Monday Morning, January 15, 2018

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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+ Author for correspondence: murakami@stat.phys.titech.ac.jp

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.

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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$_2$MnSi [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$_2$MnAl and Fe$_2$MnAl 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$_2$MnAl and superlattices terminated with Fe$_2$MnAl had 25% spin polarization. Pure Co$_2$MnAl had 65% spin polarization. Superlattice terminated with Co$_2$MnAl 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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*author for correspondence: ayost3@unl.edu

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.

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+ Author for correspondence: wangd@iccas.ac.cn [mailto:wangd@iccas.ac.cn]

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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+Author for correspondence: http:dora.bk.tsukuba.ac.jp/, hidemi@ims.tsukuba.ac.jp

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.

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