Tuesday Morning, November 11, 2014

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)$_2$].

* **Falicov Student Award Finalist**

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.

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[1] X.Z. Yu et al, Nature **465** 901 (2010)

[2] F. Jonietz et al, Science **330** 1648 (2010)

[3] S. Heinze et al, Nat. Phys. **7** 713 (2011)

[4] A. Fert et al, Nat. Nano **8** 152 (2013)

[5] J. Sampaio et al, Nat. Nano **8** 839 (2013)

[6] P. Fischer et al, JESRP **189** 196 (2013)

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 onedimensional 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.

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