

[2] K. Park and K. Alberi, *Scientific Reports*, **7**, 8516 (2017)

5:00pm **PCSI-MoA-37 Confined Lateral Overgrowth of Epitaxial InP Layers by Chemical Beam Epitaxy***, **Sukgeun Choi**, B Markman, H Tseng, S Brunelli, A Goswami, D Pennachio, J Klamkin,* University of California, Santa Barbara*; M Rodwell,* University of California, Santa Barabara*; C Palmstrom,* University of California, Santa Barbara

Recently, tunnel field-effect transistors (T-FET) have received considerable attention as a promising candidate for next-generation logic devices beyond metal-oxide-semiconductor FETs. T-FETs offer a fast transition between *on* and *off* device states with low power consumption. However, since charge carriers must "tunnel" through the bandgap of the transistor source, T-FETs tend to suffer low *on*-state current, which in turn slows device operation. In an attempt to mitigate the issue with low *on*-state current by increasing the tunnel probability, a confined hetero-junction T-FET has recently been proposed [1].

Here, we demonstrate lateral overgrowths of epitaxial InP thin layers inside threedimensional confined structures defined by SiO_2 walls in chemical beam epitaxy on InP substrates for the development of high-performance III-V hetero-junction T-FETs. Figure 1 shows a schematic of substrate structure, growth process, and a resulting top-view scanning-electron micrograph.

Suppression of undesired parasitic nucleation on SiO_2 surfaces and growth of high-quality InP layers inside the confined structure are strongly influenced by surface chemistry and chemical reactions between precursor molecules and surfaces. Dependencies of structural properties of InP layers on growth parameters such as substrate crystallographic orientation, direction of lateral growth, growth temperature, and V/III ratio are discussed. Technical challenges in the substrate preparation procedures and characterization of thin layers formed inside confined structures are also addressed. Success of confined epitaxial lateral overgrowth would pave a pathway toward the monolithic three-dimensional integration of semiconductor hetero-structures for advanced electronic and photonic device technologies.

[1] P. Long et al., IEEE Electron. Dev. Lett. 37, 345(2016).

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5:05pm **PCSI-MoA-38 Epitaxial Wafer Scale Growth of Tungsten Dichalcogenides***, **Tanushree Choudhury**, M Chubarov, X Zhang, J Robinson, J Redwing,* The Pennsylvania State University

Transition metal dichalcogenides (TMDs) have been a focus of interest due to the direct band gap of the monolayers in the range of 1.6 – 2.0 eV and large exciton binding energies, which leads to interesting electronic and optical properties. One major challenge in harnessing the potential of these materials is the growth of high quality epitaxial mono- and few-layer films over large areas. The growth on C-plane sapphire is expected to lock the domain orientations at 0° and 60° due to the hexagonal symmetry, which can result in epitaxial TMD films with reduced high-angle grain boundaries.[1] Oriented growth for TMDs like MoS_2[1] and WSe_2[2] has been demonstrated by powder vapor transport on C-plane sapphire previously. However, we find that in a cold-wall metal organic chemical vapor deposition (MOCVD) process, even though this orientation relation is maintained for WSe_2, this locking does not extend universally to WS_2. The reason for this difference is crucial in not only obtaining oriented films but also understanding the basic interactions between the TMDs themselves and/or the precursors involved and the sapphire substrate.

In this work, WS_2 and WSe_2 mono- and few-layer films were deposited by MOCVD system on 2" C-plane sapphire wafers using tungsten hexacarbonyl ($W(CO)_6$), hydrogen selenide (H_2Se) and purified hydrogen sulfide (H_2S) . The growth was carried out for 1 h at 800- 900°C for WSe_2 and 850-1000°C for WS_2 to achieve fully coalesced films with domains on the order of 1 mm in size. The results show that there is a distinct difference in the growth of WSe_2 and WS_2 films. Though both WSe_2 and WS_2 have an epitaxial relation with the underlying sapphire substrate, the WSe_2 domains are predominantly oriented at 0° and 60°, but the WS_2 films show presence of domains at other angles as well. In case of WSe_2, the orientation relation is maintained at all the growth temperatures investigated, but for WS_2, the orientation is maintained at 0° and 30° at lower temperatures between 750-850°C. Additional orientations emerge at 900-1000°C. Further details about the epitaxial relation, the interface interaction and the differences in the growth of WS_2 and WSe_2 will be presented.

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[2] L. Chen, B. Liu, M. Ge, Y. Ma, A. N. Abbas, C. Zhou*, *ACS Nano*, *9* (8),**2015**, 8368–8375.

5:10pm **PCSI-MoA-39 Structural Phenomena at the 3D/2D Interface: Epitaxy of Metals on Transition Metal Dichalcogenides***, **Kayla Cooley**, A Domask, R Alsaadi, S Mohney,* The Pennsylvania State University

Of the many emerging 2D materials, transition metal dichalcogenides (TMDs) are interesting for electronic and photonic devices as many of them are semiconducting when only a few layers thick, and they can be transferred onto flexible substrates. Successful application of these materials relies on building a fundamental understanding of the interfaces between TMDs and other materials, such as metals. Although metal/TMD epitaxy has been reported in literature, it has been observed in only a few systems to date. Much remains to be learned about this interesting phenomenon, which could offer new insights into quasi-van der Waals epitaxy for the development of novel heterostructures and for electrical contacts that may be altered or improved through epitaxy.

This work investigates a series of transition metals deposited on TMDs (MoS_2, WSe_2) at room temperature to identify metals exhibiting epitaxy on TMDs and to determine factors controlling this growth. Each metal/TMD system was analyzed by transmission electron microscopy and selected area electron diffraction to identify phases present and their crystallographic orientation. Annealed samples (4h @ 400^{o}C) were also examined to determine if thermal processing induced structural or chemical changes.

On MoS_2, many FCC metals from our work (Ag, Al, and Pd) and literature (Au, Pt, and Pb) - along with an HCP metal (Zn) from our work—were epitaxial with the following relationships: $(111)_{FCC}$ || $(001)_{TMD}$ and $<110>_{FCC}$ || $<110>_{TMD}$ or $(0001)_{HCP}$ || $(0001)_{TMD}$ and $<11\text{-}20>_{HCP}$ || $<11\text{-}20>_{TMD}$. In all cases, the close-packed plane with hexagonal symmetry grows on the basal plane of MoS_2, although lattice mismatches range from 9.4-18.6%. Like all tested BCC metals (Mo and Mn), the FCC Ni and HCP Ru and Re metals were not epitaxial on MoS_2, despite providing similar symmetry and lattice mismatches. We have discovered a strong correlation between activation energy to surface diffusion available from DFT calculations [1] and metal epitaxy on MoS_2. Our work also suggests that additional variables, such as homologous temperature, correlate almost as well.

In expanding the study to include metal/Wse_2 systems, a number of interesting differences were observed. Some metals were epitaxial on Wse_2 but not on MoS_2. Conversely, FCC Pd was epitaxial on MoS_2 after deposition, but it was epitaxial on Wse_2 only after annealing. More modeling of the surface of Wse_2 is needed to better understand these differences. Our ongoing work opens pathways for fundamental studies of Schottky barrier heights and the effect of atomic arrangement at the contact interface on this important parameter.

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5:15pm **PCSI-MoA-40 Temperature Dependence of Photoinduced Hydrogen Production and Simultaneous Purification in TiO_2 Nanotubes/Palladium Bilayer Membrane**, *J Asai, **Kei Noda**,* Keio University, Japan

Photocatalytic hydrogen (H_2) production with widegap semiconductor materials has been expected as one of the new clean energy sources. To provide H_2 gases for practical uses, all t he H_2 reforming units must be followed by hydrogen purification units for separating generated H_2 from other byproduct and residual gases such as carbon dioxide and oxygen. This issue can limit the miniaturization of H_2 production systems and the further development of on-site reformers toward mobile application of hydrogen energy. With this background, we have developed photoactive hydrogen production/separation membrane with a bilayer structure of an anodized titanium dioxide (TiO_2) nanotube array (TNA) and a hydrogen permeation film of palladium (TNA/Pd membrane) [1,2].

In this work, the temperature dependence of photoinduced H_2 production and purification in the TNA/Pd membrane was examined. This membrane was fabricated by transferring a TNA embedded in a titanium foil onto an electroless-plated 10-µm-thick palladium film. This membrane can reform a methanol/water (1:1) mixture photocatalytically under ultraviolet (UV) irradiation and concurrently purify generated hydrogen gas through the Pd layer. The H_2 production rate (r_{H2}) with the membrane at various temperatures was evaluated by using a home-made characterization system (Fig. 1(a)). As shown in Fig. 1(b), the measured r_{H2} showed larger values at higher temperature of the membrane. r_{H2} increased abruptly after several hours of UV irradiation and this inflection point appeared faster at higher temperature of the membrane. These behaviors can be probably related to the permeation characteristics of hydrogen through the Pd layer.

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5:20pm **PCSI-MoA-41 Structural Properties and Carrier Transport in Axial Silicon-Germanium Nanowire Heterojunctions**, *X Wang, **Leonid Tsybeskov**,* New Jersey Institute of Technology*; T Kamins,* Stanford University*; X Wu, D Lockwood,* National Research Council Canada, Canada

Recent advances in forming semiconductor heterojunctions within spatially confined nanoscale objects, including nanowires (NWs), show that the traditional limitations in the lattice-mismatched hetero-growth can be challenged. In various III-V semiconductor NWs, abrupt heterojunctions have been successfully demonstrated using the vapor-liquid-solid (VLS) growth for GaAs/InAs (7% mismatch) and InAs/InP (3% mismatch) heterojunctions. In group IV semiconductors, the approach is complicated not only by the 4.2% lattice mismatch between Si and Ge but also because Si and Ge both have a quite high solubility in the Au-Si catalyst. During chemical vapor deposition (CVD) based VLS growth using SiH4 and GeH4 (or similar gases), a supply of Si remains effectively "on" in the catalyst, and Si effectively intermixes with the arriving Ge even if the SiH4 flow is already switched "off". One way to address this problem is to choose a catalyst with a lower Si solubility, e.g. AlAu2 and AgAu. Another possibility is to significantly reduce growth temperature before turning a GeH4 source "on". Using the latter technique, we demonstrated Si-Ge heterojunction NWs with nearly ideal interface (Fig. 1) and only an 8 nm thick SiGe transition layer between straight and nearly micron-long Si and Ge NW segments [1].

In this work, we analyzed structural and electrical properties of axial Si-Ge heterojunction nanowires (NWs). The observed non-linear and rectifying current-voltage characteristics, strong flicker noise and damped current oscillations with frequencies of 20-30 MHz are explained using the proposed SiGe heterojunction NW energy band diagram including the energy states associated with the NW surface (and near-surface) structural imperfections revealed by transmission electron microscopy.

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5:25pm **PCSI-MoA-42 High Performance InAs Quantum Dot Lasers Grown on on-axis (001) Si with Low Threading Dislocation Density**, ***Daehwan Jung**, J Norman, M Kennedy, C Shang,* University of California, Santa Barbara*; R Herrick,* Intel Corp.*; Y Wan, B Shin, I MacFarlane, C Jan, A Gossard, J Bowers,* University of California, Santa Barbara

InAs quantum dots (QDs) epitaxially grown on Si are promising for efficient, scalable, and reliable light source for Si-based photonic integrated circuits. The effective lateral carrier confinement in QDs makes themselves less sensitive to threading dislocations that inevitably occur from the growth of GaAs on Si. Most of the previous research on QD lasers on Si employed intentional off-cut (4-6 °) substrates to circumvent electrically active antiphase domains that arise at the polar/non-polar interface. To be fully compatible with CMOS foundries, on-axis Si substrates have been recently used via various growth techniques, but the QD laser performance has been considerably diminished mainly due to the high threading dislocation density (TDD).

In this work, we demonstrate high performance 1.3 µm quantum dot lasers epitaxially grown on on-axis (001) Si using molecular beam epitaxy [1]. Thermal cycle annealing and strained-layer superlattices were performed, and the TDD was reduced from $\sim 3\times10^{8}$ cm^{-2} to $\sim 8\times10^{6}$ cm^{-2} in the metamorphic GaAs buffer layer on Si. A sample with one QD layer for photoluminescence was grown, and a very small full-width at half-maximum of 28 meV was measured at room temperature (Figure 1-a). Uncapped QDs also revealed a highly homogeneous height distribution with a density of $\sim 5.2\times10^{10}$ cm^{-2}. The high quality GaAs/Si template enabled record-low threshold current of 6.2 mA (Figure 1-b) at 20 °C. Lifetime tests were performed at Intel Corp., and the devices revealed extrapolated mean-time-to-failure (double initial threshold current) of more than one million hours for CW operation at 35 °C, which is a record-long lifetime for any lasers grown on on-axis (001) Si.

5:30pm **PCSI-MoA-43 Atomistic Mechanisms of Orientation and Temperature Dependence in Gold-Catalyzed Silicon Growth**, ***Yanming Wang**,* Massachusetts Institute of Technology*; A Santana,* Beijing Computational Science Research Center*; W Cai,* Stanford University

Gold-catalyzed vapor-liquid-solid (VLS) growth is widely used in the synthesis of silicon-based low-dimensional nano-structures. However, growth anomalies are often observed [1, 2], whose formation is believed to highly depend on the growth orientation and temperature, but a complete understanding has not been achieved yet. In this talk, we present a systematic study on the orientation and temperature dependences in the VLS process [3], by means of long molecular dynamics (MD) simulations up to 100 ns using an MEAM potential that well reproduces the binary phase diagram [4]. The Si growth velocities are extracted from the simulations under various conditions for ⟨110⟩ and ⟨111⟩ orientations respectively. Our data suggest a linear dependence of the growth velocity on the Si supersaturation for ⟨110⟩ growth, in contrast to a non-linear dependence for ⟨111⟩ growth. By analyzing the surface morphologies, this difference is linked to the continuous growth mechanism on {110} substrate and the island nucleation controlled growth on {111} substrate. Furthermore, we find that the ⟨111⟩ growth in our MD simulations operates in the regime where the nucleation rate is higher than the island expansion rate. This is traced to the formation of a gold saturated monolayer above the nucleated Si island, impeding its further growth. Also, it is found that the temperature dependent atom activity near the {111} interface is lower, explaining the smaller growth velocity of the {111} surface than that of the {110} surface.

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[2] Y. Li, Y. Wang, S. Ryu, A. F. Marshall, W. Cai, and P. C. McIntyre, *Nano letters* **16**, 1713 (2016).

[3] Y. Wang, A. Santana and W. Cai, *Journal of Applied Physics*, **122**(8), 085106 (2017).

[4] S. Ryu and W. Cai, *Journal of Physics: Condensed Matter***22**, 055401 (2010).

5:35pm **PCSI-MoA-44 Evaluation of Strain in the Oxide Covered Silicon Nanowires for Thermoelectric Devices by Raman Spectroscopy***, **Ryo Yokogawa**,* Meiji University, Japan*; S Hashimoto, M Tomita, T Watanabe,* Waseda University, Japan*; A Ogura,* Meiji University, Japan

Silicon nanowires (SiNWs) are promising candidates for the thermoelectric devices as well as next-generation channel materials of surrounding gate field-effect transistors. Especially SiNWs with cover oxide is recognized as a promising new thermoelectric material owing to their low dimensionality and the disorder strain induced at the SiO_2/SiNWs interface. To realize SiNW devices with high electric and thermoelectric performances, further improvements through the optimization of strain in the NWs are necessary to achieve a higher mobility and a lower thermal conductivity. Raman spectroscopy is a powerful strain evaluation technique in the nanostructures, because it has advantages such as a high spatial resolution and a nondestructive measurement. In this study, we evaluated the strain in the oxide covered SiNWs. We fabricated SiNWs using silicon-on-insulator (SOI) wafers with thermal oxidation under various conditions. We also performed small amount of Ar^+ ion irradiation to modify the SiO_2/SiNW interface (25 keV, 1.0×10^{14} cm^{-2}).

As a result, before Ar^+ ion irradiation, the anisotropic biaxial stresses of the along the SiNW length and width directions were confirmed to be compressive and tensile stress, respectively. On the other hand, after Ar^+ ion irradiation, we confirmed that the stress of the along the SiNW length direction became tensile stress, and the stress of the along the SiNW width direction was almost completely relaxed. We consider that an oxide-induce lattice disorder of the SiNW is relaxed by breaking strained bonds at SiO_2/SiNW interface by the ion irradiation, and tensile stress along the long direction in the SiNW is induced by SiNW lattice disorder. In conclusion, we evaluated the strain induction mechanism in the SiNW by Raman spectroscopy, sensitively.

PCSI

Room Keauhou II - Session PCSI-MoE

2D Surfaces II/2D Magnetism

Moderators: Jieun Lee, Ajou University, Gunter Luepke, College of William & Mary

7:30pm **PCSI-MoE-1 Towards Strongly Coupled van der Waals Heterostructures Using Layer-by-layer Transfer***, **Emanuel Tutuc**, K Kim, G Burg, B Fallahazad, S Larentis, H Movva,* The University of Texas **INVITED**

Layered crystals such as graphite, hexagonal boron nitride (hBN), or transition metal dichalcogenides (TMDs) can be mechanically exfoliated down to a monolayer, thereby providing a large set of two-dimensional (2D) materials with metallic, semiconducting or insulating properties. Combining such 2D materials into layered, van der Waals (vdW) heterostructures using a layer-by-layer transfer approach opens the door to realizing heterostructures with novel functionalities, which may otherwise not be possible using thin film growth techniques.

We review here key techniques and vdW heterostructures realized using layer-by-layer transfer. We demonstrate the realization of vdW heterostructures with high accuracy rotational alignment between different layers [1], which enables the realization of moiré crystals (Fig. 1) in twisted bilayer graphene [2], and gate-tunable resonant tunneling in heterostructures consisting of graphene double layers separated by hBN [1, 3].

A key parameter controlling the functionality of vdW heterostructures is the interlayer coupling in the stacking direction. Measuring such interlayer coupling, and demonstrating heterostructures with strong coupling are key issues relevant to device applications. We discuss recent results in double bilayer graphene heterostructures separated by WSe2 (Fig. 2) which show gate-tunable resonant tunneling with large current densities [4], comparable or better than values measured in epitaxial heterostructures.

[1] K. Kim, et al., Nano Lett. 16, 1989 (2016)

[2] K. Kim, et al., Proc. Natl. Acad. Sci. USA 114, 3364 (2017)

[3] B. Fallahazad, et al., Nano Lett. 15, 428 (2015)

[4] G. W. Burg, et al., Nano Lett. 17, 3919 (2017)

+ Author for correspondence: E. Tutuc (etutuc@mer.utexas.edu)

8:00pm **PCSI-MoE-7 Electronic and Optical Properties of Defects in Transition Metal Dichalcoginide Monolayers***, B Schuler, S Barja, S Wickenberg, N Borys, E Barnard, A Weber-Bargioni, **D. Frank Ogletree**,* Molecular Foundry, Lawrence Berkeley Lab

Properties of two-dimensional (2D) transition metal dichalcogenides (TMDs) are highly sensitive to the presence of defects, and a detailed understanding of their structure may lead to tailoring of material properties through 'defect engineering'. Defects in 2D semiconductors are expected to substantially modify material properties. 2D TMD semiconductors are particularly interesting because they exhibit direct bandgaps in the visible range, high charge-carrier mobility, extraordinarily enhanced light–matter interactions, and potential applications in novel optoelectronic devices.

We have investigated the structural and electronic properties of point and 1D defects in $MoSe_2$ and WSe_2 TMD monolayers through atomically resolved low temperature STM/AFM imaging and spectroscopy [1]. We have also performed scanning near-field photoluminescence hyperspectral imaging of MoS_2 monolayers [2] to image optoelectronic properties at the 40 nm length scale.

The structure and electro-optic properties of mirror-twin domain boundaries and of several types of TMD point defects will be presented and discussed.

[1] Sara Barja, Sebastian Wickenburg, Zhen-Fei Liu *et al.*, Nature Physics 12 751(2016).

[2] Wei Bao, Nicholas J. Borys , Changhyun Ko *et al.*, Nature Communications 6 7993 (2015).

8:05pm **PCSI-MoE-8 Work Function Variations in Twisted Graphene Layers***, **Jeremy Robinson**, J Culbertson,* Naval Research Laboratory*; M Berg, T Ohta,* Sandia National Laboratory

Vetting graphene and 2D materials as candidates for advanced electronics requires examination of both intrinsic and extrinsic influences on their material properties, as well as a nuanced characterization of how they respond in different heterogeneous configurations. As the field of 2D crystals expands to include stacked heterosystems, the relative orientation (or twist angle) between layers becomes important. In the simplest case, stacking two graphene layers to form twisted bilayer graphene (TBG) already leads to measureable differences in variables such as interlayer screening[1], optical absorption[2], chiral charge carriers [3], or chemical reactivity [4].

In this talk, we describe the characterization (e.g, imaging, Raman, kelvin probe force microscopy (KFPM), and photoemission electron microscopy (PEEM)) of rotationally faulted graphene. The variable inter-layer interactions in twisted graphene layers leads to a wide range of variable properties, including optical absorption and surface potential (Φ). We find that F can vary up to $\Delta\Phi$=39mV between 'small' (q_s»0°) and 'large' (q_L>16°) twist angles, and between $\Delta\Phi$=36-129mV for different layer thickness (N=1-4). The PEEM measured work function of 4.4eV for graphene is consistent with doping levels on the order of $10^{12}cm^{-2}$, and we find that F scales linearly with Raman G-peak wavenumber shift (slope = 22.2 mV/cm^{-1}) for all layers and twist angles, which is consistent with doping-dependent changes to graphene's Fermi energy in the 'high' doping limit[5]. The results discussed here emphasize that layer orientation is equally important as layer thickness when designing multilayer 2D systems.

[1] Sanchez-Yamagishi, et al., PRL 108, 076601 (2012)

[2] Robinson et al., ACS Nano 7, 637 (2013)

[3] Ding et al., Chem. Mater., 28, 1034 (2016)

[4] Kim et al., Nat Nano11, 520 (2016)

[5] Robinson et al., submitted (2017)

8:10pm **PCSI-MoE-9 Quantum Hall Effect Observed for Covalently and non-Covalently Functionalized Epitaxial Graphene***, **Evgeniya Lock**, J Prestigiacomo,* Naval Research Laboratory*; P Dev,* Howard University*; A Nath,* George Mason University*; R Myers-Ward, M Osofsky, T Reinecke, K Gaskill,* Naval Research Laboratory

We demonstrate no deterioration of electrical properties for epitaxial graphene, formed on SiC substrates via Si sublimation at elevated temperatures, functionalized using both covalent and non-covalent chemical approaches. In particular, we show that these functionalized samples exhibit the Quantum Hall Effect and possess Shubnikov-de Haas oscillations, which are typical for high quality exfoliated graphene flakes. We did not observe these phenomena on the initial pristine epitaxial graphene films. From first principle calculations, these results are likely due to reduced sheet charge density after functionalization, derived from charge transfer from the chemical molecules to the epitaxial graphene. This mechanism is supported by experimental data. This means that using our approach, and through the appropriate choice of functionalization moieties, the Fermi level of graphene can be controlled without detriment to electrical properties.

8:15pm **PCSI-MoE-10 2D Magnets and Heterostructures***, **Xiaodong Xu**,* University of Washington **INVITED**

Since the discovery of graphene, the family of two-dimensional (2D) materials has grown to encompass a broad range of electronic properties. However, until recently 2D crystals with intrinsic magnetism were still lacking. Such crystals would enable new ways to study 2D magnetism by harnessing the unique features of atomically-thin materials, such as electrical control for magnetoelectronics and van der Waals engineering for novel interface phenomena. In this talk, I will describe our recent magneto-optical spectroscopy experiments on van der Waals magnets, chromium(III) iodide CrI_3. I will first demonstrate the existence of isolated monolayer semiconductor with intrinsic Ising ferromagnetism. I will then show the layer number-dependent magnetic phases. The magnetic ground state evolves from being ferromagnetic in a monolayer, to antiferromagnetic in a bilayer, and back to ferromagnetic behavior in a trilayer. Lastly, I will discuss the emerging spin phenomena in monolayer Wse_2/CrI_3 ferromagnetic semiconductor heterostructures, including ferromagnetic control of valley pseudospin in Wse_2 via large magnetic exchange field, and optical analog of giant magnetoresistance effect.

8:45pm **PCSI-MoE-16 Antiferromagnetic Ordering in Atomically Thin 2-dimensional Materials Studied by Raman Spectroscopy***, J Lee, K Kim, S Lim,* Sogang University, Republic of Korea*; S Lee, J Ryoo, S Kang, T Kim, P Kim, C Park, J Park,* Seoul National University*; **Hyeonsik Cheong**,* Sogang University, Republic of Korea

Magnetism in low dimensional systems is attracting much interest not only for the fundamental scientific interest but also as a promising candidate for numerous applications in sensors and data storage. However, most experimental studies on magnetism in 2-dimension so far have been limited to the magnetism arising from defects, vacancies, edges or chemical dopants which are all extrinsic effects. Recent discovery of ferromagnetism in atomically thin materials [1,2] ignited much interest in magnetism in 2 dimension in general. Antiferromagnetic ordering, on the other hand, is much more difficult to detect as the net magnetism is zero. Neutron scattering, which is a powerful tool to detect antiferromagnetic order in bulk materials, cannot be used for atomically thin samples. Raman spectroscopy has proven a powerful tool to detect ferromagnetic ordering by monitoring the zone-folding due to the antiferromagnetic order [3,4] or the signal from two magnon scattering. We report on the observation of *intrinsic* antiferromagnetic ordering in the two-dimensional limit. We demonstrate that $FePS_3$ exhibits an Ising-type antiferromagnetic ordering down to the monolayer limit, in good agreement with the Onsager solution for two-dimensional order-disorder transition. The transition temperature remains almost independent of the thickness from bulk to the monolayer limit with T_N ~118 K, indicating that the weak interlayer interaction has little effect on the antiferromagnetic ordering. [4] For an XXZ-type antiferromagnet $NiPS_3$, a signal due to two-magnon scattering and the low-energy scattering signal due to spin fluctuations are monitored to find antiferromagnetic ordering down to the monolayer limit. [5]

[1] C. Gong, *et al*., Nature **546**, 265 (2017).

[2] B. Huang, *et al.*, Nature **546**, 270 (2017).

[3] X. Wang, *et al*., 2D Materials **3**, 031009 (2016).

[4] J.-U. Lee, H. Cheong, *et al*., Nano Letters **16**, 7433 (2016).

[5] K. Kim, H. Cheong, *et al*., *in preparation*.

PCSI

Room Keauhou II - Session PCSI-TuM

Scanned Probe/2D Materials and Applications/Interfaces and Heterostructures/Optical Properties of 2D Materials

Moderators: Wolfgang Windl, The Ohio State University, Michael Flatté, University of Iowa, Kirstin Alberi, National Renewable Energy Laboratory, Xavier Marie, Institut National des Sciences Appliquées, LPCNO

8:30am **PCSI-TuM-1 "Seeing'' the Covalent Bond: Simulating Atomic Force Microscopy Images***, **James Chelikowsky**,* University of Texas, Austin **INVITED**

Advances in atomic force microscopy (AFM) have made it possible to achieve unprecedented images of covalent bonds, in some cases even to resolve the bond order in polycyclic aromatics. However, fundamental questions remain about interpreting the images and modeling the AFM tip. For example, the bright spots in non-contact AFM images can have a close correspondence to the atomic structure of a given specimen, but there can be contrast changes with tip height that cannot be interpreted directly by atomic positions. While the nature of the tip can be crucial in understanding the details of the image, the atomic structure of the tip is often unknown. This situation is compounded by the difficulty in simulating AFM images. In order to perform computational studies of AFM, one must determine the interatomic forces as a function of the tip height on a fine grid above the specimen.

I will present an efficient first-principles method [1] for simulating noncontact atomic force microscopy (nc-AFM) images using a “frozen density” embedding theory. Frozen density embedding theory enables one to efficiently compute the tip–sample interaction by considering a sample as a frozen external field. This method reduces the extensive computational load of first-principles AFM simulations by avoiding consideration of the entire tip–sample system and focusing on the tip alone. I will demonstrate that our simulation with frozen density embedding theory accurately reproduces full density functional theory simulations of freestanding hydrocarbon molecules while the computational time is significantly reduced. Our method also captures the electronic effect of a Cu(111) substrate on the AFM image of pentacene and reproduces the experimental AFM image of Cu_2N on a Cu(100) surface. This approach is applicable for theoretical imaging applications on large molecules, two-dimensional materials, and materials surfaces.

9:00am **PCSI-TuM-7 Nanoscale Carrier Distribution Imaging of Layered Semiconductor Materials using Scanning Nonlinear Dielectric Microscopy***, **Kohei Yamasue**, Y Cho,* Tohoku University, Japan

Layered materials are nowadays rising class of materials owing to their various superior and anomalous properties. In particular, layered semiconductors have recently attracted much interest. For example, since molybdenum disulfide (MoS_2), one of layered semiconductors, can maintain relatively high carrier mobility even for atomic monolayer of this material, its electronic device applications have been studied extensively. Optoelectronic applications of MoS_2 are also explored, because a monolayer MoS_2 has a direct transition bandgap. For boosting research and development of layered semiconductor materials and devices, we need tools for characterization and analysis of carrier and charge distribution in a nanoscale. A promising candidate is scanning nonlinear dielectric microscopy (SNDM), which is a scanning probe microscopy method based on the detection of tip-sample capacitance. By measuring tiny variation in tip-sample capacitance to an applied voltage , SNDM can obtain information on dominant carrier (electrons or holes) and its spatial distribution in a nanoscale. In this talk, we demonstrate SNDM is even applicable to few- to mono-layer of layered semiconductors. Our images show n- and p-type MoS_2 flakes exfoliated on SiO_2/Si substrates were clearly distinguished as regions with negative and positive signals, respectively. In particular, we could obtain significant intensity even for a monolayer MoS_2. Our results suggest that SNDM will be useful for nanoscale characterization of carrier distribution in layered semiconductor materials.

9:05am **PCSI-TuM-8 Effect s of Edge Structures on the Oxygen Reduction Reaction Activity of Nitrogen-doped Graphene Nanoribbons***, **Shun-ichi Gomi**, H Matsuyama, A Akaishi, J Nakamura,* The University of Electro-Communications (UEC-Tokyo), Japan

Recently, much attention has been devoted to the oxygen reduction reaction (ORR) on nitrogen (N) -doped graphene [1]. It has been reported that N atoms prefer to be doped at the edge of graphene [2]. The structure of graphene edge can be classified into two types, zigzag and armchair edges. However, the effect of edge structures on ORR activity has not been fully understood.

We investigated the ORR activity on N-doped graphene nanoribbons with zigzag (N-ZGNRs) and armchair (N-ACGNRs) edges using first-principles calculations within the density-functional theory. Figure 1 shows the calculation models. The model of “X-Y” indicates a doping site of N (X) and a reaction site (Y). We used the computational hydrogen electrode model [3] to evaluate the maximum electrode potential. ORR mainly proceeds via the direct four-electron ($4e^-$) and the two-electron ($2e^-$) pathways. We also examined the selectivity with respect to these two pathways.

Figure 2 shows the maximum electrode potential of ORR for each doping site. The maximum potential for N-ACGNR becomes positive for each doping and reaction site. On the other hand, the maximum potential for N-ZGNR has a parity dependence with regard to the nitrogen doping site in the vicinity of the zigzag edges. For the even-numbered doping sites from the edge, the maximum potentials are larger than 0 V, while for the odd-numbered ones, the maximum potentials become negative. The reaction selectivity for the $4e^-$ pathway appears only in the vicinity of armchair and zigzag edges.

For the models showing the reaction selectivity, the sp^2 configuration of GNR is maintained, even if reaction intermediates are adsorbed on GNR. One the other hand, reaction intermediates adsorb on GNR with sp^3-like configuration for the other models. The mechanism for appearance of the selectivity will be discussed in the presentation.

[1] K. R. Lee *et al.*, Electrochem. Commun. **12**, 1052 (2010).

[2] S. F. Huang *et al*., Phys. Rev. B **80**, 235410 (2009).

[3] J. K. Nørskov, J. Rossmeisl, A. Logadottir, L. Lindqvist, J. Phys. Chem. B **108**, 17886 (2004).

[+] Author for correspondence: Shun-ichi Gomi, gomi@natori.ee.uec.ac.jp

9:10am **PCSI-TuM-9 2D or not 2D? How Nanoscale Surface Roughness Impacts the Frictional Properties of Graphene and MoS_2***, **James Batteas**, M Elinski, Z Liu, M Negtiro,* Texas A&M University

Control of friction and wear is a ubiquitous challenge in numerous machined interfaces ranging from biomedical implants, to engines, to nano- and micro-scaled devices, with the energy losses associated with friction and wear having significant impacts on the economies of the world. Notably, the combined energy losses and the associated system downtime for maintenance of machines due to friction and wear, contribute to an estimated loss of ~$200 billion/year in the United States alone. As such, developing new approaches for the control of friction at interfaces is a critical need. One of the key challenges in developing boundary lubrication schemes for such systems, is how to reduce friction and wear at the rough surfaces typical of machined interfaces, where nanoscaled asperities of ~ 10 – 20 nm rms roughness, dominate the interfacial contacts. The robust mechanical properties of two-dimensional (2D) nanomaterials has made them of significant interest for modifying surface frictional properties. It has been found that many 2D materials can readily adapt to surface structure on the atomic scale however, when deposited on substrates with nanoscopic roughness, a conformal coating cannot be fully formed due to competition between adhesion to the nanoscopic asperities of the substrate and the corresponding bending strain of the material. This often leaves a mixture of supported (bonded) and unsupported regions which respond differently to applied load. To investigate this in detail, we have developed a model platform to study friction in true nanoscaled asperity-asperity contacts using silica nanoparticles to form substrates with asperities of controlled radius of curvature (*ca.* 3 – 35 nm), matching those found in many machined interfaces. Here we describe a combination of AFM structural, nanomechanical and confocal Raman spectroscopic studies of graphene and MoS_2 on silica surfaces with controlled nanoscopic roughness, to examine the how surface roughness impacts their frictional properties. Additionally, as noted above, since substrate adhesion is a critical factor in the control of friction at these interfaces, we have also explored how the deposition of self-assembled monolayers (SAMs) of alkylsilanes with varying terminal functional groups (e.g. $-NH_2$, $-CH_3$, $-C_6H_6$) on the substrates also influence the corresponding structure, and the adhesion and friction in these 2D nanomaterials, when deposited on top of the SAM layers. The ability to tune and control roughness in these materials on the nanoscale also has other implications in the applications of these materials in electronics and catalysis.

9:15am **PCSI-TuM-10 Synthesis and Characterization of Atomic and Electronic Properties of Graphene-based Heterostructure*, Young Jae Song,*** Sungkyunkwan University, Republic of Korea

Electronic structure of graphene is affected by number of graphene layers and stacking order.[1,2] Control of layer number as well as scalability has been the main issues for device applications based on graphene. A new and unique CVD method is proposed to synthesize epitaxial multilayer graphene on copper by an iterative process of graphene growth and h-BN etching in chemical vapor deposition (CVD). A h-BN thin film is utilized to provide a gap of well-defined thickness for introducing the precursors and to play the role of the epitaxial growth of multilayer graphene. A thin h-BN film, initially-CVD grown on copper,[3] is locally etched out by hydrogen atoms decomposed from CH4 during the sequential graphene growth, which generates additional growth channels of graphene adlayers again under the first graphene layer. The crystallinity with AB stacking was confirmed by Raman analysis and selected-area electron diffraction measurements as well as statistical studies of optical microscope images. Graphene growth with a h-BN template suggests a potential way for controlling the specific layer number of large-area graphene in CVD for the device applications of graphene.

[1] A. H. Castro Neto, F. Guinea, N. M. R. Peres, K. S. Novoselov & A. K. Geim, Rev. Mod. Phys. 81 (2009) 109–162

[2] A. K. Geim & K. S. Novoselov, Nat. Mater. 6 (2007) 183–191

[3] M. Wang *et al*., Adv. Mater. 25 (2013) 2746–2752

9:20am **PCSI-TuM-11 Quantitative Relation between the Structural Stability and the Aromaticity of Graphene Nanoflakes***, M Ushirozako, H Matsuyama, A Akaishi,* ***Jun Nakamura,*** The University of Electro-Communications (UEC-Tokyo), Japan

Recently, nano-scale graphene nanoflakes (GNFs) have attracted great attention as one of the promising materials for electronics and spintronics. Kim et al. have successfully fabricated GNFs with various sizes up to 35 nm and have reported that the photoluminescence property of GNFs depends on the size and the edge shape [1]. From the view point of the structural stability of GNFs, we have not yet acquired the systematic comprehension with regard to effects of shapes and sizes of GNFs on the stability. In the present study, we have examined how the stability of GNFs is dominated by the edge shape and the size of GNFs, using first-principles calculations within the density functional theory.

In order to evaluate the stability of GNFs, we calculated the edge formation energy. First, we consider GNFs with the six-fold symmetry (D_{6h}) and classify them into zigzag GNFs (ZZGNFs) and armchair GNFs (ACGNFs). ACGNFs have two subtypes, AC(1) and AC(2), depending on whether carbon atoms are just at the corner of the outermost envelope hexagon of GNFs. In addition, we also evaluate the structural stabilities of triangular and rhombus GNFs.

Figure 1(a) shows the edge formation energy of the GNFs. The formation energy of ZZGNFs is higher than that of ACGNFs irrespective of the size of GNFs. This instability of ZZGNFs is attributed to the presence of the so-called edge state. Indeed, it has also been shown that the formation energy of the zigzag graphene nanoribbon is higher than that of the armchair one. It is noted that AC(2) is slightly more stable than AC(1), whereas the purity of AC(2) is lower than that of AC(1). Such peculiar stabilization can be reasonably explained in terms of the aromaticity of GNFs. Figure 1(b) shows the rela-tionship between the edge formation energies and the average NICS values. In addition to ACGNFs, we calculated those for trigonal-GNFs and rhombus-GNFs. As clearly seen, the edge formation energy is proportional to the average NICS value. The slope is almost the same for each type of GNFs and the intercept depends on the type. The average NICS values have one-to-one correspondence with the formation energy regardless of the GNF size. This means that the stability of the GNF edge is dominated by the degree of the aromaticity over the whole rings of GNFs. Therefore, it is concluded that the NICS values are not just the measure of aromaticity but also are relevant to the structuralstability of GNFs [2].

[1] S.Kim *et al.*, *ACS Nano*, **6**, 9, 8203 (2012)

[2] A.Akaishi, M.Ushirozako, H.Matsuyama, and J.Nakamura, *Jpn.J.Appl.Phys.***57** (2018), in press.

9:25am **PCSI-TuM-12 Formation of Water Bilayer on Graphene Surfaces*, Akira Akaishi,*** *J Nakamura,* The University of Electro-Communications (UEC-Tokyo), Japan

Water wettability of graphitic surfaces is of great interest to the fundamental understanding of graphene surfaces and for practical applications of graphene-based materials since the wettability is closely related to whether the surface is hydrophobic or hydrophilic. One of the characteristic measures of the wettability is a contact angle that is the angle of the edges of a water droplet placed on target surfaces. While graphitic surfaces are believed to be hydrophobic, in recent studies, it has been reported that the water contact angle of the graphene surfaces becomes relatively small by removing surface contamination [1]. This observation is also confirmed by evaluating the water contact angle with molecular dynamics (MD) simulations [2]. The wettability of pristine graphene surfaces is controversial.

We have examined the structure of water molecules on graphene surfaces with MD simulations. As the number of water molecules increases, the droplet covers the surface and the layered-structure of molecules on the surface is formed. This indicates that, at the level of an empirical model, a graphene surface is capable of wetting.

The formation of water layers on the surface can be seen by the density profile of water molecules. Figure 1 shows the probability density distribution of oxygen atoms, hydrogen atoms, and hydrogen bonds of water along the normal direction to the graphene surface. For the oxygen atoms, the density distribution has two peaks, indicating the bilayer of water molecules is definitely formed. Moreover, the distinct peaks of the hydrogen atoms and the hydrogen bonds distributions indicate that the oxygen-hydrogen (O-H) bonds are not randomly formed but are certainly oriented. Our analyses on the angle distribution of O-H bonds show that hydrogen bonds are formed within and between the water layers. Above the second layer, there are no dangling hydrogen bonds that are pointing perpendicular to the layer plane, which means that a graphene surface covered with the water double-layer has a hydrophobic character.

[1] Z. Li, et al., Nat. Mater. 12, 925 (2013).

[2] Y. Wu and N. R. Aluru, J. Phys. Chem. B 117, 8802 (2013).

[3] A. Akaishi, T. Yonemaru, and J. Nakamura, ACS Omega 2, 2184 (2017).

9:30am **PCSI-TuM-13 Scanning Electrochemical Microscopy of Graphene-based Hybrids: Insights into Physicochemical Interfacial Processes and Electroactive Site Distribution*, Sanju Gupta,*** Western Kentucky University

Surface (and interfacial) chemistry is found in various environments of scientific significance including biomembranes, ocean and atmospheric chemistry and applied electrochemistry. Molecular redox behavior on the surface and at the interface is drastically different than their bulk counterpart. Scanning electrochemical microscopy (SECM) is a powerful tool to investigate interfaces determining ion transfer kinetic rate, diffusion coefficient, imaging topography and electrochemical redox reactions. The significant advantage offered by SECM is its capability of probing chemical information of interfacial electron and ion transfer processes at solid/liquid interface irrespective of substrates. A constant potential is applied to the tip and electrochemical working electrode (*i.e.* the substrate in electrolyte) to drive reaction in bulk electrolyte solution of redox species (or mediator) to probe the surface of certain thickness of graphene-based hybrids. The microscaled cyclic voltammograms, probe approach (current *versus* tip–substrate distance) curves, 2D and 3D micrographs in feedback mode, were chosen for graphene/CNT, graphene/transition metal oxide as supercapacitors to probe ion adsorption and to map highly electroactive (‘hot spots’) sites. The SECM setup has a resolution of ~40 nm and can locate and relocate areas of interest precisely after a coarse image. We present our findings from viewpoint of reinforcing the roles played by heterogeneous electrode surfaces comprised of graphene nanosheets (conducting)/nanomaterials (semiconducting) via higher/lower probe current distributions. SECM approach curves as well as two dimensional scans elucidated the existence of regions of different conductivity and the data is analyzed in terms of edge plane defects distribution within the probes regions, determining diffusion coefficient and heterogeneous rate constant.

11:00am **PCSI-TuM-31 Realization of 2D Group-III Materials Through Thermal Evaporation-Based Intercalation*, Natalie Briggs,*** *B Bersch, A De La Fuente,* Pennsylvania State University*; C Lopez Pernia,* Technical University of Madrid, Spain*; K Wang, J Robinson,* Pennsylvania State University

Recent years have seen continued developments in the synthesis of 2D materials, and along with improved deposition techniques have come new strategies and approaches to realizing 2D compounds. One such strategy utilizes intercalation of metal atoms as a pathway to forming graphene-encapsulated 2D materials. This approach has allowed for the realization of a 2D form of gallium nitride (GaN) by annealing intercalated metal atoms in ammonia, as a result, expanding the pallet of materials that may be realized in 2D forms[1]. However, initial studies of 2D GaN synthesized from intercalation have relied on involved metal organic chemical vapor deposition techniques, and the resulting materials have suffered small domain sizes. We report a method of intercalating group-III (GIII) metal atoms gallium and indium through simple vaporization of metallic precursors in the presence of graphene layers. Through this method, micron-scale intercalation is possible. Following the intercalation of GIII metals, graphene-encapsulated gallium and indium layers are selenized and nitridated through exposure to selenium and ammonia at high temperatures. Ongoing work aims to elucidate the requirements of forming encapsulated 2D materials, as well as the resulting structures, and electronic and optical properties.

[1] Balushi, Z. Y. Al *et al*. Two-dimensional gallium nitride realized via graphene encapsulation. *Nat. Mater.* **15**, 1166-1171 (2016).

11:15am **PCSI-TuM-34 Strain and Compositional Fluctuations in $\mathbf{Al_{0.81}In_{0.19}N}$/GaN Heterostructures***, **Verena Portz**,* Academia Sinica, National Taiwan University, Forschungszentrum Jülich GmbH, Republic of China*; M Schnedler,* Forschungszentrum Jülich, Germany*; M Duchamp,* Nanyang Technological University, Singapore*; F Hsiao,* National Taiwan University, Republic of China*; H Eisele,* Technische Universität Berlin, Germany*; J Carlin, R Butté, N Grandjean,* École Polytechnique Fédérale de Lausanne, Switzerland*; R Dunin-Borkowski, P Ebert,* Forschungzentrum Jülich, Germany

The strain and compositional fluctuations of nearly lattice-matched $Al_{0.81}In_{0.19}N$/GaN heterostructures are investigated by cross-sectional scanning tunneling microscopy and selected area electron diffraction measurements in scanning electron transmission microscopy. The presence of strain induces height modulations governed by different roughness components at the cleavage surfaces. The surface height modulations are compatible with a relaxation of alternatingly compressive and tensile strained domains, indicating compositional fluctuations. Changes of the *a*-lattice constant are traced to interface misfit edge dislocations.

11:20am **PCSI-TuM-35 Theoretical Investigations for Strain Relaxation and Resultant Growth Mode in InAs/GaAs Heteroepitaxial System***, **Tomonori Ito**, T Akiyama, K Nakamura,* Mie University, Japan

It is well known that InAs grown on GaAs(001) produces three-dimensional (3D) island shaped quantum dots. Despite a constant lattice mismatch, InAs thin films fabricated on the GaAs(111)A and GaAs(110) exhibit two-dimensional (2D) growth contradicting the 3D growth of InAs on GaAs(001) [1]. In this study, the growth mode of InAs/GaAs depending on orientations is systematically investigated using macroscopic free energy, microscopic emprical interatomic potential, and nanoscopic ab initio calculations to clarify the contribution of strain relaxation at their interfaces and surfaces to the resultant growth modes.

Figure 1 shows the calculated free energy differences among various growth modes as a function of layer thickness *h* for InAs/GaAs with different orientations. The growth mode in (110) (Fig. 1(a)) changes from the 2D-coherent (2D-coh) to the 2D growth with misfit dislocation (2D-MD) at *h*~1 monolayer (ML), while the 2D-3D growth mode transition appears inserting $In_{0.25}Ga_{0.75}As$ layer between InAs and GaAs that reduces surface energy *g* from 51 to 49 meV/Å^2. On the other hand, (111)A (Fig. 1(b)) keeps the 2D growth mode from the 2D-coh to the 2D-MD via stacking-fault tetrahedron (SFT) formation (2D-SFT) at *h*~3 ML. The SFT formation near surface reduces strain energy more effectively than island and MD formations at the initial growth stage. For (001) (Fig. 1(c)), the strain relaxation occurs at *h*~0.5-0.6 ML where the macroscopic theory is no longer applicable. At this early stage, the strain is relaxed on the InAs reconstructed surface with missing surface dimer to substitute for In-As dimer going so far as to break the electron counting rule. These suggest that the growth mode in InAs/GaAs is closely related to the strain relaxation at the interface for (110), at both the surface and the interface for (111)A, and on the surface for (001).

11:25am **PCSI-TuM-36 Electric Field-Driven Defect Diffusion at Oxide Semiconductor-Metal Interfaces***, H Gao, G Foster,* The Ohio State University*; G Mackessy,* Columbus School for Girls*; A Hyland, M Allen,* University of Canterbury, New Zealand*; **Leonard Brillson**,* The Ohio State University

We used depth - resolved cathodoluminescence spectroscopy (DRCLS) to measure how native point defects move under applied electric fields at metal-ZnO and metal-$SrTiO_3$ interfaces. Native point defects can be electrically active, acting as donors or acceptors that increase or compensate free carrier densities, altering Schottky barrier depletion regions as well as forming interface states that "pin" Fermi levels. For many compound semiconductors, these defects exhibit pronounced segregation toward free surfaces and metal contacts, amplifying their interface electronic effects. Here we report that native point defects in ZnO and $SrTiO_3$, representative wide band gap semiconductors with and without built-in polarization fields, respectively, can move hundreds of nanometers under applied electric fields that are comparable to electric fields in conventional Schottky barriers. In turn, such voltage gradients can account for the pronounced defect segregation typically reported at oxide semiconductor interfaces.

To gauge how electric fields can affect defect distributions in ZnO, we measured DRCLS vs. increasing incident electron beam energy E_B and increasing depth below a 20 nm Pt electrode on a 0.5 mm thick commercial (MTI) ZnO single crystal. Without bias, DRCLS through the Pt showed significant increases in zinc vacancies (V_{Zn}) and Cu on Zn sites (Cu_{Zn}), analogous to previous studies.[3] An applied bias of +917V corresponding to 18.3 kV/cm across the entire crystal width increased this segregation by > 2x nearest the Pt/ZnO interface. This enhancement extends tens of nanometers into the bulk – comparable to the semiconductor depletion width, suggesting that the applied field falls primarily across the Schottky depletion region. With bias removed, these defects redistribute. Applied bias up to 2.5 kV/cm produces analogous oxygen vacancy (V_O) diffusion in commercial (Crystek) $SrTiO_3$ wafers. Here, positive bias drives the positive donors away from the anode, but with bias removed, these defects don't redistribute.

Electric fields applied laterally across ZnO surfaces also drive defect diffusion. Hyperspectral imaging (HSI) maps of V_{Zn} and Cu_{Zn} spatial distributions between a 32 nm thick, 300 nm diameter IrO_x Schottky diode and ground on a low-Li Tokyo Denpa Ltd. single crystal wafer displayed acceptor movement toward the diode with increasing positive bias corresponding to 10^4V/cm. These effects have general significance since voltage gradients of this magnitude are comparable or less than those in conventional band bending regions.

The authors gratefully acknowledge support from NSF Grant No. DMR-1305193 (T. Paskova).

11:30am **PCSI-TuM-37 General Abscence of Electron Accumulation at Stoichiometric Indium-containing Semiconductor Surfaces***, **Holger Eisele**,* Technische Universität Berlin, Germany

During recent years electron accumulation was assigned to many different indium containing semiconductor materials: it almost looked like a universal property [1]. Typically, in technologically usable samples it seems to be a persistently existing effect. But still, the question rises, whether this is an intrinsic or extrinsic semiconductor material property, meaning whether the effect is coming from the material itself or from changes in composition, complete decomposition, or due to oxidation at surfaces. Therefore, we prepared different indium containing semiconductor samples, i.e. InN, AlInN, and In_2O_3, just by cleavage without any annealing step. This process typically leads to stoichiometric surfaces, at least for a certain time of experimental investigation. After the investigation we also aged the sample in order to see changes. The investigations of the electronic states were performed by cross-sectional scanning tunneling spectroscopy, probing occupied and unoccupied states at the same time. For all materials—as long as their surfaces stay stoichiometric—we find no intrinsic electron accumulation at all non-polar surface, i.e. the ones without intrisic polarization field. For InN [2,3] we can exclude intrisic electron accumulation at both non-polar surfaces, the *a*- and the *m*-plane, for InAlN [4] at the *m*-plane, and for In_2O_3 at the (111) surface. The electronic structure of these surfaces are all different from each other: InN show no electronic surface state within the fundamental bulk bandgap, for InAlN at least one (depending on the In/Al ratio probaly more) state shifts into the fundamental bulk band gap, and In_2O_3 has different intrisic surface states within it. So the absence of electron accumulation is further independent of the intrinsic electronic properties of the material. Nevertheless, by aging In_2O_3 under ambiant conditions we receive a completely different image: the surface shows metallic behavior, as also surface electron accumulation does.

[1] P.D.C. King, *et al.*, Appl. Phys. Lett. **91**,092101 (2007).

[2] Ph. Ebert, *et al.*, Appl. Phys. Lett. **98**, 062103 (2011).

[3] H. Eisele, *et al.*, Phys. Rev. B **94**, 245201 (2016).

[4] V. Portz, *et al.*, Appl. Phys. Lett., **110**, 022104 (2017).

11:35am **PCSI-TuM-38 InAsSbBi/GaAsSbBi Type-II Heterostructures for Mid- and Long-wavelength Infrared Applications***, **Shane Johnson**, S Schaefer, R Kosireddy, A Shalindar, P Webster,* Arizona State University

Alloying bismuth with InAsSb provides an active material near the GaSb lattice constant that covers the technologically important 3 – 5 µm and 8 – 12 µm atmospheric transmission windows. A significant advantage of the InAsSbBi quaternary is that strain and bandgap can be independently selected (Fig. 1). Furthermore, independent tuning of the band offsets can be achieved when adding the larger bandgap GaAsSbBi quaternary to the mix, either as quinary random alloys or type-II quantum well/superlattice heterostructures.

The molecular beam epitaxy growth and structural and optical properties of InAsSbBi/ GaAsSbBi heterostructures on GaSb are examined using reflection high-energy electron diffraction, Rutherford backscattering spectrometry, X-ray diffraction, spectroscopic ellipsometry, and photoluminescence spectroscopy. Near stoichiometric group-V fluxes and lower growth temperatures are utilized to facilitate the incorporation of the Bi atoms. The Rutherford backscattering spectrum from InAsSbBi has a unique energy range characteristic of Bi, allowing independent determination of Bi mole fraction (Fig. 1). The As and Sb mole fractions are then uniquely determined from the layer strain provided by X-ray diffraction. The InAsSbBi bandgap and band offsets determined from photoluminescence and spectroscopic ellipsometry are parametrized in terms of mole fraction. The results indicate that the InAsSbBi material system forms a type-I band alignment with InAsSb and a type-II band alignment with GaSb and GaAsSbBi.

11:45am **PCSI-TuM-40 Excitons in MoS_2/$MoSe_2$/MoS_2 Trilayer Metal Dichalcogenides***, **Paulina Plochocka**,* LNCMI, CNRS, France **INVITED**

Monolayer transition metal dichalcogenides (TMDC) are rapidly emerging as potential building blocks for novel electronic and optoelectronic devices. In this talk I will discuss the optical properties of excitons in tri – layer transitions metal dichalcogenides (TMDC).

First, I will demonstrate a novel approach to neutralize the intrinsic defects of CVD-grown TMDCs, using transfer tools routinely employed in the fabrication of van-der-Waals heterostructures. We investigate the optical properties of trilayer stacks composed of external CVD-grown MoS_2 flakes as capping layers and an internal CVD-grown $MoSe_2$ flake which has a smaller band gap. Remarkably, this fabrication approach strongly suppresses the localized exciton emission in $MoSe_2$ yielding a low temperature PL comparable to that observed in mechanically exfoliated samples [1]. Our results pave the way for the production of large area high quality TMDCs. Furthermore, I will demonstrate that tuning the excitation laser to the A-exciton resonance of the larger band gap MoS_2 leads to a considerable charge transfer towards lower band gap $MoSe_2$. The conservation of the spin during the charge transfer opens new possibilities for spintronics and spin injection. In addition, the investigation of the charge transfer between the MoS_2/$MoSe_2$ layers allows us to demonstrate a novel way to introduce the valley polarization in $MoSe_2$, which is difficult to achieve in non resonant excitation conditions [2].

Finally, I will discuss optical properties of the long lived inter-layer exciton formed between the $MoSe_2$ and MoS_2 monolayers. Under circularly polarized excitation, the inter-layer exciton emission is intriguingly counter polarized. Such an effect has never been observed previously. Our results show that a careful choice of the TMDs forming the van der Waals heterostructure makes it possible to control the circular polarization of inter-layer exciton emission. This unexpected phenomenon gives an additional degree of freedom for tailoring the properties of van-der-Waals heterostructures [3].

[1] A. Surrente, PP et al Nano Letters 17, 4130 (2017)

[2] M. Baranowski, PP et al 2D materials 4, 025016 , (2017)

[3] M. Baranowski, PP et al Nano Letters in press DOI: 10.1021/acs.nanolett.7b03184

12:15pm **PCSI-TuM-46 Photo-assisted Modulation of Thermal Transport and Thermopower in Single-layer Transition Metal Dichalcogenides***, **Parijat Sengupta**, J Shi,* University of Illinois at Chicago

Transition metal dichalcogenides (TMDCs) have the representative formula MX_2, where *M* is a transition metal element from group IV–VI and *X* belongs to the set of elements S, Se, and Te, collectively identified as chalcogens They are layered materials of covalently bonded atoms held together by weak van der Waals forces. Thin TMDC films are considered promising thermal materials with the possibility of a large figure of merit, . Here, **S** is the Seebeck coefficient, the electrical (thermal) conductivity is denoted by $\boldsymbol{\sigma}$ ($\boldsymbol{\kappa}$), and **T**is the temperature. Beginning with a *k.p* representation of the Hamiltonian that describes the carriers in the vicinity of the two valleys, **K** and **K`,** as massive Dirac fermions, we theoretically demonstrate the modulation of **S** aided by a driven periodic perturbation. We use a high-intensity circularly-polarized illumination to drive the TMDC into a Floquet *off-resonant* phase that enlarges the fundamental band gap, say, at **K**, while **K`** suffers an equal reduction. This dual transformation is simply an outcome of the time-reversal principle connecting the two valleys and manifests as unequal conductivities for respective carriers. This inequality is also mirrored in their thermopower (**S**) behaviour. The conductivity (intra-band) calculations are performed using the Kubo formalism. To determine the thermopower for carriers (that lie close to *K* and *K`*), in the low-temperature limit, we use Mott's formula furnishing a valley-resolved thermopower. Specifically, the carriers from the valley that has an optically-lowered band gap reveal a higher thermopower vis-à-vis the ensemble located in its time-reversed counterpart. Further, a simple application of the Wiedemann-Franz law (WFL) relates σ to κ from which we obtain low-temperature *ZT*, using the pre-computed thermopower.

The thermal conductivity is integral to Peltier-type solid state cooling methods and thermopower generation; while the former requires a higher κ for unimpeded heat flow from deep-seated hot-spots in a miniaturized chip, the latter relies on localized heat production for efficient energy-conversion. To this end, in accord with WFL, to achieve a desirable κ, it is prudent to investigate conditions that permit an adjustable σ. We show that in conjunction with optical modulation, disorder, which can establish a variable hopping regime and quench σ, allows the sought control over κ within the purview of our stated applications.

PCSI
Room Keauhou II - Session PCSI-TuE
Rump Session: 2D or not 2D?

Moderator: Jun Zhu, Penn State University

7:30pm **PCSI-TuE-1 III-V Transistors for nm Logic and 100-1000 GHz Wireless*, Mark Rodwell,*** University of California, Santa Barabara **INVITED**

We examine the opportunities for nm III-V electron devices both in VLSI logic and in mm-wave (and sub-mm-wave) wireless communications.

Tunnel FETs (TFETs) are being developed for high on-off current ratios at low operating voltages, enabling low-power VLSI. III-V heterojunction TFETs offer direct (vs. phonon-assisted) tunneling, low tunnel barrier energy, and low electron effective mass. TFET on-currents are nevertheless very low; consequently TFET logic will be very slow. We are developing modified (triple-heterojunction) TFETs [1]. In these, added wide-bandgap source and channel layers increase the junction built-in potential, increasing the junction field and thereby decreasing the tunneling distance. Confinement with transport decreases the hole mass. The tunneling probability is greatly increased, proportionally increasing the on-current and logic speed. As the heterojunctions must be perpendicular to the semiconductor-dielectric interface, both convention TFETs are profoundly difficult to fabricate. Addressing this, our fabrication process, which we are developing, uses template assisted selective epitaxy [2].

Wireless communications will soon move to 5G (28, 38, 57-71, 71-86GHz); research now explores 100-1000 GHz systems. Above ~200GHz, CMOS provides little or no amplification, and scaling below ~32nm does not improve this. We must develop transistors for the low-noise and high-power stages in 100-200GHz systems, and for all stages at higher frequencies. InP HBTs, useful for power, have reached 1.1THz f_{max}. To further improve bandwidth, we are exploring TESA processes to form devices with buried dielectric layers in the base-collector junction. The base contact can be made wider for reduced resistance while the buried dielectric layer maintains low junction capacitance. InP HEMTs, useful for noise, have reached 1.5THz f_{max}. To further improve bandwidth, we are developing nm InAs MOS-HEMTs, with ALD ZrO_2 gate dielectrics, 5nm channels, and modulation-doped access regions surrounding the gate.

[1] P. Long, *et al*., 2017 Device Research Conference, June, Notre Dame.

[2] L. Czornomaz, *et al*., 2015 VLSI Symposium, June, Kyoto, Japan

8:00pm **PCSI-TuE-7 Emerging Frontiers of 2D Materials: From Low-Energy and Bendable Electronics to Quantum-, Spin-, and Valley-Enabled Devices*, Roland Kawakami,*** The Ohio State University **INVITED**

2D materials research began with graphene, but has expanded far beyond to include transition metal dichalcogenide (TMD) semiconductors, hexagonal boron-nitride (h-BN) insulators, and other 2D van der Waals systems. Most notably, the 2D materials can be stacked into vertical heterostructures, where proximity effects and transport driven processes can create properties that are not present in the individual 2D sheets. In this talk, I will review some of the exciting trends in 2D materials research as it relates to electronic and photonic devices. Some of the more near term research involves develop novel devices such as tunneling field effect transistors for low energy electronics, as well as printable inks for large area and bendable electronics. Looking further into the future for 2D materials, there are new opportunities for spin-based logic, valley-polarized electronics and photonics, and single photon emitters for quantum information. The advent of spin field effect switches in graphene/TMD heterostructures, monolayer ferromagnets, long valley lifetimes of holes and indirect excitons, and robust single photon emission from defects in h-BN are among the recent new discoveries that fuel the excitement for 2D materials research and their potential applications.

PCSI

Room Keauhou II - Session PCSI-WeM

Nanowires I/Nanowires II/Topological Properties I/Optical Studies of 2D Materials

Moderators: Ezekiel Johnston-Halperin, The Ohio State University, Paulina Plochocka, LNCMI, CNRS, Nicholas Harmon, University of Iowa

8:30am **PCSI-WeM-1 Bottom-up Grown Nanowire Quantum Devices***, **Erik Bakkers,*** Eindhoven University of Technology, Netherlands **INVITED**

InSb nanowires are used to detect first signatures of quasi particles called Majorana fermions.Recently, different schemes for performing braiding operations and uncovering the non-Abelian statistics of Majorana fermions are proposed. Such operations are fundamental for topological quantum computing. For such a universal computational architecture the realization of a near-perfect nanowire network assembly is needed in which Majorana states are coherently coupled.

Here, we demonstrate a generic process by which we can design any proposed braiding device by manipulating an InP substrate and thereby the nanowire growth position and orientation [1]. This approach combines recent advances in materials growth and theoretical proposals. Our method leads to highly controlled growth of InSb nanowire networks with single crystalline wire-wire junctions. Additionally, nanowire “hashtag” structures are grown with a high yield and contacted. In these devices, the Aharonov–Bohm (AB) effect is observed, demonstrating phase coherent transport. These measurements reveal the high quality of these structures. This generic platform will open new applications in quantum information processing. Furthermore, these structures are well suited for epitaxial shadow growth of a superconductor on the nanowire facets. We study the growth of superconductors on nanowires and reveal the electronic properties.

9:00am **PCSI-WeM-7 Dopant Profiling in Semiconductor Nanowires by Atom Probe Tomography***, A Rodil, R Plantenga, S Kolling, A Cavali, A Li, D Car, S Gazibegovic, E Bakkers, **Paul M. Koenraad,*** Eindhoven University of Technology, Netherlands

The controlled incorporation of doping atoms is essential for nearly all semiconductor devices. Devices such as transistors, light-emitting diodes, solar cells etc. are all impossible without the application of doping atoms that locally control the Fermi-level and the internal potential landscape. Nanowires comprise a relatively new class of highly interesting 3D semiconductor nanostructures in which doping also plays a crucial role. Due to their small size and special geometry it is very difficult to determine doping profiles in a straightforward manner by techniques such as SIMS and EDX. Also cross-sectional STM, which has an unprecedented capacity to determine the distribution of doping atoms in semiconductors is unfortunately not yet readily applicable for the study of doping atoms in nanowires.

At present the best and probably only technique that allows addressing this problem is Atom Probe Tomography. We have developed an improved approach [1] in which we have been able to measure doping concentrations with Atom Probe Tomography down the ppm-level or a doping level slightly below 10^{17} atoms/cm^3. We have used this approach to examine Si (n-type) and Zn (p-type) doped InP nanowires and have been able to extract the doping profiles and check the dopant incorporation efficiency, see Figure 1a. Measurements like these allow to determine the doping efficiency. We noticed that this can vary from nanowire to nanowire and that at high doping concentrations the growth of the nanowire can become unstable. Under these conditions a strong local variation of the doping concentration can occur resulting in dopant clusters, see Figure 1b. Finally we have used the Atom Probe Tomography technique to analyze details in the doping profiles that allow us to retrieve important details in the incorporation process of doping atoms in nanowires. Figure 2 shows an example of a Si doping profile along the growth axis of the nanowire. The length and the height of both doping segments was supposed to be equal but as shown strong deviations can occur. Finally we have used Atom Probe Tomography to determine the background impurity level in core/shell GaP/Si nanowires.

[1] S. Koelling, et al, “Atom-by-Atom Analysis of Semiconductor Nanowires with Parts Per Million Sensitivity” Nano Letters DOI: 10.1021/acs.nanolett.6b03109.

9:05am **PCSI-WeM-8 How Can Band Offsets in III-V Nanowires be Determined Correctly by Scanning Tunneling Spectroscopy?***, **Philipp Ebert,*** Forschungzentrum Jülich, Germany*; P Capiod,* ISEN*; T Xu,* Shanghai University, China*; M Wei, A Díaz Álvarez, X Han, D Troadec,* ISEN*; J Nys, M Berthe,* ISEN, France*; G Patriarche,* LPN-CNRS*; L Lymperakis, J Neugebauer,* MPIE*; I Lefebvre,* ISEN*; S Plissard,* LAAS-CNRS*; P Caroff,* Cardiff University, UK*; R Dunin-Borkowski,* Forschungzentrum Jülich, Germany*; B Grandidier,* ISEN, France

Scanning tunneling microscopy (STM) and spectroscopy (STS) allow a unique high resolution insight simultaneously into the structural and electronic properties of III-V semiconductor nanowires (NWs). Particularly interesting are heterostructured NWs with interfaces between different polytypes or different materials. Since the carrier transport through such NWs is expected to be affected by different band gaps and band offsets, the accurate determination of these values are critical. Although STM and STS is presented as the ideal technique for this, we demonstrate that STS measurements (and possibly other measurement techniques) are mostly wrongly interpreted and it is thus unclear if any of the published band offset values is reliable.

In this presentation we demonstrate that sidewall surfaces of III-V NWs regularly ex-hi-bit high step densities (or surface states as for III-nitrides), which induce a pinning the Fermi energy within the band gap. The pinning level is, however, different on every polytype or on every material. Hence, the relative band edge positions between different types of NW segments are extrinsically determined by the different pinning levels, but not by the intrinsic band offsets. Furthermore, extrinsic band offsets turn out to be much larger than intrinsic one. Hence, defect or surface states at the sidewall surface likely affect the carrier transport much stronger than intrinsic band offsets. Thus, it is of prime interest to determine pinning levels and extrinsic band offsets at the sidewall surfaces. We demonstrate these extrinsic band offsets using zincblende-wurtzite GaAs NW junctions.[1]

In order to nevertheless have experimental access to intrinsic band offsets, we developed a new methodology to determine accurate band offsets between different NW segments.[2] It uses a thin overgrown shell of a material with wider band gap. This allows electron tunneling through this thin shell directly into the core. The shell furthermore assures that the pinning of the overgrown and pure segments is identical. Then the differences between the band edge positions of both materials provide the correct band offset values. We applied this methodology to axial GaAs/GaAs$_{0.81}$Sb$_{0.19}$/GaAs heterostructure NWs.

[1] P. Capiod *et al*., Appl. Phys. Lett. **103**, 122104 (2013).

[2] T. Xu *et al*., Appl. Phys. Lett. **107**, 112102 (2015).

9:10am **PCSI-WeM-9 Lazarevicite-type short-range ordering in ternary III-V nanowires***, **Michael Schnedler,*** Forschungszentrum Jülich GmbH, Germany*; I Lefebvre,* Institut d'Electronique, de Microélectronique et de Nanotechnologie (IEMN), France*; T Xu,* Shanghai University, China*; V Portz,* Forschungszentrum Jülich GmbH, Germany*; G Patriarche,* Université Paris-Saclay, France*; J Nys,* ISEN, France*; S Plissard,* LAAS-CNRS*; P Caroff,* Cardiff University, UK*; M Berthe,* ISEN, France*; H Eisele,* Technische Universität Berlin, Germany*; R Dunin-Borkowski, P Ebert,* Forschungszentrum Jülich, Germany*; B Grandidier,* ISEN, France

Stabilizing ordering instead of randomness in alloy semiconductor materials is a powerful means to change their physical properties. We used scanning tunneling (STM) and transmission electron microscopy to reveal the existence of an unrecognized ordering in ternary III-V materials. The lazarevicite short-range order (SRO), found in the shell of InAs$_{1-x}$Sb$_x$ nanowires (NW), is driven by strong Sb-Sb repulsion along ⟨110⟩ atomic chains during Sb incorporation on unreconstructed {110} sidewalls. A preferred formation of lazarevicite SRO under group-III-rich growing conditions is found as shown by the pair correlation function c(x,y) and supported by our DFT calculations. Based on these observations, we present a growth model that offers the prospect to broaden the limited classes of ordered structures occurring in III-V semiconductor alloys. [1]

[1] M. Schnedler *et al.*, Phys. Rev. B **94**, 195306 (2016)

9:15am **PCSI-WeM-10 III-V Nanowire Devices: A 3D Toolbox with Contact, Interface, and Heterostructure Engineering***, **Erik Lind,** L Wernersson,* Lund University, Sweden **INVITED**

III-V nanowires are attractive for device applications. The small nanowire footprint reduces the number of propagating defects opening a path for integration of high-quality III-V materials on Si. The direct band gap and the wide range of wave lengths addressable makes the material suitable for optoelectronic applications including light emitting diodes, solar cells, and long wave length photodetectors. The advantageous transport properties find usage in transistors applications where the reduced scattering enhances the drive current. However, for the realization of these devices, processing strategies needs to be developed and the material carefully characterized to avoid detrimental parasitic effects on the device performance.

In this talk, III-V nanowire MOSFETs [1] and TunnelFETs [2] will be presented. State-of-the-art performance in terms of transconductance (g_m), drive current (I_{on}), subthreshold swing (S), and off-state leakage current (I_{off}) will be demonstrated. In particular, we will focus on InAs/InGaAs MOSFETs and InAs/InGaAsSb/GaSb TunnelFETs, where the nanowire growth technology allows for incorporation of materials with strong lattice mismatch into the transistor channel.

The transistor processing relies on understanding and control of the physics and chemistry at the transistor interfaces. Examples will be given including vertical TLM structures developed to evaluate the specific contact resistance [3]. Furthermore, a vertical gate-last process has been established to align the gate to the edges of the source and drain contact regions reducing access resistance [4]. The semiconductor/high-*k* interface has finally been evaluated and the growth and process technology optimized to reduce both interface state and border trap state densities [5].

[1] O.-P. Kilpi, et al Vertical InAs/InGaAs Heterostructure Metal–Oxide–Semiconductor Field-Effect Transistors on Si Nano Lett., (2017)

[2] E. Memisevic, et al, Individual Defects in InAs/InGaAsSb/GaSb Nanowire Tunnel Field Effect Transistors Operating below 60 mV/decade Nano Lett., 17, 4373 (2017)

[3] M. Berg, et al A transmission line method for evaluation of vertical InAs nanowire contacts Appl. Phys. Lett. 107, 232102 (2015)

[4] M. Berg, et al, Electrical Characterization and Modeling of Gate-Last Vertical InAs Nanowire MOSFETs on Si IEEE Electron Dev. Lett., 37, 966 (2016)

[5] J. Wu, et al Low Trap Density in InAs/High-k Nanowire Gate Stacks with Optimized Growth and Doping Conditions Nano Lett., 16, 2418 (2016)

9:45am **PCSI-WeM-16 The Zincblende/Wurtzite Interface in III-V Nanowires: Heterostructures with Atomically-abrupt Electronic Transition***, J Knutsson, S McKibbin, M Hjort, S Lehmann,* Lund University*; N Wilson, S Patel, C Palmstrom,* University of California, Santa Barbara*; K Dick,* Lund University*; A Mikkelsen,* ***Rainer Timm****,* Lund University, Sweden

III-V semiconductor nanowires (NWs) have a large technological potential within energy harvesting and (opto)electronics [1]. In addition, they provide a unique playground in materials science, since their small footprint allows the formation of a wide range of radial and axial heterostructures with changes in material composition, doping, or crystal phase. Recently, it became possible to purposely tune the crystal structure between Zincblende (Zb) and Wurtzite (Wz) phase over InAs or GaAs NW segments of varying length [2].

Here, we use low-temperature scanning tunneling microscopy and spectroscopy (STM/S) to monitor both the atomic surface structure and the surface local density of states (LDOS) across Zb/Wz interfaces in InAs NWs. The NWs include Zb and Wz segments of varying length, down to the shortest possible insertion of Zb phase in a Wz matrix, i.e. a Zb single bilayer stacking fault. We compare STS spectra obtained at As atoms in the stacking fault with spectra from As atoms located 1 nm, 3 nm, and 5 nm away from it. Thereby we find similar Wz LDOS signal further away and in close proximity to the stacking fault, while the stacking fault itself shows a clear Zb signature. These results demonstrate that the atomically sharp structural transition between Zb and Wz phase is accompanied by an equally abrupt electronic transition. In addition, we analyze conduction band and valence band onsets from STS results obtained at Wz segments with Zb inclusions of varying length. We obtain strong valence band offsets and a nearly flat conduction band, in agreement with previous results on extended Wz and Zb segments [3], and we observe confinement energies of up to 30 meV with decreasing length of the Zb segment.

Furthermore, we present initial tests on utilizing NWs with Wz and Zb segments for the creation of advanced 3D heterostructures with atomic precision: We expose GaAs NWs with both Wz and Zb segments to Sb and monitor the incorporation of individual Sb atoms in the surface due to Sb-for-As exchange reactions. Thereby we find a preferential incorporation of Sb in the Zb {110} surface facets, as compared to Wz {11-20} surface segments (see Fig. 1), which is also verified by density functional theory calculations [4]. Such preferential incor-poration, prior to subsequent radial overgrowth, opens up a path towards atomically thin quantum rings of tunable diameter and height.

[1] J. Wallentin et al., Science 339, 1057 (2013); E. Lind et al., IEEE J. El. Dev. Soc. **3**, 96 (2015).

[2] S. Lehmann et al., Nano Lett. **13**, 4099 (2013).

[3] M. Hjort et al., ACS Nano **8**, 12346 (2014).

[4] M. Hjort et al., Nano Lett. **17**, 3634 (2017).

9:50am **PCSI-WeM-17 Selective-area Epitaxy and Electronic Transport in in-plane InAs One-dimensional Channels***,* ***JoonSue Lee****, S Choi, M Pendharkar, A McFadden, C Palmstrøm,* University of California, Santa Barbara

One-dimensional (1D) semiconductor nanowire proximitized by a superconductor could exhibit topological superconducting phases, which host Majorana zero modes at the ends of the proximitized region. Based on the hybrid superconductor/1D nanowire systems, scalable designs for topological quantum computing processes by braiding of Majorana zero modes have been proposed [1]. Experimental efforts have been made to realize the complex nanostructures consisting of multiple Majorana zero modes: bottom-up synthesis of self-assembled nanowire networks with predefined superconducting islands has been recently reported [2], and top-down processing of the large-scale nanostructures has been suggested on a two-dimensional material platform of epitaxial superconductor/semiconductor heterostructures [3].

In this work, we study a new bottom-up approach of selective-area growth of semiconductor 1D channel networks. This approach is advantageous for scalability and for minimizing damages from further fabrication processes. We employ chemical beam epitaxy to selectively grow in-plane InAs 1D channels on pre-patterned SiO_2/InP(001) substrates. For electronic transport, InAs Hall bars with channel width of 50-500 nm and length of 500–2000 nm are selectively grown and measured with a perpendicular magnetic field at cryogenic temperatures. In order to achieve optimal transport properties, we vary 1) substrate preparation process, 2) growth conditions, such as substrate temperature, growth rate, and V/III ratio, 3) 1D channel dimensions of width and height, 4) crystallographic orientations, 5) buffer layers, and 6) capping layers. The resulting electron mobility is observed up to a few thousand cm^2/Vs with electron density of low 10^{12} cm^{-2}. Magnetoresistance also reveals universal conductance fluctuations and weak antilocalization. Further transport studies of electrostatic gating and Aharonov-Bohm oscillations will be discussed.

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9:55am **PCSI-WeM-18 Writing Gallium Oxide on GaN Nanowires With The AFM Tip***,* ***Jovana Colvin****, R Ciechonski, J Ohlsson, A Mikkelsen, R Timm,* Lund University, Sweden

Superior inherent properties of gallium nitride (GaN) semiconductor nanowires (NWs) such as defect free nature, high surface to volume ratio, wide band gap, large break-down voltage, high electron saturation velocity and mobility, high-temperature operation make them highly promising for the future metal-oxide-semiconductor (MOS) based high power and high temperature devices. However, much work will have to be done in order to achieve high quality gate oxide. Gallium (III) oxide, the native oxide of GaN, has a potential of fulfilling the aforementioned requirement [1].

Here, we study a continuous GaN film formed from GaN NWs [2]. The NWs are grown first at a low V/III ratio (1:1), and radially overgrown using a high V/III ratio on the order of 1000:1. Amplitude-modulated atomic force microscopy (AFM) characterization shows that the top c-plane of the NWs is defect free. In addition, we simultaneously monitor topography and conductivity of the GaN film. In agreement with the intended doping levels, we find significant conductivity only at the position of the GaN cores. Importantly, we observe both a height increase (see Fig. 2) and a drop in conductivity at the GaN cores upon imaging the film with a bias of 6 V or more applied between the sample and the AFM tip. This demonstrates that we can locally induce a thin gallium oxide barrier over the GaN cores, where the rest of the surface is unaffected, see Figure 2. We will present a systematic investigation of the oxide thickness as a function of growth parameters, as well as the tip loading force and applied voltage and polarity.

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10:00am **PCSI-WeM-19 Recombination processes and localization effects in GaNAsP Recombination Processes and Localization Effects in GaNAsP Nanowires***, M Jansson, S Chen,* Linköping University, Sweden*; R La,* University of California, San Diego*; J Stehr,* Linköping University, Sweden*; C Tu,* University of California, San Diego*; W Chen,* ***Irina A. Buyanova****,* Linköping University, Sweden

The GaNAsP material system, belonging to the family of dilute nitride alloys, has shown significant promises as a candidate for intermediate band solar cells (IBSCs), due to its high band gap tunability and an attractive band structure. Owing to very recent advances in fabrication techniques, it has become possible to fabricate GaNAsP in the nanowire (NW) geometry, which may reduce costs for device fabrication and also opens a door for integration of the IBSC concept with the promising NW architecture.

In this work we perform systematic optical studies of such novel GaNAsP NWs grown by molecular beam epitaxy on Si substrates, combined with comprehensive structural characterization of the wires. Based on the performed transmission electron microscopy and Raman studies, we show that the fabricated NW arrays have good structural and optical quality, in spite of a large difference in electronegativity and sizes between N and replaced As/P atoms. The arrays are also found to exhibit excellent compositional uniformity among individual wires. Based on temperature-dependent photoluminescence (PL) studies, we show that random alloy disorder causes localization of photo-generated carriers at low temperatures. The localization potential increases in N-containing wires as compared with reference GaAsP NWs. In some regions, it leads to three-dimensional carrier confinement, based on the observation of sharp and discrete PL lines in ⍰-PL spectra from individual NWs. Localization effects, however, are found to have negligible influence on carrier recombination at room temperature (RT) owing to thermal activation of the localized carriers to extended states. From time-resolved PL measurements, the prolonged roomtemperature carrier lifetime at RT was found in N-containing wires. As the carrier lifetime under these conditions is typically governed by non-radiative recombination via surface states, this finding implies N-induced suppression of surface recombination. The presented results, therefore, show that GaNAsP NWs hold great promises for future applications of this material system in nano-optoelectronic and photonic devices.

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11:00am **PCSI-WeM-31 Quantum Anomalous Hall Effect in the Magnetic Topological Insulator Thin Films***, **Cui-Zu Chang**,* The Pennsylvania State University **INVITED**

The quantum anomalous Hall (QAH) effect can be considered as the quantum Hall (QH) effect without external magnetic field, which can be realized by time reversal symmetry breaking in a topologically non-trivial system [1, 2]. A QAH system carries spin-polarized dissipationless chiral edge transport channels without the need for external energy input, hence may have huge impact on future electronic and spintronic device applications for ultralow-power consumption. The many decades quest for the experimental realization of QAH phenomenon became a possibility in 2006 with the discovery of topological insulators (TIs). In 2013, the QAH effect was observed in thin films of Cr-doped TI for the first time [3]. Two years later in a near ideal system, V-doped TI, contrary to the negative prediction from first principle calculations, a high-precision QAH quantization with more robust magnetization and a perfectly dissipationless chiral current flow was demonstrated [4]. In this talk, I will introduce the route to the experimental observation of the QAH effect in aforementioned two systems [3, 4], and discuss the demonstration of the dissipationless chiral edge state as well as the origin of the dissipative channels in the QAH state [5]. Finally I will talk about our recent progress on the QAH insulator-Anderson insulator quantum phase transition and its scaling behaviors [6].

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11:30am **PCSI-WeM-37 Molecular Beam Epitaxy of Near Surface $InAs_xSb_{1-x}$ Quantum Wells for Topological Quantum Computation***, **Mihir Pendharkar**, J Lee, A McFadden, C Palmstrom,* University of California, Santa Barbara

Topological quantum computation based on Majorana Zero Modes (MZMs) promises to be a reliable approach to fault tolerant quantum computation.[1] MZMs, created at the interface of a 1D chain of electrons with an s-wave superconductor, on application of an in-plane magnetic field, are predicted to be protected from external perturbations by the size of the topological energy gap, thus induced.[2] The size of this energy gap, can be increased by increasing the spin-orbit coupling and mobility of the semiconductor host.

In this work, we report on the Molecular Beam Epitaxy (MBE) growth of near surface, inverted, $InAs_xSb_{1-x}$ (0.4>x>0.2) quantum wells strained to $Al_{0.3}InSb$ barrier layers and compare them to InAs and InSb quantum wells. Due to band gap bowing, certain compositions of $InAs_xSb_{1-x}$ (centered around x ≈0.36) are predicted to have a higher g-factor and lower electron effective mass than either of the constituent binary compounds of InAs and InSb. Such compositions of InAsSb are hence ideal candidates for hosting MZMs providing a substantial enhancement in the topological protection. Near surface inverted QW structures with the doping layer below the 2DEG, are necessary for effective top gate control and transparent coupling to an epitaxial superconductor layer above the QW. While previous work has demonstrated MZMs in InAs and InSb nanowires and InAs QWs, demonstration of a near surface 'inverted' InAsSb QW to host MZMs had remained a challenge.

These structures were grown on GaSb and InSb substrates to study the effect of interfacial strain (compressive from GaSb and tensile from InSb) on the effective mass of electrons in the 2DEG. This work is also believed to be the first demonstration of an InAsSb QW on an InSb substrate allowing for hetero-epitaxy with drastically reduced lattice mismatch as compared to GaSb and GaAs.

The depth of the quantum well from the surface was also varied to study the effect of surface pinning on the 2D electron density. The surface of InAs is believed to be pinned at 0.2eV above the conduction band minima (electron accumulation) while InSb surface is believed to be pinned mid-gap (~0.12eV below the conduction band minima). A systematic reduction in sheet carrier density was observed with reducing depth from the surface, which also correlated to a reduced doping efficiency of n-type dopants near the surface, indicating the presence of a surface depletion layer.

This understanding of the surface pinning and the first demonstration of InAsSb QWs on InSb substrates is now expected to provide a new platform for the measurement of MZMs and consequent development of InAsSb based robust topological quantum networks.

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11:45am **PCSI-WeM-40 Exploring the Bright Side and the Dark Side of Excitons in Atomically-thin Transition Metal Dichalcogenides***, **Alex High**,* University of Chicago **INVITED**

In this talk, we will explore fundamental properties of bright and dark exciton transitions in Transition Metal Dichalcogenides (TMDs). On the bright side, we will probe a simple question: can TMDs act as an atomically-thin mirror at the bright exciton resonance? Such an experimental realization places a stringent demand on the excitons – the radiative linewidth should dominate the total transition linewidth, a criteria rarely fulfilled in solid-state systems. Remarkably, we observe resonant reflection of up to 85% of incident light from a monolayer of $MoSe_2$, indicating that the radiative decay rate of excitons can be up to an order of magnitude larger than the non-radiative and dephasing rates. Furthermore, we demonstrate that these mirrors can be electronically switched, and exhibit strong power-and wavelength-dependent hysteresis. On the dark side, because of strong spin-orbit coupling the lowest-energy excitonic states in some TMD monolayers (such as WSe_2 and WS_2) involve nominally spin-forbidden optical transitions and are thus optically dark. Probing and understanding these dark excitons provides crucial insights into the fundamental properties of TMD monolayers, however their presence typically can only be inferred through indirect measurements. We will introduce a method for probing the optical properties of two-dimensional

(2D) materials via near-field coupling to surface plasmon polaritons (SPPs). This coupling selectively enhances optical transitions with dipole moments normal to the 2D plane, enabling direct detection of dark excitons in TMD monolayers. When a WSe_2 monolayer is placed on top of a single-crystal silver film, its emission into near-field-coupled SPPs displays new spectral features whose energies and dipole orientations are consistent with dark neutral and charged excitons.

12:15pm **PCSI-WeM-46 Structure and Peierls Transition of the Indium/Si(111) 1D Model System: A Microscopic View from Raman Spectroscopy***, **Norbert Esser**, E Speiser, S Chandola,* Leibniz-Institut für Analytische Wissenschaften-ISAS e.V., Germany*; S Wippermann,* Max-Planck-Institut für Eisenforschung, Germany*; S Sanna,* 3Institut für Theoretische Physik, Justus-Liebig-Universität, Germany*; W Schmidt,* Universität Paderborn, Germany

Raman spectroscopy can be used for the analysis of surface structures by recording surface confined vibrational modes. In recent years we have demonstrated for various clean and adsorbate modified semiconductor surfaces that the related Raman signals are a general feature of solid surfaces [1], which does not depend on plasmonic/chemical Raman enhancement like for SERS.

As one example of a 1D surface structure, In nanowires on Si(111) have been analysed thoroughly by Raman spectroscopy [2]. In/Si(111) is an one-dimensional metallic nanostructure which undergoes a Peierls transition into an insulating structure upon cooling below 125K. We have recorded surface specific phonon spectra related directly to the atomic nanowire structures above and below the phase transition temperature. By performing ab-initio calculations of the structures and their vibrational properties we are able to assign Raman lines to individual surface phonon modes and verify atomic structure models. Moreover, we can follow the Peierls transition and find a clear indication of phonon softening of some particular modes, associated with a first order phase transition in the 1D-nanostructures. A microscopic picture of the whole process is achieved from ab-initio DFT based calculations.

Moreover, in 1D systems collective modes (phason, amplitudon), should arise as characteristic excitations of the correlated electron system. Such excitations have been observed with Raman spectroscopy in other correlated systems [3,4] and should also appear in the In/Si nanowire Raman spectra. We discuss the spectral signatures of such excitations in the surface Raman spectra and also their microscopic origin as a coupled electronic/vibronic excitations.

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12:20pm **PCSI-WeM-47 Charge Transfer Dynamics in Graphene-Inorganic 'hybrids' with Transition Metal Oxides Using In-Situ Raman Spectroelectrochemistry***, **Sanju Gupta**, S Carrizosa,* Western Kentucky University

We report on the electrochemical assembled two- and three-dimensional graphene variants with nanostructured cobalt oxide (CoO and Co_3O_4) polymorphs that synthesize hybrids with optimal loading and chemical attachment of cobalt oxides micro/nano particles on the functionalized graphene surface, creating tailored interfaces crucial to electrochemical property enhancement. In-situ Raman spectroscopy integrated with electrochemistry was employed to investigate ion transport and charge transfer dynamics and to determine the concomitant electrochemical tuning of Fermi level. The variation of structural bonding in these hybrids dipped in aqueous alkaline electrolyte (*e.g.* KOH) with electrochemical biasing was monitored. It is because Raman spectroscopy can detect changes in graphene/metal and graphene/metal oxide bond through various spectral features. Two of the transverse optical phonons and corresponding longitudinal optical (LO) phonons of Co_3O_4 (and CoO) above 500 cm^{-1} are observed depending on the surface morphology and particle size as well as carbon-carbon bonding via G and 2D bands at 1590 cm^{-1} and 2670 cm^{-1}, respectively. Consistent reversible and substantial variations in Raman intensity and band positions of these modes induced by electrode potential point at the fine and continuous tuning, indicative of emptying/depleting or filling of the specific bonding and antibonding states which become electroactive. The results were explained in terms of changes in the electron density of states arising due to alterations in the overlap integral of bonds between the s and p (and d)orbitals of the adjacent carbon and metal oxide atoms. We estimated the extent of variation of the absolute potential of the Fermi level and overlap integral between the nearest-neighbor atoms from modeling the electrochemical potential dependence of Raman intensity thus corroborating the synergistic coupling of graphene and cobalt oxide polymorphs. The interplay of heterogeneous basal and edge plane sites graphene and crystalline spinel cobalt oxides reinforce density of states in the vicinity of Fermi level and efficient interfacial electron transfer. We acknowledge KY NSF EPSCOR RSP, WKU Research Foundation and Graduate School internal awards in parts for financial support.

12:25pm **PCSI-WeM-48 Rydberg Excitons & Dielectric Environment Effects in Monolayer Semiconductors: Insight from High Magnetic Fields***, A Stier,* Los Alamos National Laboratory*; N Wilson,* University of California, Santa Barbara*; J Kono,* Rice University*; X Xu,* University of Washington*; **Scott Crooker**,* Los Alamos National Laboratory

Excitons in atomically-thin semiconductors necessarily lie close to a surface, and therefore their properties are expected to be strongly influenced by the surrounding dielectric environment. However, systematic studies exploring this role are challenging, in part because the most readily accessible exciton parameter—the exciton's optical transition energy—is largely *un*affected by the surrounding medium. In this work we show that the significant role of the dielectric environment on 2D materials can be directly revealed through its systematic influence on the *size* of the exciton, which can be measured via the diamagnetic shift of the exciton transition in high magnetic fields [1].

Using exfoliated Wse_2 monolayers affixed to single-mode optical fibers, we tune the surrounding dielectric environment by encapsulating the flakes with different materials [2] and perform polarized low-temperature magneto-absorption studies to 65 T. The systematic increase of the exciton's size with dielectric screening, and concurrent reduction in binding energy (also inferred from these measurements), is quantitatively compared with leading theoretical models based on the Keldysh potential for 2D materials. These results demonstrate how exciton properties and the free-particle bandgap can be tuned in 2D van der Waals heterostructures, via the surrounding dielectric environment. We also present recent 65T measurements of high-quality hBN/Wse_2/hBN structures that permit an unambiguous identification and quantification of excited *1s*, *2s*, *3s*, and *4s* Rydberg states of neutral excitons [3], which allows a direct measurement of exciton mass in 2D materials.

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PCSI

Room Keauhou II - Session PCSI-WeA

Fabrication and Processing/New Approaches to Epitaxy II/2D Surfaces III/Growth

Moderators: Patrick Lenahan, The Pennsylvania State University, Erik Lind, Lund University, Robert Wallace, University of Texas at Dallas

2:00pm **PCSI-WeA-1 Preparation and Characterization of Nanometer-thin Silicone Films for Dielectric Elastomer Transducers***, **Bert Müller**, B Osmani, T Töpper,* University of Basel, Switzerland

Nanometer-thin silicone films are essential components of low-voltage dielectric elastomer transducers and will, for example, play a vital role in future artificial muscles [1]. Organic molecular beam deposition (MBD) is a versatile technique to prepare silicone films under well-defined conditions [2,3], but the achievable growth rates of about 1 µm per hour are too low for the fabrication of multi-layer devices. Therefore, we have developed electro-spraying as an alternative deposition method with one or two orders of magnitude faster rates [4,5]. For the two approaches, spectroscopic ellipsometry (SE) has been employed for *in situ* monitoring the film's optical properties, the film thickness and the surface morphology during deposition and ultra-violet (UV) light irradiation. The derived quantities were verified by means of atomic force microscopy (AFM).

Subsequent to the silicone deposition and the cross-linking by UV light curing, Au has been deposited using MBD and sputtering. This deposition process was also quantitatively characterized using SE and controlled by means of the plasmonic fingerprints of the metal nanostructures [6]. The *ex situ* AFM measurements revealed well-known modulations characteristic for strained surface layers [7]. Recent nano-indentation tests have demonstrated that the Au-layers on the silicone near the critical stress regime hardly contribute to the overall elastic modulus and are, therefore, a sound basis for smart electrodes [8]. The nano-mechanical probing of the powered thin-film dielectric elastomer transducers evidenced the importance of the thickness homogeneity for such devices [9]. The function of planar thin-film dielectric elastomer transducers can be precisely determined taking advantage of the cantilever bending approach [10].

In conclusion, spectroscopic ellipsometry and advanced atomic force microscopy with nano-indentation capability enables us to thoroughly characterize the film morphology as well as the optical and local mechanical parameters of silicone and Au/silicone nanostructures.

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2:05pm **PCSI-WeA-2 Improving Interfacial Adhesion Between Active Material and Solid Electrolytes in Thin Film Supercapacitors***, S Ahmed, N Korivi, **Li Jiang**, B Oni,* Tuskegee University

Solid-state thin film flexible supercapacitors are of interest for emerging applications including portable and wearable electronics. Adhesion between the electrolyte (e.g. ionic conductor in a polymer matrix) and the active electrode material (e.g. carbon nanomaterial) is an important factor influencing the performance of the supercapacitor. Typically, discrete electrode and electrolyte layers are fabricated and held together by pressure clamps or mechanical vises to improve electrode-electrolyte interfacial adhesion [1, 2]. However, this approach complicates the packaging of the devices for practical applications. There is a need for simple and scalable alternatives to improve the quality of electrode and electrolyte interface.

We report a facile method for improving adhesion between electrolyte and active electrode material in solid-state supercapacitors. The method involves dispersing active electrode material in a solvent, and depositing the dispersion on the surface of a solid electrolyte. The solvent causes swelling of the polymer matrix of solid electrolyte, which results in the active material being partially embedded on electrolyte surface. This allows for enhanced adhesion between the electrode and electrolyte. The choice of solvent in the electrode material dispersion is influenced by the polymer matrix used in the solid electrolyte. The method reported here has been used to develop a flexible, solid-state thin film supercapacitor. This device was made by solution casting a dispersion of multi-walled carbon nanotubes (MWCNTs) and isopropyl alcohol (IPA) on one side of a solid electrolyte layer (composite of polyvinyl alcohol and phosphoric acid). The IPA swells the crosslinked PVA polymer matrix, and partially embeds the MWCNTs on the electrolyte surface. The process is repeated to fabricate an electrode layer on the other side of the electrolyte layer, resulting in a supercapacitor with an integrated structure. Consequently, there is no need for mechanical clamps to hold the structure together. Devices fabricated in this manner show capacitance of 1.8 F/g, with areal capacitance of 7 mF/cm^2. The energy and power densities are 0.25 Wh/kg and 1.25 kW/kg respectively. The devices are flexible and do not show appreciable degradation in performance over 2000 charge-discharge cycles and when operating at temperatures as high as 60˚C. Electrode-electrolyte interface characterization shows good adhesion between MWCNTs and solid electrolyte.

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2:10pm **PCSI-WeA-3 Physical and Chemical Modification of Graphene for High Capacitive Energy Storage***, **KwangBum Kim**,* Yonsei University, Republic of Korea

Graphene, a one-atom-thick, two-dimensional (2D) sp2 carbon structure, has attracted considerable interest as a next-generation electrode material. This can be attributed to a number of interesting properties of graphene, such as its good mechanical/chemical stability, high electrical/thermal conductivity, and a large surface area (over 2630 m2g-1) due to its high surface-to-volume ratio. The combination of these unique physical and chemical properties means that graphene has significant potential to act as either an electrochemically active material in itself or as a conductive carbon template suitable for use in energy storage devices such as supercapacitors and Li-ion batteries.[1-4] At the same time, metal oxide/graphene nanocomposites are also of considerable interest for electrochemical energy storage applications owing to their outstanding properties. These excellent properties of metal oxide/graphene nanocomposites are generated from synergistic combination of graphene with metal oxide on the nanometer scale.[5-9] In this study, we report on the physical and chemical modification of graphene for energy storage applications.

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2:15pm **PCSI-WeA-4 Interface Analysis and Phase Transition of HfO_2 Film on Si Substrate after Thermal Treatment***, **Hassan Siddique**, D Rucheng, W Zhongping, D Zejun,* University of Science and Technology of China, China*; Z Zengming,* University of Science and Technology of China, Hefei, Anhui, China

Hafnium oxide (HfO_2) thin films on Si (100) substrate was prepared by radio frequency sputtering technique. XRD patterns show that the grown films are amorphous and transform into stable monoclinic phase after annealing treatment[1]. The position and width of Raman modes vary nonlinearly with increasing temperature due to the anharmonic interaction of hafnium and oxygen [2]. XPS of the film reveals that no silicide is found after thermal treatment. However, Si_{2p} suggests the occurrence of a SiO_2 interface between HfO_2 layer and Si substrate[3-4]. Ellipsometry spectroscopy results show that amorphous HfO_2 thin films crystallize into a monoclinic phase in the range of 300- 400 °C. This observation is consistent with that of XRD and Raman spectroscopy at variable temperature. Thickness and refractive index of HfO_2 thin film are obtained by fitting ES parmeters. The total thickness of the HfO_2 thin film increases by 1.02 nm and refractive index decreases from 2.3 to 1.9 during the formation of the SiO_2 interface layer after thermal treatment. In this study, we investigated the temperature effects on the crystal structure, interface growth and optical properties of HfO_2 thin film. Furthermore, the correlations between temperature, interface growth, and optical properties have been established.

2:20pm **PCSI-WeA-5 Machine Learning for Process Development for Semiconductor and Nanotechnology Product R&D*, Mark Mueller,*** Georgia Institute of Technology

Machine Learning algorithms can be utilized to form analytic models for semiconductor or complex nanotechnology manufacturing processes. These serve as a means of mapping the process space for a manufacturing tool (such as metal deposition or oxide etch) within a manufacturing sequence. Methods described may also be extended to a “modules” or sequences of steps, such as deposition-lithography-etch-strip, and even to an entire manufacturing process.

To effectively leverage machine learning for data mining and inference formation, it is important to select variables or “attributes” for input, along with an output or predicted quantity for each set of inputs. This presentation describes how to construct an “X” matrix of inputs, along with how to process a “Y” matrix of outputs, where each row represents a wafer and each column represents an input/output variable.

Predictive modeling is compared to current methods of engineering and experiment execution. Typically, development data belongs to the engineer or group who runs an experiment, and the desired result is a report which provides technical progress or which may guide a business decision. Each experiment is designed around a particular focus, and “old” data lives in engineering notebooks or spreadsheets, while the “wisdom” derived lies in the reports and in professional experience of those involved. In contrast, by creating models based on continual collection of data, it is possible to mine this data with predictive models, such as classifier-based (example: in spec/out of spec) or regression-based machine learning algorithms.

Such models allow a thorough mapping of the process space for addressing challenges and future hardware/process development. Construction and continued extension of a model thus replaces the traditional approach of targeted experiments and design of experiments (DOE). Since the collection and analysis of data is a collaborative effort, this use of machine learning becomes a collaborative tool (such as Google Docs) where multiple team members may contribute.

Machine learning models may be utilized for more applications beyond process development. Such models can be used to measure differences between subsystems, for example, evaluating materials from different vendors or evaluating different power supplies. Machine learning can be leveraged to measure equivalence or non-equivalence between production tools within a high volume factory.

2:25pm **PCSI-WeA-6 Interlayer Assisted Growth of Polycrystalline Germanium on Silicon at Low Temperatures*, Naga Korivi,*** *N Nujhat, S Ahmed, L Jiang,* Tuskegee University*; K Das,* JBP Materials LLC

The growth of polycrystalline and heteroepitaxial germanium (Ge) on silicon (Si) is of interest for various electronic applications. Sputter deposition offers a simple and inexpensive process for deposition of homogenous Ge films on large-area substrates [1]. One challenge in growing high quality Ge on Si by sputtering method is the presence of native oxide on Si, formed during the pump down process. Also, the presence of excited and ionized oxygen created by plasma prior to Ge deposition can contribute to native oxide on Si. Our experimental observations indicate a native oxide of 1.5 - 2 nm thickness can form in the sputter chamber at mid-range vacuum ($\sim 10^{-6}$–10^{-7} Torr). This corresponds to observations made by others [2]. Some prior reports achieved high-quality heteroepitaxial Ge on Si by desorbing the native oxide from the Si substrate prior to sputtering of Ge [3]. The oxide desorption involves a high temperature in-situ anneal (> 1000 °C) in the sputtering chamber at ultra-high vacuum ($\approx 10^{-10}$ Torr). Desorption cannot be conveniently done in sputtering systems with a moderate vacuum. Also, desorption temperature is higher than the typical thermal budget for post-CMOS processing. It is relevant to investigate the growth of high-quality Ge films using a moderate pressure system without a high temperature step.

We report here a preliminary study of polycrystalline Ge film growth on Si by DC magnetron sputtering at moderate vacuum ($\sim 10^{-6}$ Torr) and at substrate temperature as low as 300 °C without a high-temperature in-situ oxide desorption step. Our approach involves the sputtering of a nanometer scale Si interlayer on the Si substrate, prior to Ge deposition. This is designed to disrupt the surface oxide on the Si substrate and ultimately assist the growth of high quality Ge on Si substrate. X-ray diffraction and Raman spectroscopic studies indicate the formation of polycrystalline Ge at 300 °C when Si interlayer is incorporated. Sputtering Ge on Si at 300 °C without a Si interlayer resulted in amorphous Ge. Prior studies have reported amorphous Ge on Si at 320 °C under similar sputtering process conditions, but without any interlayer [2]. Currently, the Ge/Si interfaces in this work are being characterized further by high resolution transmission electron microscopy.

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2:35pm **PCSI-WeA-8 Plasma-enhanced Atomic Layer Deposition of MoS_2: From 2-D Monolayers to 3-D Aligned Nanofins*, Ageeth Bol,*** Eindhoven University of Technology, Netherlands **INVITED**

Plasma-enhanced atomic layer deposition (PE-ALD) might prove to be a key enabler for tackling the current challenge of large-area growth of 2-D materials with wafer level uniformity and digital thickness controllability. In this contribution, we have implemented PE-ALD to synthesize large-area WS_2 and MoS_2 thin films with tuneable morphologies i.e. in-plane and vertically standing nano-scale architectures on CMOS compatible SiO_2/Si substrates. The large scale 2D in-plane morphology has potential applications in nanoelectronics, while the 3D nanofin structures could be ideal for catalysis applications such as water splitting.

The PE-ALD process was characterized over a wide temperature range between 150°C - 450°C by using a combination of a metal organic Mo or W precursor and a $H_2S + H_2 +$ Ar plasma as the co-reactant. The use of plasma species as reactants allowed for more freedom in processing conditions and for a wider range of material properties compared with the conventional thermally driven ALD. The number of layers in the resulting films could be controlled accurately down to a mono-layer just by tuning the number of ALD cycles. HAADF TEM analysis of the showed that during the initial ALD cycles, MoS_2 islands expeditiously extended in the lateral direction and merged to form a film which continued to grow in a layer-by-layer fashion until a certain thickness. Thereafter, an aligned out-of-plane growth mode started to dominate as shown by cross-sectional TEM analysis. The origin of this transition from in-plane to out-of-plane growth mode might be attributed to the enhanced precursor adsorption on high surface energy locations such as grain boundaries, kinks or ledges. Due to crowding effects at these favourable adsorption sites subsequent vertical growth of MoS_2 is observed.

We show that the in-plane grown 2D structures can be successfully applied in electronic devices, while the 3D aligned fins a very suitable catalysts for the Hydrogen Evolution Reaction. These results show that plasma enhanced ALD might be instrumental in realizing not only the large area growth of high-quality 2-D materials but can also be applied as a tool to control the morphology of thin films.

3:05pm **PCSI-WeA-14 Phase Control of Ga_2O_3 Films Grown by Atomic Layer Epitaxy**, *V Wheeler, N Nepal,* U.S. Naval Research Laboratory*; L Nyakiti,* Texas A&M University*; D Boris, S Walton, D Meyer,* ***Charles Eddy, Jr.,*** U.S. Naval Research Laboratory

Ga_2O_3 has attracted significant interest as an ultra-wide bandgap material for next generation high-power, high-temperature electronic device applications. While there are five polymorphs of Ga_2O_3, the β-Ga_2O_3 (monoclinic) is the most stable and most widely studied to-date. By comparison, the α-Ga_2O_3 phase is less energetically favorable but has a similar bandgap (5.3 eV) and a rhombohedral corundum crystal structure. The ability to attain this metastable state can encourage bandgap engineering between α-Al_2O_3 and α-In_2O_3 similar to other III-V alloys. In addition, Schottky barrier diodes made with α-Ga_2O_3 films have shown improved performance over both β-Ga_2O_3 and SiC [1], demonstrating the benefit of this polymorph in next generation devices. Here, we use atomic layer epitaxy (ALE) to produce high-quality, heteroepitaxial Ga_2O_3 films and demonstrate phase selectivity with variations in growth temperature, plasma chemistry and gas pressure.

ALE Ga_2O_3 films were grown on c-plane sapphire substrates in a Veeco Fiji 200 reactor. All films were produced using trimethylgallium and O_2 plasma precursors with pulse/purge times of 0.015s/10s and 10s/10s, respectively.

The growth temperature, plasma gas flow, and pressure were varied to assess their impact on resulting film crystallinity and phase composition. Independent of growth conditions, all films were crystalline and highly resistivity with Ga/O ratios between 0.68-0.70 and no indication of C contamination by XPS.

Decreasing chamber pressure an order of magnitude during the plasma step drastically effected the resulting phase, yielding pure β-Ga_2O_3 at 80 mTorr and pure α-Ga_2O_3 at 8 mTorr. Additionally, at 350°C and 8 mTorr, the phase could be altered by a varying the O_2 plasma flow from 5-100 sccm. For these conditions, optical emission spectroscopy and ion flux measurements were made to correlate the impact of ions and other plasma species on the preferential promotion of different phases. By varying the growth temperature from 300 to 500°C at 8 mTorr, films went from mixed phase, to pure α-Ga_2O_3 at 350°C, to pure β-Ga_2O_3 at 500°C. High-quality β-Ga_2O_3 films were produced at 5sccm O_2 that had an RMS roughness of 0.38nm and XRD FWHM of 268 arc-sec for a 30nm film. At 40sccm, high-quality α-Ga_2O_3 films were obtained with an RMS roughness of 0.15nm and XRD FWHM of 250 arc-sec for a 30nm film. Thus, using ALE high-quality, phase selective films can be achieved to satisfy application requirements.

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3:10pm **PCSI-WeA-15 Low-temperature Homoepitaxial Growth of Two-dimensional Antimony Superlattices in Silicon***, **April Jewell**, A Carver, S Nikzad, M Hoenk,* Jet Propulsion Laboratory

Silicon-based imaging arrays have a variety of scientific and commercial applications, and are at the heart of NASA's optical space telescopes and instruments. Operation in space brings the challenge of dealing with radiation effects. For example, protons cause displacement damage within the silicon lattice, resulting in stable defects or "traps" within the device. Traps accumulate over time leading to increased dark current, hot pixels, and charge transfer inefficiency; adversely affecting performance and science return. JPL-invented delta-doped and superlattice-doped ("2D-doped") detectors offer high durability, high stability and high sensitivity to wavelengths spanning the UV, visible, and near IR spectral regions. Importantly, JPL's 2D-doped detectors offer a vast improvement in stability against damaging radiation over conventional devices.

For device passivation by 2D-doping, dopant concentrations in the range of 10^{13}-10^{14} cm^{-2} are typically used, and delta layers are confined to within a few nanometers of the surface. P-type doping with boron from an effusion cell is relatively straightforward. Boron evaporates as an atomic beam, and the small boron atoms incorporate with the silicon crystal lattice. Conversely, n-type doping of silicon using antimony presents many challenges, arising primarily from the tendency of antimony to segregate to the surface. This phenomenon can be avoided by employing low temperature growth to kinetically limit dopant segregation. However, this approach may compromise epitaxial growth (leading to amorphous layers) and often results in poor dopant incorporation and activation.

Despite these challenges, it has been shown that at sufficiently slow silicon deposition rates it is possible to maintain epitaxial growth for finite thicknesses even at low temperatures [1]. We previously reported on the low-temperature growth of antimony delta-doped silicon [2]. We demonstrated ~85% dopant activation, activated dose concentrations as high as 2×10^{14} cm^{-2}, and sharp dopant profiles (~35 Å FWHM). We also showed that the low temperature antimony delta-doping process is effective for passivating back-illuminated, high-purity, p-channel CCDs [3,4]. In this presentation, we will discuss the extension of our n-type delta doping capabilities to the growth of n-type superlattices. Electrical characterization and preliminary device measurements will be included.

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3:15pm **PCSI-WeA-16 Unraveling Atomic-level Self-organization at the Plasma-material Interface***, **Jean Paul Allain**, A Shetty, B Holybee, M Cheng, C Jaramillo,* University of Illinois at Urbana Champaign

The intrinsic dynamic interactions at the plasma-material interface and critical role of irradiation-driven mechanisms at the atomic scale during exposure to energetic particles require *a priori* the use of *in-situ* surface characterization techniques [1]. Characterization of "active" surfaces during modification at atomic-scale levels is becoming more important as advances in processing modalities are limited by an understanding of the behavior of these surfaces under realistic environmental conditions. Self-organization from exposure to non-equilibrium and thermalized plasmas enable dramatic control of surface morphology, topography, composition, chemistry and structure yielding the ability to tune material properties with an unprecedented level of control. Deciphering self-organization mechanisms of nanoscale morphology (e.g. nanodots, ripples) and composition on a variety of materials including: compound semiconductors, semiconductors, ceramics, polymers and polycrystalline metals via low-energy ion-beam assisted plasma irradiation are critical to manipulate functionality in nanostructured systems.

By operating at ultra-low energies near the damage threshold, irradiation-driven defect engineering can be optimized and surface-driven mechanisms controlled. Tunability of optical, electronic, magnetic and bioactive properties is realized by reaching metastable phases controlled by atomic-scale irradiation-driven mechanisms elucidated by novel *in-situ* diagnosis coupled to atomistic-level computational tools. In this work we present data *in-operando* the mechanisms responsible for low-energy (250-1000 eV) Ar, Kr and Ne irradiation of III-V semiconductors and Si nanopatterning. We conduct measurements of surface composition and chemistry with environmental XPS and low-energy ion spectroscopy (LEISS) illustrating the importance of *in-operando* and *in-situ* characterization of the surface and sub-surface regions from first ML down to about 10-nm. High-pressure low-energy ion scattering spectroscopy and mass spectrometry are also combined to elucidate mass redistribution and ion-induced desorption mechanisms at play during nanostructuring. Additional examples including ZnO nanoparticles on PDMS and nanopatterning of 70-nm TiO_2 thin films on biosensors are presented to illustrate *in-situ* PMI techniques.

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4:30pm **PCSI-WeA-31 Excitonic Linewidth Approaching the Homogeneous Limit in MoS_2 based Van der Waals Heterostructures***, **Xavier Marie**,* Institut National des Sciences Appliquées, LPCNO, France **INVITED**

Transition metal dichalcogenides such as MoS_2 and Wse_2 are layered materials that are semiconductors with a direct bandgap when thinned down to one monolayer (ML). The strong light matter interaction and the valley selective optical selection rules make these monolayers an exciting 2D material for fundamental physics and optoelectronics applications. But so far optical transition linewidths even at low temperature are typically as large as a few tens of meV and contain large inhomogeneous contributions [1].

In this work we show that encapsulation of ML MoS_2 in hexagonal boron nitride can efficiently suppress the inhomogeneous contribution to the exciton linewidth, as we measure in photoluminescence and reflectivity a FWHM down to 2 meV at T = 4 K [2]. Similar results are obtained with encapsulated $MoSe_2$, Wse_2 and WS_2 monolayers [3,4]. This indicates that surface protection and substrate flatness are key ingredients for obtaining stable, high quality samples. These encapsulated monolayerss allow accessing the optical and spin properties of these materials with unprecedented detail for neutral and charged excitons (trions).

Among the new possibilities offered by the well-defined optical transitions we evidence the optical selection rules for in-plane propagation of light. These studies yield a direct determination of the bright-dark exciton splitting, for which we measure 40 meV and 55 meV for Wse_2 and WS_2 monolayer, respectively [5]. The dark exciton fine structure is also revealed [6]. We also uncover new information on spin and valley physics and present the rotation of valley coherence in applied magnetic fields perpendicular to the ML [7].

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5:00pm **PCSI-WeA-37 Out-of-Plane Electromechanical Response of TMDs***, **Christopher Brennan**, K Koul, N Lu, E Yu,* University of Texas, Austin

The electromechanical properties of materials are inherently interesting for sensors, actuators, and energy harvesters in which deformation is coupled with electronic or optical properties. 2D materials offer a promising platform for such devices because when atomically thin, they can withstand large strains and strain gradients. Theory [1] and experiments [2, 3] have revealed that transition metal dichalcogides (TMDs) are intrinsically piezoelectric in-plane due to their lack of centrosymmetry in or close to the monolayer limit. Recently, we have shown that MoS$_2$ also exhibits an out-of-plane electromechanical response, potentially a result of the flexoelectric effect [4]. Theory suggests that flexoelectricity may depend on lattice constant, allowing for the opportunity to study the fundamental nature of the effect by looking at similar TMDs with varying lattice constants.

In this work, the out-of-plane electromechanical response of other monolayer TMDs is measured using piezoresponse force microscopy. A conductive atomic force microscope probe is used to apply an AC voltage across the sample and a lock-in amplifier is then used to measure the resultant deflection. Exfoliated WS$_2$ and WSe$_2$ are transferred onto gold for the measurements. Figure 1 shows optical images, topography, and piezoresponse (PR) amplitude and phase images for both WS$_2$ and WSe$_2$. Clear contrast between both TMDs and the underlaying gold in the PR images confirms that out-of-plane electromechanical coupling is present. Preliminary analysis suggests a correlation between the magnitude of the response and the lattice constant as indicated by the stronger contrast in the WS$_2$. A more detailed analysis of the results will be presented as well as their possible flexoelectric origin.

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$^+$ Author for correspondence: Edward T. Yu: ety@ece.utexas.edu

5:05pm **PCSI-WeA-38 Infrared Problem in Cold Atom Adsorption on Graphene***, **Dennis Clougherty,*** University of Vermont

There has been some controversy [1] concerning the phonon-assisted adsorption of atomic hydrogen to suspended graphene at low energies; one numerical calculation predicts an enhancement of the adsorption rate in comparison to the rate on graphite [2], while another work has argued for a suppression of adsorption [3]. Recent theoretical results of the adsorption rate of atomic hydrogen to suspended graphene are presented using four different methods that include contributions from processes with multiphonon emission. We compare the numerical results of the atom self-energy obtained by: (1) the loop expansion of the atom self-energy, (2) the non-crossing approximation (NCA) [4], (3) the independent boson model approximation (IBMA) [5], and (4) a leading-order soft-phonon resummation method (SPR) [6].

The loop expansion reveals an infrared problem, analogous to the infamous infrared problem in QED. The 2-loop contribution to the sticking rate gives a result that tends to diverge for large membranes. The latter three methods remedy this infrared problem for a membrane at zero temperature and give results that are finite in the limit of an infinite membrane. At finite temperature, the divergence problems are exacerbated; only SPR gives a finite adsorption rate in the limit of an infinite membrane. For micromembranes (sizes ranging 100 nm to .01 mm) at zero temperature, the latter three methods give results that are in good agreement with each other and yield sticking rates that are mildly *suppressed* relative to the lowest-order golden rule rate; however, the SPR sticking rate decreases to *zero* with increasing membrane size for all temperatures. Thus, approximations to the sticking rate are sensitive to the effects of soft-phonon emission for large membranes, and multiphonon processes suppress the rate.

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5:10pm **PCSI-WeA-39 Measuring and Modeling Liquid-Filled Nanobubbles Trapped by 2D Materials***, **Daniel Sanchez,** Z Dai,* The University of Texas at Austin*; P Wang,* The University of Texas at Austin, China*; A Cantu-Chavez, C Brennan, E Yu, R Huang, N Lu,* The University of Texas at Austin

Layered systems of van der Waals bonded two-dimensional (2D) materials are widely explored for new physics and devices. In many cases, 2D atomic layers are transferred on a foreign substrate, including other 2D materials. It has been extensively reported that nanometer-scale interfacial bubbles form spontaneously after the transfer. So far, there is no consensus on whether these nanobubbles are filled by liquid, solid, or gas.

We have carried out time-lapse atomic force microscopy scans on nanobubbles trapped between graphene and SiO2. The bubbles deflate slower than ideal-gas-filled 2D membranes over a course of 92 days indicating that liquid is likely trapped under the 2D membrane. We therefore develop a theoretical framework built upon the membrane equations for a thin, elastic membrane trapping incompressible liquid to form interfacial bubbles. Our final analytical solution suggests that adhesion between the 2D material and its substrate is related to the fourth power of the aspect ratio of the blister, which is a constant irrespective of the blister diameter. Our model is applied to estimate the adhesion energy of various 2D material interfaces using the experimentally measured aspect ratios of the bubbles. Good agreement between the estimated adhesion energies of graphene-SiO2 and MoS2-SiO2, and those reported in the literature substantiates our model. In conclusion, liquid-filled nanobubbles trapped by 2D materials can be used as a simple but generic metrology for the adhesion of 2D materials.

5:15pm **PCSI-WeA-40 Stress Relaxation Mechanism in the Si-SiO$_2$ System and its Influence on the Interface Properties***, **Daniel Kropman**, T Laas,* Tallinn University, Estonia*; V Seeman,* Tartu University*; A Medvids,* Riga University*; J Kliava,* Universityte de Bordeaux

It is known that internal mechanical stresses (IMS) due to the differences in the thermal expansion coefficients between films and substrates and lattice mismatch appear in the Si-SiO$_2$ system during the process of its formation and that point defects (PD) generation and redistribution could be used to reduce partially the surface stress. However, this process on the atomic scale is till not studied. The goal of the present report is to investigate the stress relaxation mechanism in the Si-SiO$_2$ system using EPR, IR absorption spectroscopy, scanning elektron microscopy (SEM) and samples deflection measurements. PD density and stresses in the Si-SiO$_2$ system were varied by oxidation condition (temperature, time, cooling rate, ambient) and by Si$_3$N$_4$ deposition on SiO$_2$. Different sign of the thermal expansion coefficient of the SiO$_2$ and Si$_3$N$_4$ on Si allow to modifay the IMS at the interface. It has been found that samples deflection decreases or increases simultaneously with EPR signal intensity depending on the oxidation condition (temperature).

At oxidation temperature 1100^{0}C the deflection of the samples(h) decreases with the increase of EPR signal intensity (vacancies),while at a oxidation temperature 1200^{0}C EPR signal (I) and deflection increase simultaneously. Those allows to suggest that at lower oxidation temperature PD (vacancies) reduce the tensil IMS in Si, while at higher oxidation temperature compressive IMS created PD in SiO$_2$ (E' centers).At an intermediate oxidation temperature tensil stresses in Si and compressive stresses in SiO$_2$ may be equal and compensate each others. It has been find that at oxidation temperature 1130^{0}C IMS at the Si-SiO$_2$. interface are lower than at 1100^{0}C and 1200^{0}C. Lower defect dencity on samples crossection microphotos obtained by SEM and PD dencity diminishing.in samples oxidized at 1130^{0}C confirmed thise suggestion.In Fig,2 the EPR signal and IR absorbtion line-width dependence on the oxidation time is shown. It can bee seen ,that EPR signal and IR absorbtion line-width at 1100 cm^{-1} dependence on the oxidation time (oxide thickness) is nonmonotonous and depended on the cooling rate .In slowly cooled samples the increase of the EPR signal is accompanied by the decrease of $\Delta\nu$ but,in fast cooled samples EPR signal and $\Delta\nu$ increase simultaneously with increase oxidation time.

Absent of the cooling rate influence on the PD density and $\Delta\nu$ dependence on the oxidation time at I(t) and $\Delta\nu$(t) dependence intersection points show, that IMS by an appropriate choice of the SiO$_2$ film thickness dissapear. The obtained results may bee explained by the PD generation kinetic model in the Si-SiO$_2$ system proposed by T.U.Tan and U.Gösele.

5:20pm **PCSI-WeA-41 Characterization of Barium Hexaferrite Thick Films Deposited by Aerosol Deposition with an *in situ* Magnetic Field*, Scooter Johnson,*** U.S. Naval Research Laboratory*; D Park,* Korean Institute of Materials Science*; A Hauser, S Ranjit, K Law,* University of Alabama*; H Newman, S Shin, S Qadri, E Gorzkowski,* Naval Research Laboratory

Devices utilizing magnetic materials such as circulators, inductors, and filters are critical components in many of today's electronics [1]. The need for ferromagnetic materials in these devices poses many difficulties for minimizing device size, weight, and cost. One issue that hampers integration of ferromagnetic materials is the high-melting temperature of the ferrite compared with the low-melting temperature component structure [2]. Furthermore, the need for low-loss and narrow bandwidth operation adds another significant barrier to the advancement of integration of ferromagnetic materials. The high-frequency operation regime and strong uniaxial anisotropy of barium hexaferrite ($BaFe_{12}O_{19}$, BaM) makes this material particularly interesting to utilize as an oriented film for microwave components. In this study, we characterize BaM films deposited onto sapphire by a room-temperature thick-film growth technique called aerosol deposition. We performed alternating gradient magnetometry depth studies on a series of as-deposited films that show a variation in magnetization with depth. Cross-sectional SEM images indicate laterally uniform film density. Electron dispersive spectroscopy of the interfacial region suggest significant Al_2O_3 mixing into the film volume. Fe XPS spectra indicate a change in peak weighting as a function of thickness, possibly indicative of modified structure or oxygen incorporation due to Al incorporation. To explore the possibility of magnetically orienting the films we deposited additional films in the presence of a 4 kOe static magnetic field. We report VSM, FMR, and XRD results of these films as-deposited and after sintering from 700C to 1000C. The Figure shows the results of VSM measurements of 5-um-thick films deposited with no applied field compared to films deposited in a 4 kOe applied field. The films deposited in the field presence show an increased saturation magnetization and remanence. Annealing improves the overall properties of the films further increasing the magentic orientation and saturation.

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5:25pm **PCSI-WeA-42 Surface Science Studies During Plasma-Assisted Atomic Layer Epitaxial Growth of InN on GaN Substrates*, Samantha Rosenberg,*** U.S. Naval Research Laboratory*; D Pennachio,* University of California, Santa Barbara*; V Anderson, S Johnson, N Nepal,* U.S. Naval Research Laboratory*; C Wagenbach,* Boston University*; M Munger,* SUNY Brockport*; A Kozen,* U.S. Naval Research Laboratory*; Z Robinson,* SUNY Brockport*; S Choi,* University of California, Santa Barbara*; J Hite,* U.S. Naval Research Laboratory*; K Ludwig,* Boston University*; C Palmstrøm,* University of California, Santa Barbara*; C Eddy, Jr.,* U.S. Naval Research Laboratory

III-N semiconductors such as GaN, AlN, and InN are the basis for creating many compound ternary and quaternary semiconductor materials well suited for applications in several important technological areas, including high current, normally-off power switches. [1-3] While atomic layer deposition (ALD) is a versatile technique and has gained wide use, it does not offer the required level of crystallinity and purity needed for high-performance III-N semiconductor devices. Therefore, we have developed a technique adapted from ALD, called low temperature plasma-assisted atomic layer epitaxy (ALEp). [2]Using surface science techniques we plan to develop a fundamental understanding of the ALEp growth process to further enable the method as a powerful new technique for growth of semiconductor materials.

Here we employ *in-situ* and *in-vacuo* surface studies of GaN substrate preparation and InN ALEp growth to advance fundamental understanding of the ALEp process as well as the effect of variation in nitrogen plasma pulse conditions on ALEp of InN. We conduct *in-situ* grazing incidence small angle x-ray scattering (GISAXS) experiments at the Cornell High Energy Synchrotron Source and The National Synchrotron Light Source-II at Brookhaven National Laboratory, utilizing morphological evolution monitoring to investigate the growth surface during sample preparation and film deposition, as well as using this technique to understand how the nitrogen plasma pulse affects nucleation and growth kinetics of InN on GaN substrate surfaces. GISAXS information is complemented with *in-vacuo* x-ray photoelectron spectroscopy and reflection high-energy electron diffraction studies conducted at the Palmstrøm Lab at UCSB, where we consider traditional molecular beam gallium flash-off [4] in contrast to our ALEp based gallium flash-off as ways to produce the most suitable GaN surface for our ALEp-based approach. We have been able to determine with GISAXS that ALEp based gallium-flash off experiments run at higher temperatures (500°C) produce a less roughened starting surface than lower temperatures. We have also determined with *in-vacuo* XPS that traditional molecular beam gallium flash-off greatly reduces the oxygen content at the GaN interface (<40% remaining), while our ALEp based approach does not reduce the oxygen as effectively.

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Wednesday Evening, January 17, 2018

PCSI
Room Keauhou II - Session PCSI-WeB
PCSI Banquet

7:30pm **PCSI-WeB-13 Dynamic Materials Inspired by Cephalopods***, **Alon Gorodetsky**,* University of California, Irvine **INVITED**

Cephalopods, such as the squid shown below in Figure 1, have captivated the imagination of both the general public and scientists for more than a century due to their visually stunning camouflage displays, sophisticated nervous systems, and complex behavioral patterns. Given their unique capabilities and characteristics, it is not surprising that these marine invertebrates have recently emerged as exciting models for novel materials and systems. Within this context, our laboratory has developed various cephalopod-derived and cephalopod-inspired materials with unique functionalities. Our findings hold implications for next-generation adaptive camouflage devices, sensitive bioelectronic platforms, and advanced renewable energy technologies.

PCSI

Room Keauhou II - Session PCSI-ThM

Topological Properties II/2D Surfaces IV/New Techniques II

Moderators: Xiaodong Xu, University of Washington, Hidemi Shigekawa, University of Tsukuba

8:30am **PCSI-ThM-1 A Valley Valve and Electron Beam Splitter in Bilayer Graphene***, J Li, R Zhang, Z Yin, J Zhang,* Penn State University*; K Watanabe, T Taniguchi,* National Institute of Materils Science, Japan*; C Liu,* ***Jun Zhu,*** Penn State University **INVITED**

Conventional CMOS field effect transistors control current transmission by controlling the charge of carriers. The advent of two-dimensional materials with hexagonal crystal symmetry offers a new electronic degree of freedom, namely valley, the manipulation of which could potentially be exploited to develop new paradigms of electronic applications dubbed “Valleytronics”. I will discuss our work on realizing a valley valve and tunable electron beam splitter in bilayer graphene[1][2].

In high-quality bilayer graphene, the application of a perpendicular electric field opens a tunable band gap, the sign of which can be reversed by reversing the polarity of the applied E-field. Theory predicts the existence of valley-momentum locked one-dimensional conducting channels at the artificial domain wall of two oppositely gapped bilayer graphene regions[3]. Known as the “kink states”, they are hallmarks of the quantum valley Hall effect. The helicity of the kink states can be controlled by the polarity of the applied E-field. This unique attribute allows the design of a novel valve and electron beam splitter, where electrically controlled transmission and guiding of the kink states at a four-way intersection have been proposed [4].

Here, we will show our experiments realizing the kink states in bilayer graphene and the operations of a waveguide, a valley valve and beam splitter. The conductance of the kink states exhibits well-developed plateaus with values close to the expected quantization of $4e^2/h$ at zero magnetic field. We will show the transmission of the kink states in the “on” state of the valve and the expected valley blocking effect in the “off” state of the valve. The on/off ratio is about 800% at B=0 and T=1.5 K. The control of the Fermi level in a magnetic field enables a chirality-based beam splitting mechanism. We demonstrate a continuous tuning of the splitting ratio from 0 to close to 100%. The high quality, in-situ electrical control, and scalabilty of the system open the door to many exciting opportunities in valleytronics and fundamental inquiries.

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9:00am **PCSI-ThM-7 Topological Phase Transition and Isostructural Phase Transitionin 1T-TiTe2 Single Crystal Under Pressure***, Z Zhang,* ***Min Zhang,*** University of Science and Technology of China, China

Trigonal TiTe$_2$ (1T-TiTe$_2$) has been studied for a few decades, showing some novel properties such as the enhanced superconductivity under uniaxial strain and the charge density wave (CDW) transition in monolayer form. However, there has been no experimental exploration for its high pressure behavior. In this work, the pressure-induced phase transitions were investigated by Raman scattering and electric resistivity for 1T-TiTe$_2$ single crystal under high pressure up to 17 GPa at room temperature. The result indicated that 1T-TiTe$_2$ single crystal undergoes three phase transitions at 1.7 GPa, 3 GPa and 8 GPa, respectively. The first-principles calculations manifest that the first two transitions at 1.7 GPa and 3 GPa are accompanied with the band inversion near Fermi level, from which parity analysis show two topological phase transitions occur here. Meanwhile, the structural distortion marked by the calculated c/a minimum was observed and proposed to induce the isostructural phase transition at 8 GPa. The observation of the two topological phase transitions and one isostructural phase transition for 1T-TiTe$_2$ single crystal under high pressure immensely enriches the physical understandings for this material family.

9:05am **PCSI-ThM-8 Chemical Potential Tuning and Strain Engineering in Topological Half-Heusler Thin Films***,* ***Shouvik Chatterjee****, J Logan, N Wilson, H Inbar, T Brown-Heft,* University of California, Santa Barbara*; A Fedorov,* Lawrence Berkeley National Lab*; C Palmstrøm,* University of California, Santa Barbara

Heusler compounds have emerged as an exciting material system where realization of functional and tunable novel topological phases might be possible [1-2]. PtLuSb is one such compound that has recently been shown to host topologically non-trivial surface states [3]. However, the chemical potential was found to lie below the Dirac point of the surface states, consistent with p-type Hall conductivity, in our thin films [4]. One way to shift the chemical potential above the Dirac point is to substitute a few of the platinum (Pt) atoms in PtLuSb with gold (Au), which has one more electron compared to Pt. We have successfully synthesized thin films of Au alloyed PtLuSb with different Au concentrations, up to 50% (Pt$_{0.5}$Au$_{0.5}$LuSb). Employing a combination of the techniques of angle-resolved photoemission spectroscopy via a UHV vacuum suitcase transfer and *in-situ* scanning tunneling spectroscopy along with *ex-situ* transport measurements we will provide evidence of our ability to tune the chemical potential via substitution alloying in Pt$_{x1-x}$LuSb thin films.

Furthermore, PtLuSb being a semimetal does not possess a bulk band gap. As a result, exotic transport and thermodynamic properties expected from topological surface states are often obscured by contributions from trivial bulk carriers. In this talk, I will present our efforts to address this issue by synthesizing compressively strained thin films on lattice mismatched substrate that is expected to lift the degeneracy of Γ_8 manifold, thereby opening a bulk band gap.

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9:10am **PCSI-ThM-9 Spin-dependent Processes of Interfacial Charge Transfer Excitons in Polymer-fullerene Solar Cells***, Y Puttisong, F Gao, Y Xia, I Buyanova, O Inganäs,* ***Weimin M. Chen,*** Linköping University, Sweden

Efficient solar energy conversion in bulk hetero-junction (BHJ) organic photo-voltaic devices relies on photo-generation of charges at the donor and accepter hetero-interfaces. An important requirement in further improving device efficiency is our understanding of the photo physics of interfacial charge transfer (CT) states - the precursors for charge generation, and their contributions to both charge generation and energy losses. Earlier studies have shown that spin and localization of the interfacial CT states play crucial roles in ultrafast charge generation and the subsequent recombination loss in polymer/fullerene blend systems. However, a direct proof for such roles on the microscopic level is still lacking.

In this work, we focus on the direct probing of the optically-excited lowest CT exciton states (CT$_1$) and their associated spin-dependent processes in a model polymer/fullerene solar cell based on TQ1/PCBM blends. By combining selective optical excitation and detection with the optically detected magnetic resonance (ODMR) technique, we are able to identify the triplet CT$_1$ states and the associated spin-spin interaction. With this, we estimate the electron-hole separation of the CT$_1$ exciton to be about 1 nm, within the physical dimension of a one-polymer-one-fullerene unit. The size of the CT$_1$ exciton is found to be identical in the blends regardless of the fullerene load and aggregation that are known to affect the degree of delocalization of CT excited states. We therefore conclude that the exciton localization of the CT$_1$ state is not responsible for the observed different efficiency of the solar cells with different fullerene loads. In addition, we provide direct evidence that CT$_1$ can mediate charge loss by facilitating intersystem crossing between the singlet and triplet of CT$_1$, trapping and bimolecular recombination of separated charges via CT$_1$, and electron back transfer from CT$_1$ to the polymer triplet. Interestingly, we also observe at the same time efficient charge generation via the CT$_1$ state. As such, we purpose a dual role of CT$_1$ in both charge loss and charge generation. We furthermore suggest the physical principle and possible pathways to turn CT$_1$ from a loss channel into a charge generation channel.

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9:15am **PCSI-ThM-10 2D Materials: Surfaces, Interfaces, and Defects***, **Robert Wallace,*** University of Texas at Dallas **INVITED**

The size reduction and economics of integrated circuits, captured since the 1960's in the form of Moore's Law, is under serious challenge. Current industry roadmaps reveal that physical limitations include reaching aspects associated with truly atomic dimensions, and the cost of manufacturing is increasing such that only 2 or 3 companies can afford leading edge capabilities. To address some of the materials physical limitations, "2D materials" such as graphene, phosphorene, h-BN, and transition metal dichalcogenides have captured the imagination of the electronics research community for advanced applications in nanoelectronics and optoelectronics. Among 2D materials "beyond graphene," some exhibit semiconducting behavior, such as transition-metal dichalcogenides (TMDs), and present useful bandgap properties for applications even at the single atomic layer level. Examples include "MX_2", where M = Mo, W, Sn, Hf, Zr and X = S, Se and Te

In addition to the potentially useful bandgaps at the monolayer thickness scale, the atomically thin layers should enable thorough electric field penetration through the channel, thus enabling superior electrostatic control. Further, with such thin layers, the integration with suitable gate dielectrics can result in a mobility enhancement. From an interface perspective, the ideal TMD channel material should have a dearth of dangling bonds on the surface/interface, resulting in low interface state densities which are essential for efficient carrier transport. The ideal TMD materials have much appeal, but the reality of significant densities of defects and impurities will surely compromise the intrinsic performance of such device technologies. This presentation will examine the state-of-the-art of these materials in view of our research on semiconductor device applications, and the challenges and opportunities they present for electronic and optoelectronic applications.[1]

This work is supported in part by the SWAN Center, a SRC center sponsored by the Nanoelectronics Research Initiative and NIST. It is also supported in part by Center for Low Energy Systems Technology (LEAST), one of six centers supported by the STARnet phase of the Focus Center Research Program (FCRP), a Semiconductor Research Corporation program sponsored by MARCO and DARPA, the US/Ireland R&D Partnership (UNITE) under the NSF award ECCS-1407765, and the Erik Jonsson Distinguished Chair.

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9:45am **PCSI-ThM-16 Synthesis, Properties and Tunability of Lateral 2D Heterostructures***, **Shruti Subramanian**, D Deng,* The Pennsylvania State University*; K Xu,* University of Pittsburgh*; N Simonson, K Wang,* The Pennsylvania State University*; J Li, R Feenstra,* Carnegie Mellon University*; S Fullerton-Shirey,* University of Pittsburgh*; J Robinson,* The Pennsylvania State University

Heterogenous combinations of two-dimensional (2D) layered materials provides us with an ability to tune properties tailored for specific applications. Transition metal dichalcogenides (TMDs) are attractive 2D materials in the "beyond graphene" realm of materials. Low resistance contacts are instrumental to utilize their unique electronic properties. Graphene is a promising candidate and has been shown to produce low-resistance contacts to a few TMDs[1] via manual stacking. We have developed a reproducible method to grow lateral heterostructures of graphene and TMDs like MoS_2, thus allowing for the graphene to be used like an "as-grown" near-Ohmic contact[2]. Here, we discuss electronic properties resulting from the interface of these as-grown lateral hetero-structures.

Cross sectional high-resolution transmission electron microscopy is able to demonstrate that the actual interface is a vertical overlap (a few hundred nms) of the MoS_2 onto the edge of the graphene pattern. The van der Waals stacking is maintained at the interface, leading to a pristine and unique combination, which allows for the reduced contact resistance to MoS_2 using graphene as the contacting material instead of conventional metals like Ti/Au. The flexibility of being able to tune the doping of the epitaxial graphene allows us to explore the option of type-matching the graphene contact to the TMD, thus reducing the barrier for electrons and making contacts much superior to conventional metals. This study also explores the impact of this interface in electronic band alignments via low energy electron reflectivity and temperature dependent current measurements.

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9:50am **PCSI-ThM-17 Surface Potential and Photoresponsive Behavior at Graphene-Metal Interfaces***, **Matthew DeJarld**, P Campbell, A Friedman, M Currie, R Myers-Ward, A Boyd, S Rosenberg, S Pavunny,* U.S. Naval Research Laboratory*; K Daniels,* University of Maryland*; K Gaskill,* U.S. Naval Research Laboratory

Graphene has remarkable photonic properties and, combined with its exceptional electronic transport properties, has led to a number of unique photonic devices.[1-3] Among these are photodetectors utilizing the photo thermoelectric effect, where devices are fabricated having metal contacts with differing work functions.[2,3] Yet, since metals contact-dope graphene, the (unintentional) formation of junctions at the edge of each contact may increase contact resistance as well as generate a photoresponse when illuminated. Despite the ubiquitous presence of metal junctions in all device types, little work exists that describes the behavior of non-noble metals on graphene. Hence, we present a preliminary study of the interactions between graphene and wide range of metals.

Here, we measure the work function, of a wide variety of metals deposited on monolayer epitaxial graphene synthesized on SiC. We find a discrepancy between the measured and reported work functions of metals traditionally considered to have low values, with the work function measured on graphene being consistently higher. We also characterize the films with photovoltage and Raman spectroscopy. For example, Yb films exhibit the strongest photovoltage response despite having a modest work function, and we identify several metals having significant adhesion issues to graphene. In addition, Eu films on graphene have unique phonon signatures with strong Raman peaks at high energies ($>1900 cm^{-1}$) in the spectrum. These peaks may be due to Eu-adsorption within the graphene lattice.[4] A closer look at the graphene-metal interface of Er films via Raman Spectroscopy (Fig. 1) shows evidence of disorder in the graphene lattice at the metal-graphene-air contact point, suggesting bonding with the graphene lattice may occur during oxidation. Such interactions are candidates to influence electronic transport across graphene-metal contacts.

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10:30am **PCSI-ThM-25 Force Measurement by Atomic Force Microscopy with a Molecular Tip at Low Temperature***, **Shigeki Kawai,*** National Institute for Materials Science, Japan **INVITED**

Recent progress in atomic force microscopy allows us to see inner structures of molecules adsorbed on surfaces [1]. In such measurements, a reactive metal tip is usually terminated by a small molecule or an inert rare gas atom. Such high-resolution imaging is beneficial to study single and self-assembled molecules as well as chemical reactions. Besides high-resolution imaging, force measurements became more reliable and even quantitative since the structure of the tip apex, at least the front-most-atom, can be controlled in experiment.

In this presentation, force spectroscopic measurements with different molecular tips (i.e. Xe-tip for van der Waals force detection [2] and CO-tip for the intermolecular bond detection [3]) will be discussed (Fig. 1). Besides the small atom and molecule, the tip can be also terminated with a large molecule or a polymer. By moving the tip vertically, we measured desorption phenomena of repeat polyfluorene units [4]. We found that the incommensurability between the unit length and the lattice distance plays a role in the friction. Since the fluorene units are connected to each other by a single bond, the incommensurability is not high. Using a stiffer material in-plane, a lower friction can be expected. In fact, the super lubricity was detected when graphene nanoribbon was slid on Au(111) [5].

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11:00am **PCSI-ThM-31 Local Deep Level Transient Spectroscopy Imaging for MOS Interface Trap Distribution***, N Chinone,* ***Yasuo Cho****,* Tohoku University, Japan

Physical properties of metal-oxide-semiconductor (MOS) interface are critical for semiconductor devices. There are several techniques for characterizing MOS interface properties. Deep level transient spectroscopy (DLTS) [1] is one of powerful techniques capable of macroscopic quantitative evaluation of trap density at/near MOS interface. But it is easily imagined that actual trap is not homogeneously distributed but has two dimensional distributions in atomic scale and even in mesoscopic scale. Therefore, it is very important to characterize MOS interface microscopically. Unfortunately, it is impossible to observe such inhomogeneity by using conventional macroscopic DLTS method.

In this paper, a new technique for local DLTS imaging using scanning nonlinear dielectric microscopy (SNDM) [2] is proposed. This method enables us to observe two dimensional distribution of trap density at/near MOS interface and is demonstrated with oxidized SiC wafer.

We measured three n-type silicon face (4°-off) 4H-SiC wafer samples on which 45-nm-thick thermal silicon dioxide film was formed. Two of them were followed by post oxidation annealing (POA) in nitric oxide ambient with different annealing conditions: (a) 10 min in 1250°C and (b) 60 min in 1150°C. We labeled the samples without POA, with POA in condition (a) and with POA in condition (b) as #S-45-1, #S-45-2 and #S-45-3, respectively. These three samples were scanned on 1.5×1.5mm^2 square area with a resolution of 30×30 pixels and analyzed using the proposed local DLTS method. By analyzing the acquired images, time-constant and magnitude of transient capacitance response were obtained at each pixel. As shown in Figure 1, highest brightness was obtained from #1 and lowest one was obtained from #3, which is consistent with macroscopically obtained result (#1 sample has highest trap density and #3 sample has lowest one.). Furthermore, in the local DLTS images, we detected dark and bright areas, which can be translated as two dimensional trap distribution. This means that this is the first demonstrations of two dimensional imaging of trap distributions in MOS interfaces.

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11:15am **PCSI-ThM-34 Interaction and Topological Effects in Two-dimensional Materials***,* ***Steven G. Louie****,* UC Berkeley **INVITED**

Symmetry, interaction and topological effects, as well as environmental screening, dominate many of the quantum properties of reduced-dimensional systems and nanostructures. These effects often lead to manifestation of counter-intuitive concepts and phenomena that may not be so prominent or have not been seen in bulk materials. In this talk, I present some fascinating physical phenomena discovered in recent studies of atomically thin two-dimensional (2D) materials. A number of highly interesting and unexpected behaviors have been found – e.g., strongly bound excitons (electron-hole pairs) with unusual energy level structures and novel optical selection rules; massless excitons; tunable magnetism and plasmonic properties; electron supercollimation by disorders; and novel topological phases – adding to the promise of these 2D materials for valuable applications.

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