Actinides and Rare Earths Focus Topic
Room 202C - Session AC+MI+SA-WeM

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

Moderators: Melissa Denecke, University of Manchester, UK, David Geeson, AWE, James Tobin, UW Oshkosh

8:00am **AC+MI+SA-WeM-1 Strong electron-electron Interactions in the Actinides: Using Organometallics to Probe Delocalization Effects**, *Corwin Booth*, Lawrence Berkeley National Laboratory **INVITED**

Systems exhibiting strong electron-electron interactions remain at the forefront of inquiry into complex properties of condensed matter systems due to their exciting properties (eg. superconductivity) and their resistance to being understood on a fundamental level. A bottleneck toward a better understanding has been the difficulty of the required many-body calculations for extended solids. Alternatively, calculations on small molecules require fewer and better approximations, potentially offering a better description. Although strong electron-electron interactions are well established in extended solids, recent work on lanthanide organometallic coordination compounds has demonstrated the importance of such interactions, fueled by the propensity for certain 4f orbitals to be partially delocalized. Meanwhile, recent work on the actinides challenges the canonical view that the 5f electrons can bond in the light actinides but are essentially localized in the heavier actinides. A major stumbling block for such work is the paucity of known structures for elements beyond Am in the periodic table.

For the discussion presented here, work on Ce and Yb organometallics will provide context in terms of f-occupancy and in bonding characteristics and the effect on magnetism. The role of strongly electron interactions will be described in terms of configuration interaction (CI) and related calculations. Occupancy is measured using Ln L_{III}-edge x-ray absorption near-edge structure (XANES) techniques, and local structure (EXAFS) measurements demonstrate the final effect on the bonding at the metal center. Of particular interest is what happens in formally Ce(IV) systems that exhibit strong interactions.

XANES measurements of actinides are more difficult to interpret and will be discussed. The focus will be, however, on EXAFS measurements across the An series in the presence of strongly oxidizing ligands. Chosen ligands include hydroxypyridonone (HOPO), with less oxidizing ligands, such as diethylenetriaminepentaacetic acid (DTPA) used for comparison. Cations include Th, U, Pu, Am, Cm, Bk, and Cf. Discussions will center on nearest-neighbor bond lengths, using DFT calculations as a guide. The surprising role of covalency in the late actinides will be considered, both in terms of the EXAFS results and in terms of the edge shifts.

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8:40am **AC+MI+SA-WeM-3 Structure and Magnetism of U-based Thin Films and Heterostructures**, *Evgeniya Tereshina-Chitrova*, Institute of Physics, Academy of Sciences of the Czech Republic, Czech Republic; *L Havela*, Charles University, Prague, Czech Republic; *T Gouder, Z Bao*, Institute for Transuranium Elements, Germany; *M Dopita*, Charles University, Prague, Czech Republic; *R Caciuffo*, Institute for Transuranium Elements, Germany **INVITED**

Uranium is the basic component of most nuclear fuels. The production of uranium-based films has advantage over bulk materials studies as it allows performing advanced physics and chemistry experiments on small amounts of radioactive material and on its clean and smooth surfaces. Other interesting field is uranium magnetism. Although uranium itself is non-magnetic, uranium compounds display a rich variety of magnetic phenomena intimately related to the variable character of the 5f electron states [1]. Additional degrees of freedom can be used in thin films, in which the reduced dimensionality and structure modifications far exceed the limits imposed by thermodynamics, obeyed in bulk systems. We review the achievements in the field of sputter-deposited films, in which variations of deposition conditions can dramatically suppress crystallinity of the deposited material. The 5f itinerant magnetic systems (as US or UN [2]) react to the low substrate temperatures and high deposition rates by decreasing ordering temperatures and eventually by the loss of U magnetic moments. The strong ferromagnetism of uranium hydride is, on the other hand, almost insensive, which underlines its local-moment character.

The possibility to combine films of various materials on the nanostructure scale can also give rise to new functionalities. For example, the exchange bias (EB) effect [3], arising as a result of combination of a ferromagnet biased by exchange interaction at the interface to an antiferromagnet, is particularly interesting if uranium magnetics are involved. The new ingredient, strong spin-orbit interaction, can lead to very strong magnetic anisotropy, which represents an essential parameter. We have been systematically studying films of Fe_3O_4 (ferromagnet) grown using different substrates on the top UO_2, playing the role of biasing antiferromagnet [4]. The resulting high bias field (> 0.2 T) and a proximity effect, in which the high Curie temperature of Fe_3O_4 provides the EB functionality even at temperatures exceeding ordering of UO_2, demonstrate the promising aspects of using actinides in this non-traditional way.

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9:20am **AC+MI+SA-WeM-5 Field Induced Lifshitz Transitions in URu2Si2**, *E Calegari*, Univ Federale Santa Maria, Brazil; *S Magalhaes*, Universidade Federale Rio Grande do Sul, Brazil; *Peter Riseborough*, Temple University **INVITED**

We report calculations on an unusual phase of the Under-screened Anderson Lattice (UAL) model, the so called spin-dependent inter-orbital density wave that has been proposed as describing the ``Hidden Order" (HO) phase of URu2Si2.

We determine the effects of an applied magnetic field. Since the order parameter describes an ordering in the x-y plane, the electronic properties of the system are anisotropic below the critical temperature THO. We show that the magnetic susceptibility becomes anisotropic below THO. Furthermore, for fields applied along a spontaneously chosen hard axis, THO decreases towards zero and that the HO transition changes from second order to first order at a large value of the magnetic field. Also, we find that the system undergoes a cascade of field-induced Lifshitz transitions and also show how these properties originate from the dependence of the quasi-particle bands on the orientation of the applied field. The good qualitative agreement with experimental findings provides strong support for the proposed description of the HO phase as a spin-dependent inter-orbital density wave phase.

11:00am **AC+MI+SA-WeM-10 New Form of Uranium Hydride - UH2**, *Ladislav Havela*, M Paukov, M Dopita, L Horak, P Minarik, M Divis, I Turek, Charles University, Prague, Czech Republic; *D Legut*, VSB-Technical University of Ostrava, Czech Republic; *T Gouder, A Seibert, F Huber*, European Commission - Joint Research Centre; *E Tereshina-Chitrova*, Institute of Physics, Academy of Sciences of the Czech Republic, Czech Republic

Most of *f*-elements form with hydrogen both di- and trihydrides. Actinide and rare-earth dihydrides occur, as a rule, in the CaF_2 structure type. Uranium represents an exception, only UH_3 is present in the binary phase diagram. It exists in two different structure types. The metastable form α-UH_3 forms in the Cr_3Si structure type, which is in fact *bcc* U lattice filled with hydrogen. The stable form β-UH_3 has a larger cubic cell with two different U sites. Both forms are ferromagnets with the total U moment of ≈ 1 μ_B/U and the Curie temperature T_C ≈ 165 K. We have recently synthesized UH_3 thin films using a reactive sputter deposition. XRD analysis indicated the β-UH_3 structure, modified by a pronounced (00l) texture and compressive residual strains imposed by the deposition dynamics. Magnetization measurements proved T_C = 165 K.

The sputter deposition on a cooled substrate (*T* = 170 K) using Si wafer the crystal structure turned different. The deposited material is undoubtedly cubic, of the *fcc* type, and the lattice parameter a = 5.3598 ± 0.0014 Å is very close to that of PuH_2 (a = 5.359 Å) and NpH_{2+x} (a = 5.343-5.355 Å). Hence we can assume that UH_2 in the fluorite structure has been formed. The key role in stabilization plays likely the effect of substrate (Si has a = 5.431 Å) in combination with low temperature deposition. The UH_2 film was subsequently subjected to magnetization measurements, which indicated a ferromagnetic ground state with T_C ≈ 125 K. This is lower than in the UH_3 phases, although the U-U spacing in UH_2 should be higher, 3.78

Å, than in both UH_3 phases (3.31 and 3.60 Å for β- and α-UH_3, respectively). This fact points to the U-U interaction being more important than the U-U spacing. The ferromagnetic state is also the ground state obtained from ab-initio calculations. Scalar relativistic calculations (LDA) for experimental lattice parameter yield the spin moment μ_S = 2.0 μ_B/U. LDA+U (U = 2.25 eV) gives the equilibrium lattice parameter a = 539.9 Å, i.e. 0.7% larger than the experimental one, the ferromagnetic ground state with (111) easy-magnetization direction and the magnetic anisotropy energy E_a = 9 meV. The total moment 0.45 μ_B/U consists of 2.59 μ_S and -3.04 μ_L.

11:20am AC+MI+SA-WeM-11 Tuning of Electronic Properties of U- and RE-Metallic Systems by H Absorption, *Silvie Maskova,* Charles University, Prague, Czech Republic; *K Miliyanchuk;* Ivan Franko National University of Lviv, Lviv, Ukraine; *A Kolomiets,* Lviv Polytechnic National University, Lviv, Ukraine; *L Havela,* Charles University, Prague, Czech Republic

The sensitivity of the interactions in the intermetallic systems to modification of the crystal structure makes the experimental techniques involving alteration of the atomic arrangement especially important. Various studies under compression are well-known examples of such methods. From this point of view hydrogenation can be treated as a complementary technique that provides „negative" pressure. Hydrides can be defined as compounds for which the hydrogen absorption leads to the modifications of the crystal structure, such as pure lattice expansion or the formation of a new structure. As a result, the new compounds (hydrides) exhibit qualitatively new physical properties and such modifications provide us with additional information on the peculiarities of interatomic interactions in the initial compounds.

As an example, we will compare the impact of H absorption on U- and RE-compounds using A_2T_2X (A = Rare-Earth (RE) or actinide, T = transition metal, X = p-metal) compounds crystallizing in the tetragonal Mo_2FeB_2 structure type (space group $P4/mbm$). U_2T_2X interact with H_2 only at high pressure (≈ 100 bar) reaching 2 H/f.u. The H absorption produces a lattice expansion (lower than 10 %), while the tetragonal structure is preserved. Higher H concentrations, which can be achieved in some RE_2T_2X compounds (up to 8 H atoms/f.u), lead to amorphization or structure symmetry changes (with volume expansion exceeding 20 %), imposed by a minimum H-H distance requirement.

Magnetic properties of U-compounds strongly depend on the U-U distances. Hydrogen intrusion modifies the lattice by expanding it without changing the crystal-structure type leading to a 5f band narrowing. As a consequence, doping of U intermetallics by interstitial hydrogen leads to stronger magnetic properties. On the other hand, the hydrogen absorption has opposite effect on magnetic properties of RE_2T_2X compounds. For RE compounds, hydrogenation affects mainly the inter-site exchange interaction, which is weakened presumably by reducing the concentration of conduction electrons, responsible for the RKKY interaction.

11:40am AC+MI+SA-WeM-12 Magnetic Structures of U_nRhIn_{3n+2} Materials, *Attila Bartha,* M Klicpera, Charles University, Prague, Czech Republic; *P Cermak,* Forschungszentrum Juelich GmbH, Germany; *B Ouladdiaf,* Institute Laue-Langevin, France; *J Custers,* Charles University, Prague, Czech Republic

In the past decade, U-compounds crystallizing in the $HoCoGa_5$-type structure (P4/mmm), frequently referred to as 115, have been in the focus of attention in experimental and theoretical research. Vigorous activities have been motivated by the high superconducting transition temperature of T_c = 8.7K in $PuRhGa_5$ [1] and T_c = 18.5K in $PuCoGa_5$ [2]. No further superconductivity has been reported in neither U-115 nor in the closely related U_2TGa_8 compounds (T = transition metal). However, interesting magnetic properties have been observed: neutron scattering experiments revealed that $UNiGa_5$ exhibits the G-type antiferromagnetic (AFM) phase, while $UPdGa_5$ and $UPtGa_5$ exhibit the A-type AFM state. Note that G-type indicates a 3D Néel state, while A-type refers to a layered AF structure where spins align FM in the ab plane and AFM along the c axis [3]. The difference in the two magnetic structures is significant since it implies a sign change of the nearest-neighbor (NN) interaction.

Here we report on the magnetic structures of $URhIn_5$ and U_2RhIn_8, two new members of the $U_nT_mX_{3n+2m}$ (X=In,Ga) family of compounds [4]. $URhIn_5$ displays AFM order below T_N = 98K. The observed increase of the resistivity for current parallel [100], [110] and [001] are reminiscent to a spin-density

wave (SDW) type of transition with the gap opening first along the [001] direction [5]. U_2RhIn_8 enters the AFM state at T_N = 117K. No increase in resistivity in the vicinity of T_N is found which would hint to a SDW gap opening. Neutron diffraction experiments on $URhIn_5$ were performed at the Heinz Maier-Leibnitz Zentrum (MLZ) in Garching using the triple axis spectrometer PANDA. Single crystals with accumulated mass of 10mg where glued on an Al-plate. Our results confirmed the magnetic propagation vector **k**=(1/2,1/2,1/2) predicted by NMR experiments [6] and a magnetic moment of 1.65 μ_B/U^{3+}. The neutron study on U_2RhIn_8 has been conducted at ILL, Grenoble using D10 on only one single crystal with m ≈ 1mg. Analysis revealed a propagation vector **k**=(1/2,1/2,0) and an ordered moment of 1.7 μ_B/U^{3+}. UIn_3, $URhIn_5$ and U_2RhIn_8 all show G-type AFM phase. While the c-axis parameter differs significantly the a lattice parameter equals 4.601Å, 4.621Å and 4.6056Å respectively, being a change of less than 1% pointing to the fact that the NN coupling is important for the type of magnetic structure.

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12:00pm AC+MI+SA-WeM-13 Insights into the Magnetic Dead Layer in $La_{0.7}Sr_{0.3}MnO_3$ Thin Films from Temperature, Magnetic Field and Thickness Dependence of their Magnetization, *Navid Mottaghi,* M Seehra, R Trappen, S Kumari, C Huang, S Yousefi, G Cabrera, A Romero, M Holcomb, West Virginia University

Detailed dc magnetization (M) measurements of a 7.6 nm $La_{0.7}Sr_{0.3}MnO_3$ thin film samples is investigated. The sample was fabricated by pulsed laser deposition. Zero-field-cooled (ZFC) M vs. applied field (H) cooled down to T = 5 K reveal the presence of negative remanent magnetization (NRM) as well as in ZFC M vs. temperature (T) measurements in H = 50 Oe and 100 Oe. ZFC and FC (field-cooled) protocols are used to determine the blocking temperature T_B in different H. Isothermal hysteresis loops at different T are used to determine the temperature dependence of saturation magnetization (M_S), remanence (M_R) and coercivity H_C. The M_S vs. T data are fit to the Bloch law, $M_S(T) = M_0(1 - BT^{3/2})$, showing a good fit for T < 100 K and yielding the nearest-neighbor exchange constant $J/k_B \cong 18$ K. The variations of T_B vs. H and H_C vs. T are well described by the model often used for randomly oriented magnetic nanoparticles with magnetic domain diameter ≈ 9 nm present in the dead-layer of thickness d =1.4 nm. Finally, the data available from literature on the thickness (D) variation of Curie temperature (T_C) and M_S of LSMO films grown under 200, 150, and 0.38 mTorr pressures of O_2 are analyzed in terms of the finite-size scaling, with M_S vs. D data fit to $M_S(D) = M_S(b)(1-d/D)$ yielding the dead layer thickness d = 1.1 nm, 1.4nm and 2.4 nm respectively.

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