## Magnetic Interfaces and Nanostructures
## Room: 311 - Session MI+MG-TuM

### Advanced Materials Discovery
**Moderator:** Markus Donath, Muenster University, Germany

8:00am **MI+MG-TuM1 Combinatorial Approach to Novel Functional Materials**, ***Ichiro Takeuchi***, University of Maryland **INVITED**

Throughout the history of mankind, scientists and engineers have relied on the slow and serendipitous trial-and-error approach for materials discovery. In 1990s, the combinatorial approach was pioneered in the pharmaceutical industry in order to dramatically increase the rate at which new chemicals are identified. The high-throughput concept is now widely implemented in a variety of fields in materials science. We have developed combinatorial thin film synthesis and characterization techniques in order to perform rapid survey of previously unexplored materials phase space in search of new inorganic functional materials. Various thin film deposition schemes including pulsed laser deposition, electron-beam deposition, and co-sputtering are implemented for fabricating massive arrays of compositionally varying samples on individual combinatorial libraries. A suite of high-throughput characterization tools are employed to screen the combinatorial libraries and map different physical properties of materials as a function of sweeping composition changes. They include room-temperature scanning SQUID microscopy, microwave microscopy, and micromachined MEMS cantilever arrays. Advanced characterization techniques at synchrotron beam lines are used for rapid diffraction as well as x-ray magnetic circular dichroism measurements.

8:40am **MI+MG-TuM3 Discovery and Design of Two-Dimensional Materials by Data-Mining and Genetic Algorithm Approaches**, ***Richard Hennig***, University of Florida, Gainesville **INVITED**

The rapid rise of novel single-layer materials, presents the exciting opportunity for materials science to explore an entirely new class of materials. This comes at the time when mature computational methods provide the predictive capability to enable the computational discovery, characterization, and design of single-layer materials and provide the needed input and guidance to experimental studies. I will present our data-mining and genetic algorithm approaches to identify novel 2D materials with low formation energies and show how unexpected structures emerge when a material is reduced to sub-nanometers in thickness. We discovered several 2D materials in the families of group III-V compounds and group-II oxides with promising properties for electronic devices and identify suitable metal substrates that can stabilize several of these as-yet hypothetical materials. In the families of group-III monochalcogenides and transition metal dichalcogenides we identify several 2D materials that are suitable for photocatalytic water splitting. We show that these 2D materials in contrast to their 3D counterparts have appropriate bad gaps and alignments with the redox potentials of water, and exhibit high solvation energies, indicating their stability in aqueous environment. We show that strain can be used to tune the electronic and optical properties of these materials. Our results provide guidance for experimental synthesis efforts and future searches of materials suitable for applications in energy technologies.

9:20am **MI+MG-TuM5 Complexities in the Molecular Spin Crossover Transition**, ***Xin Zhang****, *S. Mu,* University of Nebraska-Lincoln, *J. Chen,* Columbia University, *T. Palamarciuc, P. Rosa, J.-F. Létard,* Université de Bordeaux, France, *J. Liu, D. Arena,* Brookhaven National Laboratory, *B. Doudin,* Université de Strasbourg, France, *P.A. Dowben*, University of Nebraska-Lincoln

The electronic structures of three different spin crossover molecules have been obtained by temperature dependent X-ray absorption spectroscopy (XAS). We show compelling evidence that the electronic structure changes associated with the spin crossover transition occur at significantly lower temperature than observed for the change in the molecular spin state. The transition temperatures indicated by XAS is about 20~60 K lower than that given by the magnetic moment switching. The changes in electronic structure are in agreement with density function theory (DFT) results that shows that the molecular electronic structures are different for high spin (HS) and low spin (LS) states. The conclusion that the electronic structure changes occur at significantly lower temperature than observed for the change in the molecular spin state associated with the spin crossover transition are also supported by transport measurements and the temperature dependence of the dielectric properties of SCO molecular system: [Fe(PM-AzA)$_2$(NCS)$_2$].

9:40am **MI+MG-TuM6 Controlling and Imprinting Topological Spin Textures**, *R. Streubel, L. Han,* IFW Dresden, Germany, *M.-Y. Im,* Lawrence Berkeley National Laboratory, *F. Kronast,* Helmholtz-Zentrum Berlin für Materialien und Energie/Elektronenspeicherring BESSY II, Germany, *U.K. Roessler,* Institute for Theoretical Solid State Physics, IFW Dresden, Germany, *F. Radu, R. Abrudan,* Ruhr-Universitaet Bochum, Germany, *G. Lin, O.G. Schmidt,* IFW Dresden, Germany, ***Peter Fischer***, Lawrence Berkeley National Laboratory, *D. Makarov*, IFW Dresden, Germany

Topological states in magnetism, such as chiral skyrmions, with an integer topological charge are currently a topic of intensive fundamental research [1-3]. If one was able to control their properties in a digital manner, such as switching their topological charge deliberately in storage devices, a novel path in spintronics would be opened [4]. However, so far, most of these topological spin textures have been only observed in exotic materials with low symmetry and at low temperatures, making them rather impractical for applications. Here, we offer an alternative route by designing synthetic magnetic heterostructures where specific spin textures resembling swirls, vortices or skyrmions with distinct topological charge densities can be tailored at ambient temperatures. This is achieved by vertically stacking two magnetic nanopatterns with in-plane and out-of-plane magnetization and imprinting the in-plane non-collinear spin textures into the out-of-plane magnetized material. Key mechanisms of our concept are demonstrated both by micromagnetic simulations and experimental observations with element-specific magnetic soft x-ray microscopy [6] in a common ferromagnetic thin film element stack, e.g. Co/Pd multilayers coupled to Permalloy. Utilizing the interlayer coupling strength as tuning parameter, a gradual transition in the magnetic pattern of the out-of-plane layer from the decoupled magnetized state to a strongly coupled state with a vortex spin texture is achieved. At an intermediate coupling strength, magnetic spirals with tunable opening angle and in particular donut textures form which can be referred to as skyrmion system with $D_n$ symmetry. Applying a small magnetic field, a controlled and reliable switching between two topologically distinct donut textures is realized.

Supported by the German Science Foundation (DFG) grant MA 5144/1-1, the European Research Council under European Union's Seventh Framework program (FP7/2007-2013)/ERC grant agreement n.306277. M.-Y.I. and P.F. acknowledge support by the Director, Office of Science, Office of Basic Energy Sciences, Materials Sciences and Engineering Division, of the U.S. Department of Energy under Contract No. DEAC02-05-CH11231 and by Leading Foreign Research Institute Recruitment Program through the National Research Foundation (NRF) of Korea funded by the Ministry of Education, Science and Technology (MEST)(2012K1A4A3053565).

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11:00am **MI+MG-TuM10 Growth and Properties of Skyrmionic MnSi Nanowires and Thin Film on Silicon**, ***Jieyu Yi***, *S.W. Tang,* University of Tennessee, *I.I. Kravchenko, G.X. Cao,* Oak Ridge National Laboratory, *D.G. Mandrus,* University of Tennessee, *Z. Gai*, Oak Ridge National Laboratory

Magnetic skyrmion lattice, a vortex-like spin texture recently observed in chiral magnets, is of great interest to future spin-electronic data storage and other information technology applications . The origin of the magnetic skyrmion phase can be traced to the anti-symmetric Dzyaloshinski-Moriya (DM) interaction that is allowed in space groups lacking inversion symmetry. The combined effect of a large ferromagnetic exchange and a weak DM interaction is to twist the magnetization into a long-period spiral that can be tens to hundreds of nanometers in length. As these spirals are only weakly bound to the underlying lattice in cubic systems, they can be readily manipulated with modest applied fields. Prototypical materials with the skyrmion ordering are those compounds with B20 structure, like MnSi and FeGe. The skyrmion lattice in MnSi appears in a small region (known as the A phase) of the H-T phase diagram in bulk samples, but in 2D samples like thin films the skyrmion phase is much more robust. It is of great interest to determine the properties of the skyrmion phase in quasi-1D nanowires and 2D thin films. If skyrmion ordering can persist in one-

*** Falicov Student Award Finalist**

dimensional MnSi nanowires and 2D films, then these systems may be very promising for spintronics applications as the magnetic domains and individual skymions could be manipulated with small currents. We have systematically explored the synthesis of single crystal MnSi nanowires via controlled oxide-assisted chemical vapor deposition and observed a characteristic signature of skyrmion magnetic ordering in MnSi nanowires. The $SiO_2$ layer pla ys a key role for the high yield, correct stoichiometric and crystalline growth of the B20 MnSi nanowires. A growth phase diagram was constructed. For the thin films, an unique growth receipt was developed for the growth of high quality of thin films. The structure and magnetic properties of the films at different thickness were studied.

11:20am **MI+MG-TuM11 Depth Dependent Mapping of Valence and Other Factors in $LaSrMnO_3/PrZrTiO_3$ Magnetoelectric Heterostructures**, ***Mikel Holcomb***, *C.-Y. Huang, R. Trappen, J. Zhou,* West Virginia University, *Y.-H. Chu*, National Chiao Tung University, Taiwan, Republic of China

Our group focuses on the ability to study the unique properties occurring at material surfaces and interfaces. One of the most interesting types of interfaces are magnetoelectric, because they offer the ability to electrically control magnetism or vice versa. This magnetoelectric control offers potential advantages in computing, magnetic sensors, energy scavenging and more. Magnetoelectric interfaces offer advantages over single layer magnetoelectrics as the ordering temperatures can be above room temperature and the coupling can be significantly stronger. Despite these advantages, the mechanism responsible for magnetoelectric coupling is currently unknown, which limits our ability to improve these systems to the parameters required for applications. In order to understand the mechanism for magnetoelectric multilayers, we investigated $LaSrMnO_3$ on $PbZrTiO_3$. By varying the sample thickness and utilizing both surface and bulk sensitive synchrotron radiation techniques, we are able to map out the Mn valence throughout the $LaSrMnO_3$ layer. We have also studied how strain and magnetization change with layer thickness. I will discuss our how results enable us to understand the charge origin of magnetoelectric interfaces.

11:40am **MI+MG-TuM12 Strain Measurements in $LaSrMnO_3/PbZrTiO_3$ Magnetoelectric Heterostructures**, ***Chih-Yeh Huang***, *J. Zhou,* West Virginia University, *Y.-H. Chu,* National Chiao Tung University, Taiwan, Republic of China, *M.B. Holcomb*, West Virginia University

LaSrMnO3/PbZrTiO3 (LSMO/PZT) magnetoelectric heterostructures make them attractive not only for data storage applications but also for studying strain measurements. There are many reasons why LSMO/PZT magnetoelectric heterostructures were selected for our studies such as the excellent lattice matching and high ordering temperatures. X-ray micro diffraction technique is used to observe local strain behavior at the interface of LaSrMnO3/PbZrTiO3 magnetoelectric heterostructures. Due to high spatial resolution in X-ray spot size (~1 mm) laterally, the observation of strain measurements in thickness-dependent PbZrTiO3 reveals shiftings of LSMO and PZT peaks, allowing an understanding of the behavior of strain at the interface which can be related to the mechanism of magnetoelectric coupling.

12:00pm **MI+MG-TuM13 Bit-Patterned Media Using Block Copolymer Templating on FePt**, *S. Gupta, H. Su,* ***Allen Owen***, *R. Douglas*, University of Alabama

Block copolymer (BCP) templating has been used to pattern perpendicular magnetic anisotropy media. Large-area arrays of magnetic dots with diameter of ~30nm have been obtained by BCP templating in FePt films. FePt was deposited by dc cosputtering of elemental targets and in situ annealing in the sputtering system at 550°C for 1hr. The polystyrene polyferrocenyldimethylsilane (PS-b-PFS) was spin-coated onto the film and annealed to cause phase separation, followed by oxygen plasma treatment to remove the polystyrene matrix and expose the PFS nanospheres[4]. The FePt films were subsequently etched using an ion mill. Then post-patterning annealing at 600°C was also performed to reverse the ion damage of the film. SEM and XRD were utilized to characterize the morphology and structural properties respectively, while magnetometry was carried out to show the magnetic properties. Response surface methodology was performed to optimize the power, etching time and etching angle of the block copolymer mask and magnetic film. The effects of these patterning parameters on structural and magnetic properties were discussed.

**Accelerating Materials Discovery for Global Competitiveness Focus Topic**
**Room: 302 - Session MG-TuA**

**Multi-scale Modeling in the Discovery of Advanced Materials**
**Moderator:** Alberto Roldan, University College London, Veena Tikare, Sandia National Laboratories

2:20pm **MG-TuA1 Search for Substitutes of Critical Materials with Targeted Properties by Scale-Bridging and High-Throughput Modelling and Simulation**, ***Christian Elsässer***, Fraunhofer Institute for Mechanics of Materials IWM, Germany **INVITED**

In this lecture three case studies will be addressed on how sustainable substitutes for materials, which have outstanding functionalities but also constraining criticalities, can be discovered and developed efficiently by employing multi-scale-coupling and high-throughput-screening concepts.

In the first case, a multi-scale chain from atomic-level first-principles theory to microstructure-level phase-field theory for ferroelectric piezoelectrics is set up for the still best material $Pb(Zr,Ti)O_3$ (PZT), which contains the biomedically health-critical element Pb, and then transferred to $(K, Na)NbO_3$ (KNN), which is a potential substitute for PZT. [1]

The second case is on the modelling of structure-property relationships for transparent and conductive oxides (TCO), which are free of the geologically ressource-limited element Indium and therefore potential substitutes for the still best TCO material Indium Tin Oxide (ITO) for front electrodes on, e.g., smart phones or solar cells. [2]

In the third case, a combinatorial high-throughput-screening approach is employed to search for crystal structures and chemical compositions of intermetallic phases of transition-metal (TM) and rare-earth (RE) elements, which have sufficiently good intrinsic ferromagnetic properties for permanent magnets but contain less amounts of the geopolitically supply-critical RE elements than, e.g., the still best permanent magnets based on $(Nd,Dy)_2Fe_{14}B$. [3]

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3:00pm **MG-TuA3 Monte Carlo Simulations of Nanoscale Focused Electron Beam Induced Etching**, *R. Timilsina,* ***Philip Rack,*** The University of Tennessee Knoxville, *K. Wolff, M. Budach, K. Edinger*, Carl Zeiss SMS, Germany

Focused beam (electron-ion-photon) induced processing has long been utilized as a micro-/nano-scale direct synthesis method for both additive (via deposition) and subtractive (via etching) machining for a variety of editing and prototyping applications. Nanoscale lithography mask editing is one critical area which is pushing the limits for these beam induced processing methods. Beam damage associated with liquid gallium and the recently developed gas field ion source limits their utility in lithography mask repair due to the stringent optical requirements. Thus, electron beam induced processing for mask repair of both clear and opaque defects is the method of choice. To understand the fundamental electron-solid-precursor interactions, a Monte Carlo electron-solid simulation has been developed with a dynamic precursor gas routine which emulates adsorption/desorption, surface diffusion and electron stimulated reactions. The simulation was recently modified to handle electron beam induced etching. The electron beam induced etching of silicon dioxide is studied at low and high energies, short and long dwell times and various etch precursor gas conditions to elucidate important rate limiting regimes. Furthermore, the temporal behavior of the high-aspect ratio etch process is demonstrated. In this presentation we will overview the Monte Carlo simulation and will illustrate how various parameters affect the resolution and etch rate of the electron beam stimulated etch process. We will demonstrate how beam parameters (beam energy, current, and dwell and refresh time) precursor parameters (flux, residence time, surface diffusion coefficient, dissociation cross-section) and material (secondary electron yield, density) all contribute to the nanoscale etching process.

4:20pm **MG-TuA7 Advances in Multiscale Mathematical Modeling of Materials: From Phase Diagrams to Interface Dynamics**, ***Maria Emelianenko***, George Mason University **INVITED**

This talk will survey recent developments in two areas critical for advancing materials design. First is the mesoscale kinetic modeling of polycrystalline materials, focused on the task of understanding how statistical distributions develop in the process of coarsening of materials microstructure and how these distributions in turn relate to materials properties. The challenges here include the design of reliable benchmarks for curvature-driven growth, vertex and Monte Carlo grain growth simulation codes, as well as the development of coarse-grained kinetic theories capable of capturing realistic materials behavior. These and other questions will be discussed in the context of nonlocal evolution theory and particle gas dynamics, and unexpected connections with other fields of science will be revealed. The other part of the talk will be concerned with phase diagram calculation methods, where robust and accurate numerical optimization methods are required to prevent costly mistakes. A universal Gibbs energy minimization formulation will be discussed that allows to link traditional Calphad codes and databases to state-of-the-art optimization engines, paving the road to a more intelligent automated phase data exploration.

5:00pm **MG-TuA9 Discrete All-Atom Simulations: Predicting Fit-for-Purpose Properties of Fuels**, *M.T. Knippenberg,* High Point University, ***BarbaraL Mooney***, *J.A. Harrison*, United States Naval Academy

Hydrotreated renewable fuels are complex blends of hydrocarbons produced by catalytic treatment of oils from such materials as corn, algae, and tallow. These fuels are of potential interest to the US Navy for use in their fleet, but due to their complexity it is not obvious which blends are suitable, and which are not. To this end, we use computational modeling for the prediction, based upon chemical composition, of the fit-for-purpose (FFP) properties of these alternative fuels. Low-cost, high-throughput assessment of fuel space from molecular dynamics (MD) simulation accelerates fuel discovery by: 1) identifying suitable candidate fuels out of a large phase space of possible fuel mixtures and environmental conditions; 2) providing an informed starting point for experimental investigations; and 3) reducing waste by eliminating the need to perform expensive, time-consuming measurements on unviable candidates. We are able, through MD with the modified-AIREBO potential, to obtain excellent agreement with experimental measurements of density, enthalpy of vaporization, and bulk modulus for a range of example surrogates containing up to 12 hydrocarbon components, as well as for binary mixtures of the straight-chain alkane *n*-dodecane with the branched 2,2,4,4,6,8,8-heptamethylnonane over the full range of mole fractions.

**Magnetic Interfaces and Nanostructures**
**Room: 311 - Session MI+MG-TuA**

**Development of Multiferroic Materials (2:20- 5:00PM)**
**MIND Panel Discussion (5:00-6:30 pm)**
**Moderator:** Peter Fischer, Lawrence Berkeley National Laboratory

2:20pm **MI+MG-TuA1 Versatile Abilities of Lattice Instabilities: New Design Strategies for Emergent Ferroics**, ***James Rondinelli***, Drexel University **INVITED**

I describe in this talk the design methodology and theoretical discovery of a new class of “rotation-induced” ferroelectric materials. By tailoring the instabilities of the $BO_6$ octahedral rotations common to $ABO_3$ perovskites oxides, I show these lattice distortions provide a new structural “sand box" from which to design and discover such ferroic phases. Bottom-up engineering of the transition metal octahedra at the unit cell level, is applied to realize ferroelectricity in artificial perovskites superlattices formed by interleaving two bulk materials with no tendency to such behavior. This emergent, chemistry-independent, form of ferroelectricity – octahedral

rotation-induced ferroelectricity – offers a reliable means to externally address and achieve deterministic electric-field control over magnetism. I discuss the required crystal-chemistry criteria, which are obtained from a combination of group theoretical methods and electronic-structure computations, to select the compositions and stoichiometries giving polarizations comparable to the best known ferroelectric oxides. Much rarer in crystalline materials with an electric polarization, however, is the appearance of a ferri-electric (FiE) state, vis-à-vis ferrimagnetism, where local electric dipoles of different magnitude are anti-aligned to yield a net non-zero electric polarization. The underlying reason is that the long-range Coulomb forces in oxide-based dielectrics favor the cooperative alignment of all electric dipoles in the crystal through cation displacements that occur against an oxygen ligand framework. I conclude by describing our recent discovery of a first-order, isosymmetric, transition between a ferrielectric (FiE) and ferroelectric (FE) state in A-site ordered perovskite superlattices and offering new areas for ferroic discovery

3:00pm **MI+MG-TuA3 Voltage-controlled Exchange Bias and Exchange Bias Training**, ***Christian Binek***, *W. Echtenkamp*, University of Nebraska-Lincoln **INVITED**

Voltage-controlled exchange bias (EB) is a seminal achievement in nanomagnetism. It enables dissipationless electric control of interface magnetic states with major implications for room temperature spintronic applications. Numerous prototypical solid-state spintronic devices rely on switchable interface magnetism, enabling spin-selective transmission or scattering of electrons. Controlling magnetism at thin-film interfaces, preferably by purely electrical means, i.e. in the absence of electric currents, is a key challenge to better spintronics. Currently, most attempts to voltage-control magnetism focus on potentially large magnetoelectric (ME) effects of multiferroics.

Here, we report on the use of antiferromagnetic (AF) ME $Cr_2O_3$ (chromia) for voltage-controlled magnetism [1,2]. Electrically switchable boundary magnetization (BM) can overcome the weak linear ME susceptibility of room temperature bulk ME antiferromagnets. BM is a roughness insensitive equilibrium property of ME antiferromagnets which is in sharp contrast to the surface magnetic properties of conventional antiferromagnets. Voltage-controlled BM is the key property enabling isothermal voltage-controlled switching of exchange bias (EB) which emerges at the interface of adjacent ferromagnetic (FM) and the ME antiferromagnetic (AF) thin film. The inter-layer exchange alters the magnetization reversal shifting the FM hysteresis loop along the magnetic field axis. In this presentation I introduce voltage-control of EB and EB training [2]. Electric switching between stable EB fields is investigated in heterostructures based on single crystal $Cr_2O_3$(0001)/PdCo heterostructures and compared with recent results in MBE grown all thin film EB heterostructures. In addition to voltage-switching of EB we electrically and isothermally tune chromia into distinct AF multi-domain states. As a result, EB training, which originates from triggered rearrangements of the AF interface magnetization during consecutively cycled hysteresis loops, is tuned between zero and sizable effects. We quantify and interpret the peculiar voltage-controlled training effect in $Cr_2O_3$(0001)/PdCo by adapting our recently developed theory which is based on a discretized Landau-Khalatnikov dynamic equation [3].

We acknowledge the Center for NanoFerroic Devices, C-SPIN, part of STARnet, a SRC program sponsored by MARCO and DARPA for partial funding of this work.

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4:20pm **MI+MG-TuA7 Multiferroic $Z_6$ Vortices in Hexagonal $ErMnO_3$**, *Y. Geng, X.-Y. Wang, S.-W. Cheong,* ***Weida Wu***, Rutgers University

Multiferroics are materials with coexisting magnetic and ferroelectric orders, where inversion symmetry is also broken [1-5]. The cross-coupling between two ferroic orders can result in strong magnetoelectric coupling. Therefore, it is of both fundamental and technological interest to visualize cross-coupled topological defects in multiferroics. Indeed, topological defects with six interlocked structural antiphase and ferroelectric domains merging into a vortex core were revealed in multiferroic hexagonal manganites [6, 7]. Numerous $Z_6$ vortices are found to form an intriguing self-organized network, and may be used to test Kibble-Zurek model of early universe [8, 9]. Many emergent phenomena, such as enhanced conduction and unusual piezoelectric response, were observed in charged ferroelectric domain walls protected by these topological defects [10, 11]. In particular, alternating uncompensated magnetic moments were discovered at coupled structural antiphase and ferroelectric domain walls in hexagonal manganites using cryogenic magnetic force microscopy (MFM) [12], which demonstrates the coupling between ferroelectric and spin orders ($B_2$ phase). The appearance of correlated net moments at the coupled domain walls is in excellent agreement with a phenomenological Landau theory [13], suggesting that the 120° antiferromagnetic order ($B_2$ phase) rotates 4pi in each $Z_6$ vortex. This is further corroborated by the magnetic field dependence of domain wall moments.

*This work is supported by NSF grant # DMR-0844807.

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4:40pm **MI+MG-TuA8 Two-Dimensional Manganese Gallium Quantum Height Islands on Wurtzite GaN (000-1)**, ***Jeongihm Pak***, *A. Mandru, A.R. Smith*, Ohio University

We describe the spontaneous formation of five and six-monolayer quantum height manganese gallium islands on gallium-rich, nitrogen polar GaN(000$\underline{1}$). From ex-situ MOKE measurements at room temperature, we expect these MnGa islands to be ferromagnetic. The structural evolution is followed from the beginning of growth using reflection high energy electron diffraction, in which a dotted 2× pattern is observed to form. In-situ scanning tunneling microscopy is also used to investigate the islands' structures with atomic resolution. Based on all the observations, we propose the possible bulk and surface models for the islands. A possible bonding structure at the substrate/island interface is also discussed in which Mn atoms substitute for Ga atoms on the Ga adlayer thus making the MnGa islands bonded to the GaN substrate. Atomic chains are observed only on the six-layer island surface and the model for the chains is also discussed. STM observations of atomic-chain interconnection on the six-layer island surface indicate a dynamic system at room temperature. The models presented here should serve as useful starting points for theoretical calculations.

5:20pm **MI+MG-TuA10 Current Topics in Magnetism: The Importance of Interfaces**, ***Mark Stiles***, National Institute of Standards and Technology

Interfaces play a crucial role in many magnetic systems. As magnetoelectronic devices shrink, this role is becoming more and more important. Unfortunately, many times these interfaces are not well enough characterized to allow measurements to constrain physical models of the behavior in these systems. In this talk, I give several examples from my own experience of systems of both historical and current interest in which the interfaces play a dominant role but for which very little is known. A historical example is exchange bias, the study of systems in which the behavior of a ferromagnetic film is modified by coupling to it to an antiferromagnet. In spite of decades of study on a wide variety of systems, structural characterization of the interfaces has only been done several times on model systems, despite the fact that all of the coupling occurs at this interface. A topic of recent interest is the study of current induced torques in magnetic bilayers consisting of ferromagnetic thin films coupled to non-magnetic materials with strong spin-orbit coupling. The spin orbit coupling dramatically affects the current induced torques in these systems. An outstanding question is what role the interfacial spin-orbit coupling plays. This can be addressed theoretically by first-principles calculations, but these necessarily assume ideal interfaces between perfectly coherent lattices for material pairs with lattice mismatch on the order of ten percent. Without real characterization of the structure of these interfaces, it is almost impossible to definitively determine which parts of the system are playing important roles. Both of these topics are useful or potentially useful for applications, a characteristic that tends to drive research focused on achieving dramatic results rather than doing the time intensive work necessary to characterize the samples adequately to support a deeper understanding of the underlying physics.

5:40pm **MI+MG-TuA11 Optical Spectroscopy of Nanomaterials within Magnetic Fields**, ***Angela Hight Walker***, NIST

Transition-metal dichalcogenides are a new system in which to study the effect of temperature and magnetic field on optical properties. Recent experiments will be discussed from a novel set up which couples a confocal optical microscope into fields up to 9 Tesla and temperatures down to 3.5 K, with several laser sources throughout the visible range. As these dichalengenides or 2D materials are certainly under study for use in nanoelectronic devices they are of general interest to the Magnetic Interfaces and Nanostructures (MIN or MI) Division. Other areas where MIND members see as future foci will be explored. Methods to ensure that the Division draw upon the widest possible spectrum of talented individuals from all segments of society will also be discussed.

**Accelerating Materials Discovery for Global Competitiveness Focus Topic**
**Room: 302 - Session MG-WeM**

**Design of New Materials**
**Moderator:** Christian Elsässer, Fraunhofer Institute for Mechanics of Materials IWM, Susan Sinnott, University of Florida

8:20am **MG-WeM2 Hydrogen Molecules Distribution in Multi-Cathodes Funneling Gun**, ***Erdong Wang***, *I. Ben-Zvi, J. Skaritka, T. Rao,* Brookhaven National Laboratory, *R. Bothell, J. Bothell, A. Henry*, Atlas Technologies

The high average current polarized electron source for future electron ion collider (EIC) requires extremely high vacuum. Currently, we have constructed a DC gun based on principle of beams funneling and this gun is under commissioning. Superlattice GaAs cathodes will be used as our electron source. The lifetime of these cathodes is dependent on ion back bombardment which caused by the residual gas pressure. Multiple GaAs cathodes with almost same lifetime are extremely crucial for the operation of this gun. Therefore, produce a uniform extremely high vacuum environment is essential in gun design. We studied residual molecules distribution in funneling gun by Molflow+ and a python based Monte-Carlo simulator. Twenty cathodes testing is under planning. Cathodes lifetime changes will give us indication on vacuum distribution inside the gun. This articles describes our coding and modeling for the gun vacuum, analyzes the residual gas distribution on the gun and discusses on multiple cathodes lifetime measurement test. We also discusses the XHV achievement in our gun test.

8:40am **MG-WeM3 Tailored Functionality of Wide Band Gap Semiconductors**, *B.E. Gaddy, Z.A. Bryan, I.S. Bryan, R. Kirste,* North Carolina State University, *J. Xie, R. Dalmau, B. Moody,* Hexatech Inc., *Y. Kumagai,* Tokyo University of Agriculture and Technology, Japan, *T. Nagashima, Y. Kubota, T. Kinoshita,* Tokuyama Corporation, Japan, *A. Koukitu,* Tokyo University of Agriculture and Technology, Japan, *R. Collazo, Z. Sitar,* ***Douglas Irving***, North Carolina State University

Semiconductors obtain new functionality by the incorporation of dilute concentrations of impurities. This principle has been utilized to tailor the properties of narrow gap semiconductors, such as Si or GaAs, but tailoring the properties of wide band gap materials for optical or high power applications has been extremely challenging. As a result, there has been slow progress in identifying *new material* combinations (bulk material + dilute dopants) to enable *novel functionality*. To help overcome these obstacles, we have developed and implemented a point defects database in which we store formation, ionization, and optical transition energies determined by hybrid exchange-correlation density functional theory methods. These predictions from first principles are then strongly coupled with synthesis and characterization efforts to identify troublesome point defects and also suggest routes to realizing desired properties if particular defect cannot be removed. The stored data is also used to solve mass balance equations to determine the number of carriers and compensating defects. In this talk, I will present our recent efforts in applying these tools to determine solutions for unwanted optical absorption in AlN grown by PVT. With our data we have demonstrated that substitutional carbon on the nitrogen site is a deep acceptor. When ionized it is the source of unwanted optical absorption. This was confirmed by PL, SIMS, and HVPE. Solution of mass balance equations reveals that the compensating defect is a singly ionized nitrogen vacancy for relevant growth conditions. The presence of this defect has been confirmed by an optical emission predicted to originate from a donor acceptor pair recombination and measured by PLE spectroscopy. When carbon cannot be removed from the growth process, we have used our database to determine mechanisms important to removing unwanted optical absorption in high carbon samples. In total, this approach has accelerated the design of new materials and also led to deeper understanding of the important mechanisms, which will impact future efforts to tailor properties of AlN and its alloys.

9:00am **MG-WeM4 Substitution and Strain Control of Polarization in Multifunctional Materials**, *M. Ashton, A. Chernatynskiy,* ***Susan Sinnott***, University of Florida

Density functional theory (DFT) calculations are used to analyze the combined effects of substitution and strain on spontaneous polarization in multiferroic perovskites, such as $BiFeO_3$. In particular, DFT calculations are used within the Vienna Ab-initio Simulation Package (VASP) to examine the macroscopic spontaneous polarization in $BiFeO_3$ systems with varying percentages of substitution and epitaxial strain. Substitutional elements considered for the A-site (Bi), B-site (Fe), and A/B co-substitution combination include Ba and La (A-site), Co, Cr, and Ni (B-site), and Ca/Mn and La/Ru (A/B site combination). In addition, strain values between +/- 2% are considered for each system. The results provide new insights into the roles of each of these factors on polarization and will be analyzed with data mining techniques to extrapolate design principles for high-$T_c$ perovskites with controllable polarization. This work is supported by the National Science Foundation (DMR-1307840).

9:20am **MG-WeM5 Manipulation of Site Reactivity at the Au Nanoparticle – Titania Interface through Alloying: Insights from Density Functional Theory**, ***Sampyo Hong***, *T.S. Rahman*, University of Central Florida

It has been shown that in methanol decomposition, as in CO oxidation, on titania supported Au nanoparticle, the interfacial atoms are the most reactive [1]. When we replace the Au atom, to which methoxy is bonded at the interface of $Au_{13}/TiO_2(110)$, by other 3d (Cr, Ni, Cu) and 5d (Pt, W) atoms, we find that the dopant atoms at the interface become more cationic than the original Au atom and the relevant activation energies for a H-C bond scission of methoxy bonded to them is reduced as compared to that for methoxy bonded to the original Au atom. On the basis of these results we propose that the activity of $Au/TiO_2$ interface for reactions involving C-H scission of hydrocarbons would be enhanced by increasing the density of interfacial atoms with higher oxidization state than that of gold at the interface. Work supported in part by DOE Grant No. DOE-DE-FG02-07ER15842 [1] S. Hong and T. S. Rahman, *J. Am. Chem. Soc.***2013**, *135*, 7629.

9:40am **MG-WeM6 Structural Descriptors for Hole Traps in Hydrogenated Amorphous Silicon Revealed through Machine Learning**, ***Tim Mueller***, Johns Hopkins University, *E. Johlin, J.C. Grossman*, Massachusetts Institute of Technology

The discovery and design of new materials can be accelerated by the identification of simple descriptors of material properties. However the identification of the most relevant descriptors and how they relate to the properties of interest is not always obvious. We demonstrate how machine learning, in the form of genetic programming, can be used to identify relevant descriptors for predicting hole trap depths in hydrogenated nanocrystalline and amorphous silicon. Amorphous silicon is an inexpensive and flexible photovoltaic material, but its efficiency is limited by low hole mobility. We have evaluated 243 structural descriptors of amorphous silicon to identify those that are most indicative of the hole trap depth. Our calculations reveal three general classes of structural features that influence hole trap depth and predict that multiple interacting defects may result in deeper traps than isolated defects. These results suggest a possible mechanism for the Staebler-Wronski effect, in which exposure to light degrades the performance of amorphous silicon over time.

11:00am **MG-WeM10 Integration of Meso-scale Microstructural Modeling for Engineering Materials Development**, ***Veena Tikare***, Sandia National Laboratories **INVITED**

The meso-scale materials modeling community, over the last two decades, has developed vast capabilities in microstructurally-based modeling of complex ceramic and metals. While several modeling techniques have been developed, the Potts kinetic Monte Carlo model and the phase-field model form the foundation of most materials modeling efforts for a variety of microstructural evolution processes experienced by ceramics and metals during fabrication and engineering service. Harnessing these modeling capabilities and applying them to design materials to tailor their microstructure for optimal engineering performance properties and designing fabrication processes to obtain the desired microstructure can greatly accelerate development and optimizing of materials for a large number of technologies. This presentation will give a general overview of the core capabilities of the microstructural evolution modeling capabilities by reviewing the two most commonly used methods, Potts and phase-field. The former is a discrete, statistical-mechanical model that has been successfully used to simulate many microstructural evolution processes, such as grain growth, sintering, coarsening in the presence of mobile and immobile pinning phase, and recrystallization. The phase-field model is a continuum, thermodynamic model that has been used to successful simulation solidification, phase transformation and coarsening processes. The capabilities and limitation of each model will be reviewed and appropriate application of the models to different materials microstructural evolution processes will be discussed. The presentation will also

demonstrate how these two models can be applied to understand and predict materials processes including coarsening, sintering and phase transformations. Specific examples of microstructural modeling and their application to design materials microstructure for optimal performance will be presented and discussed. Examples will included simulation of microstructural evolution during sintering of complex powder compacts; the generation, transport and release of fission gases from nuclear fuels during service in a reactor; and development of grain shapes and sizes during welding processes. Finally, the current trends in microstructure model development will be discussed.

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

11:40am **MG-WeM12 Insights on the $CO_2$ Reduction Mechanism on Bio-inspired Iron Sulphide**, ***Alberto Roldan***, *N.H. de Leeuw*, University College London, UK **INVITED**

Carbon dioxide capture and utilisation is gaining attention, driven not only by environmental factors but also by the potential to use it as chemical feedstock. One plausible utilisation route is its conversion to form small organic molecules, however, CO2 is thermodynamically very stable and its reduction is energy intensive. The CO2 conversion takes place under mild conditions in chemoautotrophic bacteria catalysed by enzymes.1 These enzymes often contain Fe4S4 clusters (cubanes), which have been shown to act as electron-transfer sites2,3 but they can also be catalytically active centres for molecule transformations.4 An iron thiospinel mineral is structurally similar to the cubane,5 fact that brings us to suggest it as a novel heterogeneous catalyst. We present a theoretical investigation using the iron sulphide greigite mineral (Fe3S4) as a catalyst to transform CO2 into small organic molecules. In agreement with the experiments, the adsorbed species depends on the solution pH as well as both concentration and actual products formed. The reduction consists of a sequential hydrogenation steps that we studied by the common Langmuir-Hinshelwood mechanism. We have identified ~170 steady states describing the different reaction pathways where the most favourable ones lead to formate and carboxyl intermediates yielding two different products, HCOOH and CH3OH, also identified experimentally under conditions of room temperature and pressure.

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(4) Seino, H.; Hidai, M. Chemical Science 2011, 2, 847.

(5) Martin, W.; Russell, M. J. Philosophical Transactions of the Royal Society of London Series B-Biological Sciences 2003, 358, 59.

**Biomaterial Interfaces**
**Room: 317 - Session BI+MG-WeA**

**Design and Discovery: Biointerfaces**
**Moderator:** Morgan Alexander, The University of Nottingham, UK

2:20pm **BI+MG-WeA1 Discovery of Materials for Stem Cell Control using Polymer Microarrays**, ***Morgan Alexander***, The University of Nottingham, UK

Polymer micro arrays have proven to be useful tools for the discovery of new synthetic materials which control cells.[1] This high throughput (HT) materials discovery approach is attractive because the paucity of understanding of the cell-material interface hinders the *ab initio* rational design of new materials.[2] The large number of polymer chemistries that can be investigated on a single polymer micro array act as a wide "net" in the search for materials that can achieve a certain cell response. Micro array *hits* are the starting point from which new materials may be developed.

Combinatorial acrylate libraries formed on standard glass slides were presented as a HT platform by Anderson and Langer of MIT.[3] To complement materials screening, we developed the approach of *HT surface characterisation* employing a range of analytical techniques in collaboration with the MIT group.[4] This surface characterisation step is necessary to directly relate the effect of the material on attached cells to the actual surface on which they sit, and to enable effective scale up from micro array to culture ware dimensions. Application of chemometrics, to handle the large amounts of complex data, reveals the importance of certain surface moieties, guiding the process of materials discovery and increasing our understanding of the cell-material interface.

We have applied this approach to the identification of materials which resist bacterial attachment and biofilm formation with application in the reduction of medical device centred infection.[5,6] In the mammalian cell field, we have identified materials which show promise as synthetic substrates for pluripotent stem cell culture.[7,8] These materials require pre-treatment with expensive proteins such as vitronectin, a constraint which limits their commercialisation.[9]

In this talk, screening of arrays with greater chemical diversity than ever before, incorporating up to 140 monomers[10], is reported which leads to the identification of materials which support pluripotent stem cell expansion without pre-treatment of the substrate with protein. Materials which support differentiation to mature cardiomyocytes which have potential application in in vitro toxicology screening have also been discovered.

1 Hook, A. L. **Biomaterials** (2010).

2 Kohn, J., **Nature Materials** (2004).

3 Anderson et al. **Nature Biotechnology** (2004).

4 Urquhart, A.et al. **Advanced Materials** (2007).

5 Hook, A. L. et al. **Nature Biotechnology** (2012).

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7 Mei, Y et al. **Nature Materials** (2010).

8 Saha, K. et al **PNAS** (2011).

9 Celiz, A. D et al. **Nature Materials** (2014).

10 Celiz, A.et al. **Biomaterials Science** (2014).

3:00pm **BI+MG-WeA3 Interfacial Force Field Parameterization in CHARMM for the Accurate Molecular Dynamics Simulation of Peptide Adsorption on High-Density Polyethylene**, ***Tigran Abramyan***, *J.S. Snyder, J.Y. Yancey, S.S. Stuart, R.A. Latour*, Clemson University

A fundamental molecular-level understanding of protein-surface interactions (PSIs) is crucial for many applications in biotechnology and bioengineering. All-atom molecular dynamic (MD) simulation methods hold great promise as a valuable tool for understanding and predicting PSIs. However, current MD force fields have not been validated for this application. In this study, adsorption free energy ($\Delta G_{ads}$) of small TGTG-X-GTGT host-guest peptides (T = threonine, G = glycine, and X = variable amino acid residue) on a high-density polyethylene (HDPE) surface (110 crystalline plane) using the CHARMM force-field were calculated and compared with experimental results in order to find inaccuracies. In order to accurately calculate $\Delta G_{ads}$ in our simulation studies, advanced sampling methods such as umbrella sampling and replica-exchange MD were used to provide adequate conformational sampling of the peptides over the HDPE surface. Results revealed substantial discrepancies between the simulation and the experimental $\Delta G_{ads}$ values (i.e., differences exceeding 1.0 kcal/mol). To correct the adsorption behavior, an *in-house-developed* interfacial force-field (IFF) was incorporated into the simulation program with IFF parameters adjusted until satisfactory agreement with the experimental data set was achieved. Subsequent studies are planned to apply the tuned IFF to simulate the adsorption behavior of lysozyme and ribonuclease A proteins to HDPE, for which synergistically matched experimental studies have also been conducted to validate the developed method for protein-adsorption simulations.

3:20pm **BI+MG-WeA4 Degradable Silica Nanoshells for Ultrasonic Imaging and Therapy**, ***Alexander Liberman***, *C. Barback, R. Viveros, S.L. Blair, D. Vera, L. Ellies, R. Mattrey, W. Trogler, A.C. Kummel*, University of California at San Diego

As a safe alternative to intrasurgical guidewires and implantable radioactive seeds, gas-filled hollow Fe-doped silica particles have been developed, which can be used for ultrasound-guided surgery for multiple foci. The function of the Fe doping is to render the silica shells biodegradable. The particles are synthesized through a sol-gel method on a polystyrene template, and calcined to create hollow, rigid nanoshells. The Fe-doped silica shell is derived from tetramethyl orthosilicate (TMOS) and iron ethoxide, which forms a rigid, nanoporous shell upon calcination. The nanoshells are filled with perfluoropentane (PFP) vapor or liquid. The flourous phase is contained within the porous shell due to its extremely low solubility in water. *In vitro* studies have shown that continuous particle imaging time is up to approximately three hours non-stop. *In vivo* particle injection longevity studies have been performed in tumor bearing mouse models show signal presence with color Doppler imaging up to ten days post injection. To study biodistribution, nanoshells were functionalized with DTPA and radiolabeled with Indium-111 and then imaged by gamma scintigraphy over 72 hours. Scintigraphic imaging and gamma counting confirm that particles undergoing IV delivery to tumor bearing mice will passively accumulate in the tumors which may allow for tumor detection and therapuetic applications. Additionally, long term biodistribution studies in mice have shown a steady decrease in silicon content over the course of 10 weeks by inductively coupled plasma optical emmision spectroscopy (ICP-OES).

These silica shells break under acoustic excitation to release uncovered gas pockets which increase acoustic energy absorption and reduce acoustic cavitation threshold locally. Therefore they may also be employed as a sensitizing agent in high intensity focused ultrasound (HIFU) therapy. Traditional ultrasound agents which can be used as a HIFU senstizing agent pose several potential drawbacks such as poor *in vivo* persistence (minutes) and high risk during continuous perfusion. Preliminary *in vivo* HIFU ablation studies show that very few particles are needed in order to develop a sensitizing effect to HIFU thereby substantially reduce the amount of HIFU exposure necessary to achieve an ablative effect. It was found that nanoshells systemically adminstered to breast tumor bearing mice could be cavitated by HIFU 24 hours after administration. This mechanical cavitation caused liquification within the focal volume of the HIFU which contained the nanoshells within seconds of the HIFU application. This may potentially allow for a larger area to be ablated in less time with less power.

4:20pm **BI+MG-WeA7 An Encapsulation Technique for Adenovirus to Enhance Viral Gene Therapy**, ***Natalie Mendez***, *V. Herrera, L. Zhang, F. Hedjran, W. Trogler, S.L. Blair, A.C. Kummel*, University of California at San Diego

Oncolytic viruses (OVs) constitute a promising class of cancer therapeutics which exploit validated genetic pathways known to be deregulated in many cancers. To overcome an immune response and to enhance its potential use to treat primary and metastatic tumors, a method for liposomal encapsulation of adenovirus has been developed. The encapsulation of adenovirus in anionic 140-180nm diameter PEG containing non-toxic liposomes has been prepared by self-assembly of lecithin around the viral capsid. The encapsulated viruses retain their ability to infect cancer cells. Furthermore, an immunoprecipitation (IP) technique has shown to be a fast and effective method to extract non-encapsulated viruses and homogenize the liposomes remaining in solution. 76% of adenovirus plaque forming units were encapsulated and retained infectivity after IP processing. Additionally, encapsulated viruses have shown enhanced transfection efficiency up to 4X higher compared to non-encapsulated Ads. Extracting non-encapsulated viruses from solution may prevent an adverse in vivo immune response and may enhance treatment for multiple administrations.

4:40pm **BI+MG-WeA8 Sequential and Competitive Adsorption of Peptides at Pendant PEO Layers**, *X.W. Wu, M.R. Ryder, J.M. McGuire,* ***Karl Schilke***, Oregon State University

A more quantitative understanding of peptide entrapment and elution from otherwise protein-repellent polyethylene oxide (PEO) brush layers will provide direction for development of new strategies for drug storage and delivery. Here we describe criteria for peptide integration and structural change within the PEO brush, and discuss the reversibility of peptide entrapment with changing solvent conditions. For this purpose, three cationic peptides were used: the arginine-rich amphiphilic peptide WLBU2, the chemically identical but scrambled peptide S-WLBU2, and the non-amphiphilic homopolymer poly-*L*-arginine (PLR). Circular dichroism (CD) was used to record the adsorption and conformational changes of WLBU2 and S-WLBU2, and polyarginine peptides at PEO-coated silica nanoparticles. UV spectroscopy and a quartz crystal microbalance with dissipation monitoring (QCM-D) were used to quantify changes in the extent of peptide elution. Peptide conformation was controlled between disordered and α-helical forms by varying the concentration of perchlorate ion. We show an initially more ordered (α-helical) structure promotes peptide adsorption into the PEO layer. Peptide interaction with the PEO chains resulted in entrapment and conformational change that was irreversible to elution with changing solution conditions in the case of the amphiphilic peptide. In contrast, the adsorption and conformational change of the non-amphiphilic peptide was reversible. We also evaluated the effects of peptide surface density on the conformational changes caused by peptide-peptide interactions, and using CD, QCM-D, and UV spectroscopy, showed that these phenomena substantially affect the rate and extent of peptide elution from PEO brush layers. Specifically, for amphiphilic peptides at sufficiently high surface density, peptide-peptide interactions result in conformational changes which compromise their resistance to elution. In contrast, elution of a non-amphiphilic peptide is substantially independent of its surface density, presumably due to the absence of peptide-peptide interactions.

The sequential and competitive adsorption behavior of WLBU2, S-WLBU2 and PLR at pendant PEO layers was studied by optical waveguide lightmode spectroscopy (OWLS), time-of-flight secondary ion mass spectrometry (TOF-SIMS), CD and UV spectroscopy. Results strongly indicate that amphiphilic peptides are able to displace non-amphiphilic peptides that are adsorbed in PEO layers, while non-amphiphilic peptides cannot displace amphiphilic ones. In summary, peptides of high amphiphilicity are expected to dominate the competitive adsorption with less amphiphilic peptides in PEO layers.

5:00pm **BI+MG-WeA9 Moulding Cells and Materials in High Throughput**, ***Clemens van Blitterswijk***, *R. Truckenmuller, L. Moroni, N. Rivron, P. Habibovic, J. De Boer*, Maastricht University, The Netherlands **INVITED**

The interaction of cells and materials at their interface is crucial for the performance of devices that are applied in regenerative medicine.In general the approach to optimize interaction is characterized by a mechanistic low throughput research cycle where researchers try to move forward by improving performance based on fundamental insights and related small volume in vitro/in vivo experiments. Although this approach has successes it has its disadvantages. First as the field of regenerative medicine is young we currently lack fundamental insights into many of aspects that are relevant to our field.Second, the research cycle is slow, so if our experiments do not give the anticipated results we may lose several years.Third,the conventional approach only allows us to test a maximum of ca.10 experimental conditions in one cycle forces us to leave out many other possibly equally interesting, opportunities.

In our lab we are convinced on how influential surface geometry of material can be on cell behavior and in vivo response by recently inducing prominent bone formation in muscle tissue in large animals by modulating the biomaterial surface in the submicrometer range.The effects of these instructive materials are equivalent to the use of growth factors while no biological agents or cultivated cells were applied.As we have no complete insight in the underlying mechanism,a conventional low throughput mechanistic approach does not seem the method of choice for further optimizing this performance and applying it to other tissue types.

Therefore,we developed multiwell screening systems that allow us to test a selection of thousands of surfaces from a truly designed high throughput library of 150 million different surface features in a single run. We have shown that this method allows us to modify cell shape and function in a remarkable way,both as far as cell attachment,proliferation and differentiation are concerned.As the above topochip platform is focused on 2D single cell performance and actual tissues are 3D and multicellular we have developed alternative platforms that allow us the build 3D mesoscale complex tissues in the thousands,while we have also generated so called 2,5 D muliwell systems that present convex surface features. Applying such systems allowed us to demonstrate that the mechanism of function follows form not only holds for individual cells but equally for millimeter scale cell aggregates.We are currently applying these technology platforms to create deeper insights in formation of tissues for regenerative medicine by introducing very early(embryonic)tissues in these systems while actively collaborating with developmental cell biologists.

6:00pm **BI+MG-WeA12 The Influence of Structural Array of Polymorphic hIAPP fibrils to its Mechanical Properties**, ***HyunJoon Chang***, *M. Lee,* Korea University, Republic of Korea, *G. Yoon,* Boston University, *S. Na*, Korea University, Republic of Korea

Amyloid proteins are misfolded, denatured proteins that are responsible for causing several degenerative and neuro-degenerative diseases, such as type II diabetes, Alzheimer's disease, Huntington's disease, and so on. Determining the mechanical stability of these amyloids is crucial for understanding the disease mechanism, which will allow us to provide guidance in treatment. Furthermore, many research groups also recognized amyloid proteins as a functional biological materials that can be used in nano sensor, bacterial biofilms, coatings, etc. There have been many *in vitro* studies to determine the material characteristics via force spectroscopy methods, Atomic Force Microscopy and Optical Tweezers to exemplify. However, computational methods (e.g. Molecular Dynamics (MD) and Elastic Network Model) not only reveal the mechanical properties, but also provide a more in-depth information on the amyloids by visualizing the conformation. In this study, we have discovered the material properties of four different polymorphic structures of Human Islet Amyloid Polypeptide (hIAPP) by using MD simulations under tensile Steered Molecular Dynamics (SMD) conditions. Also, from our results, we have observed how these mechanical properties may differ in respect of their structural formation. This study will help us to take a step forward for treating degenerative disease and also establish a template for the functional biological materials.

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