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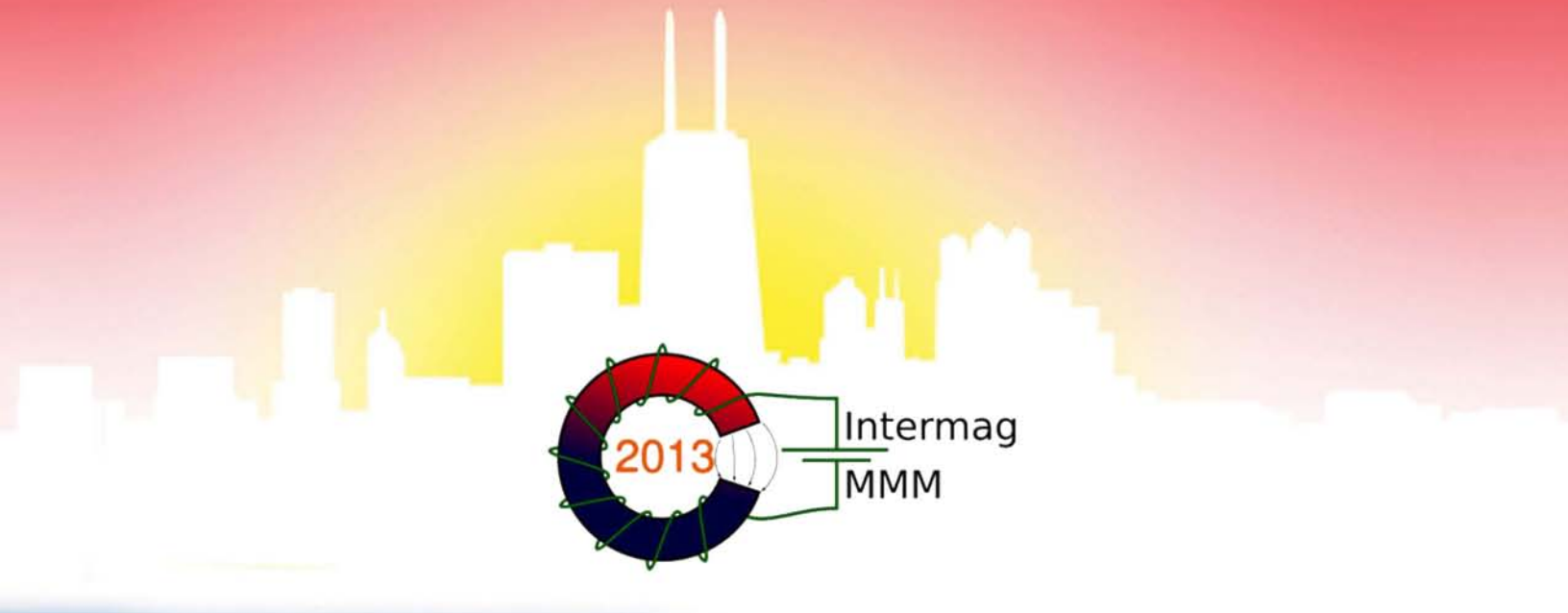

ABSTRACTS

IEEE MAGNETICS

AIP American Institute of Physics

TUESDAY MORNING, 15 JANUARY 2013 RIVERSIDE CENTER, 9:00 TO 12:00

Session AS
FUNDAMENTAL PROPERTIES AND COOPERATIVE PHENOMENA I (POSTER SESSION)

Daniel Haskel, Co-Chair
Xiaofeng Jin, Co-Chair

CONTRIBUTED PAPERS

AS-01. Electronic, structural, and magnetic properties of O and Py deficient CoO/Py interfaces. *U. Schwingenschlogl*[1] and S. Grytsyuk[1] *1. KAUST, Thuwal, Saudi Arabia*

The development of magnetic devices based on coupling between a ferromagnet and an antiferromagnet (such as spin-valves, metal-oxide-metal diodes, and magnetic recording media) depends strongly on the interfacial magnetic structure. In this work we investigate the CoO(111)/Ni(111) interface focusing on its structure and stability. To satisfy the 5:6 ration of the CoO and Ni lattice constants, we construct a supercell with 5x5 Co (O) and 6x6 Ni atoms per layer in the bulk regions. For the interface Ni layer and the adjacent Ni layer we consider different configurations. We study the binding energy and work of adhesion by first principles calculations. We find for an ideal CoO interface terminated by 5x5 O atoms that the structure is more stable if there are 5x5 Ni atoms next to it instead of 6x6 as in the bulk. In addition, we observe that a transition layer with 31 Ni atoms located between the interface 5x5 Ni and bulk 6x6 Ni layers (which partially reflects the structures of both these layers) enhances the stability of the CoO/Ni interface. We also extrapolate the behavior for the case that the interface is Co terminated. The electronic and magnetic modifications induced by the interface formation are discussed.

AS-02. Soft x-ray magnetic circular dichroism study of valence and spin states in FeT_2O_4 (T=V, Cr) spinel oxides. J.S. Kang[1], J. Hwang[1], D.H. Kim[1], E. Lee[1], W.C. Kim[2], C.S. Kim[2], H. Lee[3], J.Y. Kim[3], B. Kim[4] and *B.I. MIN*[4] *1. Physics, The Catholic University of Korea, Bucheon, Republic of Korea; 2. Physics, Kookmin University, Seoul, Republic of Korea; 3. Physics, Pohang Accelerator Laboratory, Pohang, Republic of Korea; 4. Physics, POSTECH, Pohang, Republic of Korea*

The crystal distortion due to the co-operative Jahn-Teller (JT) effect plays a crucial role in leading to charge ordering (CO) or orbital ordering (OO) in magnetic oxides. FeT_2O_4 (T=V, Cr) are good candidates for studying the effect of competition and/or cooperation between the orbital degrees of freedom at different sites. Electronic structures of spinel oxides FeT_2O_4 (T=V, Cr) have been investigated by employing soft x-ray magnetic circular dichroism (XMCD) and soft x-ray absorption spectroscopy (XAS). The measured XAS spectra reveal that Cr and V ions are trivalent and that Fe ions are nearly divalent in FeT_2O_4 (T=V, Cr). Finite XMCD signals are observed for FeV_2O_4, while negligibly weak XMCD signals are observed for $FeCr_2O_4$. The signs of the V and Fe 2p XMCD signals are opposite to each other, reflecting that the ordered magnetic moments of Fe^{2+} and V^{3+} ions are antiparallel to each other. It is found that the orbital ordering of V t_{2g} states occurs from the real orbital states and that the orbital moment of a V^{3+} ion is mostly quenched.

AS-03. Strain-engineered new magnetic order in YTiO3: a first-principles study. X. Huang[1] and *S. Dong*[1] *1. Department of Physics, Southeast University, Nanjing, 211189, China*

Transition metal oxides with the perovskite structure exhibit a wide variety of electronic phases with various electronic, magnetic, and orbital structures. Among these oxides, the RTiO3 family (R is a trivalent rare earth cation) also show plenty electronic phases just like manganites or cuprates, but have not been extensively studied yet. Here a first-principles calculation has been performed to study the epitaxial strain effects on the magnetic ground state in YTiO3 grown on LaAlO3 substrates. The experimental magnetic phase diagram of RTiO3 shows an antiferromagnetic (AFM)-to-ferromagnetic(FM) phase transition with the decreasing size of R cation. For example, LaTiO3 bulk with the largest cell and smallest lattice distortion is G-type AFM at low temperatures. In contrast, YTiO3 bulk is a rare example of a Mott insulator with a FM ground state. With epitaxial strain, it is possible to tune the physical properties and even creat some unique properties in thin films which do not exist in bulks. Here LaAlO3 is adopted as the substrate to give a in-plane compressive strain to YTiO3 film since the in-plane lattice constant of LaAlO3 is smaller than that of YTiO3. First, we compared four magnetic orders (FM, A-type, C-type and G-type AFM) for YTiO3 bulk. Our DFT calculations confirmed that the FM order has the lowest energy while the energy gap between FM and A-type AFM is the smallest. Second, by fixing the in-plane lattice constants to fit the LaAlO3 substract, the lattice of YTiO3 was relaxed along c-axis and the internal atomic positions are also relaxed. As expected, by varying the lattice constant along c-axis from 6.8Å to 8.6Å, our calculations show that the A-AFM order is stabler than FM order in a wide region, while the optimized the lattice constant along c-axis is 7.954Å which is just located in this region. This conclusion remains robust when the GGA+U method (U=3.2 eV for the d-electrons of Ti3+ ions) is adopted. In summary, by engineering a large out-of-plane lattice constant and small in-plane ones via substrate strain, a new magnetic order (A-type AFM) is induced in YTiO3 films which does not exist in any RTiO3 bulks.

M. Mochizuki and M. Imada, New J. Phys. 6, 154 (2004)

AS-04. Electronic structure and transport properties of superconducting Heusler topological insulators. *C. Shekhar*[1], A.K. Nayak[1], M. Nicklas[1], S. Ouardi[1], G.H. Fecher[1], W. Schnelle[1] and C. Felser[1] *1. Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany*

The discovery of topological insulators (Tls) has attracted much attention in not only understanding of their properties but also for potential applications [1, 2]. Tls are a class of quantum materials and belong to a new state of matter with topologically protected gapless Dirac fermionic states [1, 3]. The Heusler compounds are one of a major series predicted as 2D-topological properties. Besides topological property [4], YPtBi and LaPtBi also have non-centrosymmetric superconductors [5, 6]. The lack of crystalline inversion symmetry and nontrivial electronic topology are signatures for unconventional superconductivity and Majorana fermions. Therefore, it is encouraging and worthwhile to investigate the electronic structure and transport properties of theses superconducting Heusler topological insulators. The electronic structure was investigated by means of polarization dependent hard x-ray photoelectron spectroscopy. The linear dispersion of the bands at the Fermi energy is one hint for a topological insulator at the phase transition. In quantum mechanical systems, such a linear dispersion is a typical fingerprint of massless particles. YPtBi and LaPtBi show superconductivity below 1K remarkable features of the observed magneto resistance (MR). The MR is positive, nonsaturation and shows systematic variations with temperature