Actinides and Rare Earths Focus Topic
Room A215 - Session AC+LS+MI-MoM

Magnetism, Complexity, Superconductivity, and Electron Correlations in the Actinides and Rare Earths

Moderators: Krzysztof Gofryk, Idaho National Laboratory, Ladislav Havela, Charles University, Prague, Czech Republic

8:20am **AC+LS+MI-MoM1 Possible Structural Quantum Phase Transition in UCr2Si2 Accessed Through Cr → Ru Chemical Substitution***, Ryan Baumbach,* Florida State Universityy **INVITED**

Materials with intertwined magnetic, electronic, and structural degrees of freedom often can be tuned (e.g., using pressure or chemical substitution) to induce novel behavior, including unconventional superconductivity. Examples include the cuprates, iron based superconductors, and lanthanide/actinide-based compounds, and despite the their diversity of structure, chemistry and interaction mechanisms, their individual phase diagrams often conform to a semi-universal format that features a quantum phase transition. As a result, there have been prolonged efforts to develop new families of materials based on this paradigm. Even so, there still are few examples of f-electron intermetallics that combine both magnetic and structural quantum phase transitions. In this talk, we will present results from recent efforts to tune the ordered states of UCr_2Si_2, which is a Kondo lattice metal with antiferromagnetic ordering near $T_N \approx 24$ K and a structural phase transition near $T_S \approx 200$ K. In particular, we will focus on the influence of Cr to Ru chemical substitution, where we find that both T_N and T_S are rapidly suppressed towards separate quantum phase transitions. The impact of the quantum phase transitions on the structural, magnetic, and electronic properties will be examined in detail.

9:00am **AC+LS+MI-MoM3 Dynamic Spin Transport in Antiferromagnetic Insulators: Angular Dependent Spin Pumping in $Y_3Fe_5O_{12}$/NiO/Pt Trilayers***, Fengyuan Yang,* The Ohio State University **INVITED**

In recent years, pure spin transport driven by ferromagnetic resonance (FMR) spin pumping or a thermal gradient has attracted intense interest and become one of the most active frontiers in condensed matter and materials physics. Extensive research efforts have demonstrated pure spin currents in a broad range of materials, which enrich our understanding of dynamically-driven spin transport and open new paradigms for energy-efficient, spin-based technologies. Antiferromagnetic (AF) insulators possess various desired attributes, such as low loss and high speed up to THz frequencies, for future spintronic applications.

To probe the dynamic spin transport phenomena and the underlying mechanisms in AF insulators, we use high-quality $Y_3Fe_5O_{12}$ (YIG) epitaxial thin films excited by FMR as a source to inject spins into AF insulator NiO layers and detect the transmitted spin current using inverse spin Hall effect (ISHE) signals in YIG/NiO/Pt trilayers [1, 2]. We observed robust spin currents from YIG to Pt across AF insulators, which initially enhances the ISHE signals and can transmit spin currents up to 100 nm thickness, demonstrating highly efficient spin transport through an AF insulator carried by magnetic excitations. Recently, we studied the angular dependence of spin pumping in a series of YIG/NiO/Pt trilayers as the orientation of the applied magnetic field is rotated out of plane [3]. A simple sinusoidal angular dependence of V_{ISHE} has been viewed as a signature of spin pumping. Surprisingly, we observe an extensive plateau in the V_{ISHE} vs. ϑ_H plots with a pronounced peak feature at an out-of-plane angle of 45° to 60° when the measurement temperature is close to the Néel temperature (T_N) of NiO. This phenomenon can be understood as arising from the competition between the exchange coupling at the YIG/NiO interface, the easy-plane and in-plane easy-axis anisotropies of NiO, and the effect of the applied magnetic field. While insulating antiferromagnetic films can efficiently transmit spin currents and show promise for integration in spintronic devices, the underlying physics of spin ordering and dynamics is richer than currently understood.

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9:40am **AC+LS+MI-MoM5 Pressure Studies of Strongly Correlated Phases in Rare Earth Compounds***, Rena Zieve,* University of California, Davis **INVITED**

Various strongly correlated materials have complex low-temperature phase diagrams, exhibiting magnetism and superconductivity as well as spin glass, non-Fermi liquid, and other behaviors. Since each material has its own quirks, determining the underlying universal influences has been challenging. Pressure is a key tool in these efforts, since pressure can tune the interactions within a material without changing its chemical composition or impurities. I will discuss how hydrostatic or uniaxial pressure can probe strongly correlated materials by changing valence, breaking crystal symmetry, or altering the dimensionality of the electron system. I will draw examples from various rare earth compounds. Finally, I will mention recent pressure application techniques that expand the range of possible characterization measurements.

10:40am **AC+LS+MI-MoM8 Fermi Surface Reconstructions and Transport Properties in Heavy-fermion Materials***, Gertrud Zwicknagl,* Institut f. Mathemat. Physics, TU Braunschweig, Germany

The search for new types of exotic topological orders has recently rekindled the interest in Fermi surface reconstructions. Of particular interest are Electronic Topological (Lifshitz) transitions where the number of FS sheets changes abruptly under the influence of external parameters like chemical doping, pressure, or magnetic field. Lifshitz transitions (LTs) are generally associated with the presence of critical points in the electronic band structure, i. e., maxima, minima, or saddle points whose presence follows directly from lattice periodicity. As their separation from the Fermi energy is of the order of the bandwidth the critical points usually do not a ect the low temperature behavior. In heavy-fermion materials, however, magnetic fields can drive LTs which are reflected in pronounced anomalies in thermodynamic and transport properties. Here we demonstrate that the magnetic field-dependent anomalies in the Seebeck coefficient provide detailed information not only on the critical points, i. e., their character and position relative to the Fermi energy but also on the quasi-particle dispersion in the vicinity of the critical points, i. e., the effective mass tensor. For lanthanide-based HFS, the theoretical analysis is based on Renormalized Band (RB) structure calculations assuming that the heavy quasiparticles result from a Kondo effect. For U-based HFS, on the other hand, we adopt the "dual nature" model which allows for a microscopic description of the heavy bands. The calculated Lifshitz transitions reproduce the observed positions of anomalies in the Seebeck coecients surprisingly well.

11:00am **AC+LS+MI-MoM9 Direct Measurement the 5 $f_{5/2}$ and 5 $f_{7/2}$ Unoccupied Density of States of UO_2***, James G. Tobin,* University of Wisconsin-Oshkosh*; S. Nowak,* SLAC National Accelerator Laboratory*; C.H. Booth,* Lawrence Berkeley National Laboratory*; E.D. Bauer,* Los Alamos National Laboratory*; S.W. Yu,* Lawrence Livermore National Laboratory*; R. Alonso-Mori, T. Kroll, D. Nordlund, T.C. Weng, D. Sokaras,* SLAC National Accelerator Laboratory

In a world of ever increasing population and diminishing resources, the need for abundant and inexpensive energy remains critical. [1] Despite the problems associated with radioactive contamination/disposal and nuclear proliferation, electricity generated by nuclear power remains immensely important, [2] providing for 20% of the electrical grid of the USA and 50% or more for several European nations. [3-6] Uranium Dioxide (UO2) is by far the widely used nuclear fuel for the generation of electricity. [7] Thus, a fundamental understanding of the electronic structure of UO2 is crucial, if only to provide the best theoretical models for its disposal and storage. [7, 8]

Using High Energy Resolution Fluorescence Detection (HERFD) in a Resonant Inelastic Scattering (RIXS) experiment and electric dipole selection rules, the U 5f5/2 and U 5f7/2 Unoccupied Densities of States (UDOS) were determined. Significant changes were observed in going from UF4 (localized, 2 5f electrons) to UCd11 (localized, 3 5f electrons), consistent with the predictions of the Intermediate Coupling Model. The results for UO2 were experimentally confirmed by direct comparison with the Bremstrahlung Isochromat Spectroscopy for Uranium Dioxide.

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11:20am **AC+LS+MI-MoM10 Optimizing the Magnetic Performance of Tetragonal $ReFe_{12-x}M_x$ Phases by First Principles Computational Simulations**, ***Heike Christine Herper***, *O.Y. Vekilova, P. Thunström, O. Eriksson,* Uppsala University, Sweden

The increase of environmentally friendly energy production is coupled to an increasing demand for new magnetic materials. Especially, new Rare earth (Re) lean permanent magnets are highly sought after as possible replacement for high-performance magnets based on Nd-Fe-B and Dy to limit costs and supply risk. In this context the tetragonal 1:12 phase ($TmMn_{12}$) which contains 35% less Re than commercial Nd-Fe-B magnets are rediscovered. To stabilize this phase with light Re and Fe instead of Mn a nonmagnetic phase stabilizing element is needed but this degrades the magnetic performance.

To identify new 1:12 phases being suitable for permanent magnet applications materials design based on computational simulations has become an important tool. Here we focus on $ReFe_{12-x}M_x$. with Re = Y, Ce, Nd, Sm and M = Ti and V. We use state of the art density functional theory methods (VASP; full potential LMTO (RSPt)). The phase stability and the magnetic properties were calculated depending on the M concentration. Aiming to reduce the Re amount we monitor the performance depending on the Nd/Y ratio.

The key quantities are the magnetocrystalline anisotropy (MAE) and the magnetization. To capture the correct magnetic behavior, it is crucial to describe the localization of the 4f electron properly for each Re. While for Sm-based systems the spin-polarized core approximation is sufficient to describe the localized 4f electrons, it fails for Nd, e.g. the low temperature MAE of $NdFe_{11}Ti$ would be uniaxial instead of conic. Using a DFT+U approach with U = 5 eV, J = 1.1 eV for $NdFe_{11}Ti$ reproduces the experimentally observed behavior. Ce is special since the uniaxial MAE of $CeFe_{11}Ti$ is obtained independent from the treatment of the 4f electron. However, an analysis of the hybridization function analogue to [1] shows that a spin polarized core approximation is more appropriate for Ce-based 1:12 phases. For a deeper insight additional studies are carried out to examine the crystal field splitting.

With $SmFe_{11}V$ system a new phase was found leading to an increase of the magnetization by 17% compared to the commonly used concentrations of V. In view of the MAE a replacement of Nd by Y turned out to be preferable over a reduction of Ti. MAE values of 1.3 MJ/m^3 ($(NdY)Fe_{11}Ti$) and 1.7 MJ/m^3 ($SmFe_{11}V$) are predicted [2]. The latter could already be verified in recent experiments [2].

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11:40am **AC+LS+MI-MoM11 Optical Excitation Effect on Magnetodielectric and Photodielectric Properties of Rare Earth doped ZnO:Na Nanoparticles**, ***Mohammed Bsatee***, *F.P.N. Inbanathan,* Ohio University*; R. Martínez,* University of Puerto Rico*; H. Huhtinen,* University of Turku, Finland*; R. Palai,* University of Puerto Rico

There have been ongoing efforts in developing rare earth (RE) ions doped semiconductors responsive to optical and magnetic stimuli for developing multifunctional devices. ZnO is considered as a promising semiconductor with wide range of applications in optoelectronics and spintronics due to its optical properties (*i.e*. direct band gap, high electron mobility, high thermal stability, strong absorption of UV), and at the same time being an attractive host for RE doping resulting in enhanced spin polarization in ZnO:RE matrix [1]. In this project, undoped and RE ions (Er and Yb) doped and co-doped ZnO:Na nanoparticles were studied with an aim to understand recently reported magnetodielectric and photodielectric effects stimulated by magnetic field and UV excitation stimuli [2]. After synthesizing well-defined Er and Yb-co-doped ZnO:Na by sol-gel route, evaluation of structural, optical, magnetic and electrical characteristics of synthesized nanoparticles was performed. Structure, morphology, and composition of the samples were analyzed by XRD and SEM showing high quality hexagonal crystal structure. The absence of secondary phases was confirmed by Raman spectroscopy and XPS analysis of all elements in ZnO:NaErYb compound. Optical properties were investigated by optical reflectance spectroscopy, photoluminescence (PL), PL excitation, and PL kinetics with photons excitation energy corresponding to above and below bandgap energy. PL spectra were investigated under magnetic field of up to 2 Tesla in 7 K – 400 K temperature range. It was observed that PL spectra exhibit broad green-yellow defects emission band without NBE excitonic peak. PLE spectra revealed that both Er^{3+} and Yb^{3+} ions are optically active and involved in complex energy transfer between ZnO:Na host and 4f-shall levels of RE^{3+} ions dopants. PL spectra show features related to intra-shell 4f-4f transitions of the Er^{3+} ion (at 522 nm) and Yb^{3+} ion (at 980 nm). It was observed that luminescence decay of the ZnO defect band is unexpectedly long (> tens of 10^{-3} second), strongly affected by RE^{3+} ions doping and depends on the magnetic field strength when excited at 3.814 eV. In the presentation we will attempt to correlate reported magnetodielectric and photodielectric properties of the Er,Yb-co-doped ZnO:Na [2] with observed optical characteristics.

References

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