Actinides and Rare Earths Focus Topic
Room 318 - Session AC+LS+MI-WeM

Magnetism, Electron Correlation, and Superconductivity in the Actinides/Rare Earths

Moderators: James G. Tobin, University of Wisconsin-Oshkosh, **Ladislav Havela**, Charles University, Czech Republic, **Gertrud Zwicknagl**, Technical University Brauschweig, Germany

8:00am **AC+LS+MI-WeM-1 The Relation between Crystal Chemistry and Superconductivity in Actinide-Based Superconductors***, **Eteri Svanidze,*** Max Plank Institute, Dresden, Germany **INVITED**

Crystallographic features play an important role in the physical and chemical properties of a given solid-state material. In particular, actinide-based systems exhibit a wide range of properties – from unconventional superconductivity to peculiar magnetic orders. In this talk, I will highlight some of the old and new actinide-based superconductors, in which a delicate interplay between chemistry and physics is observed. A comprehensive characterization of properties of UBe_{13} has revealed a deep interrelation between the physical and chemical features. Notably, single crystals of this material tend of include many defects which have a dramatic effect on superconducting state [1]. Motivated by this issue, an alternative method of studying intrinsic properties is investigated [2-4]. By creating a micro-scale device, it is possible to measure intrinsic superconductivity of UBe_{13}, whichhas so far remained out of reach [4]. The properties of UBe_{13} are compare to those of other actinide-based superconductors – UTe_2 [5] and $Th_4Be_{33}Pt_{16}$ [6] – in which a strong coupling of lattice and superconducting properties is observed. By studying these systems, it is possible to expand the understanding of crystal chemistry of solid-state materials, while simultaneously providing an insight into which crystallographic parameters impact the physical properties of a given solid-state material.

[1] A. Amon *et al.*, “Tracking aluminium impurities in single crystals of the heavy-fermion superconductor UBe_{13},”*Sci. Rep.***8**, 10654 (2018)

[2] E. Svanidze *et al.*, “Revealing intrinsic properties of UBe_{13}”, *in preparation* (2022)

[3] A. Amon *et al*., "Interplay of atomic interactions in the intermetallic semiconductor Be_5Pt", *Angew. Chem. Int. Ed.***58**, 2 (2019).

[4] I. Antonyshyn *et al*., "Micro-scale device - an alternative route for studying the intrinsic properties of solid-state materials: case of semiconducting TaGeIr", *Angew. Chem. Int. Ed.***59**, 2 (2020)

[5] E. Svanidze *et al.*, “Intrinsic crystal structure of UTe_2”, *in preparation* (2022)

[6] P. Kozelj *et al.*, “A noncentrosymmetric cage superconductor $Th_4Be_{33}Pt_{16}$”, *Sci. Rep.***11**, 22352 (2021)

8:40am **AC+LS+MI-WeM-3 Revealing The Beauty of Uranium Compounds:the UMB_4 (M=V, Cr, Fe, Co, Mo, W, Re, Os) and UFe_xSb_2 Cases***, **Antonio Pereira Gonçalves,*** Instituto Superior Técnico, Univ. Lisboa, Portugal **INVITED**

Uranium-based phases with d-metals show a vast and rich variety of physical properties, some of them unique, which are mainly driven by the large 5*f* spin-orbit coupling and the degree of delocalization of the 5*f* states. The understanding of such behaviors is critical for the advance of Solid State Sciences and can lead to the discovery of new phenomena and ground states. In this talk, examples of uranium compounds with unusual properties are presented, the focus being on UMB_4 materials and UFe_xSb_2 alloys.

UMB_4 (M=V, Cr, Fe, Co, Mo, W, Re, Os) compounds are quite notable, crystallizing in the $YCrB_4$-type (for V, Cr, Fe, Co) and $ThMoB_4$ type (for Mo, W, Re, Os) polymorphs. Both structures are closely related, containing the same number of atoms in the unit cell and similar coordination polyhedral, which allows the comparison of their properties as a function of the d-metal. Their electronic structure is influenced by a strong hybridization between the B-2*p* states and both the *d*-metals *d*-states and the uranium (5*f*) valence band states. This avoids the formation of narrow bands with high density of states at the Fermi level, even if the 5*f*-*d* hybridization is weak, i.e. for late d-metals. Hence, the explored UMB_4 compounds are weak Pauli paramagnets, with a density of states at Fermi level of only ~4 times higher than for α-U. Those crystalizing in the $ThMoB_4$ structure show anomalous lattice vibrations, in particular the presence of low-energy Einstein modes, which can lead to superconducting ground states.

UFe_xSb_2 alloys crystallize in the $HfCuSi_2$ type structure and present a remarkable ground state evolution with Fe concentration. $UFe_{0.5}Sb_2$ shows a non-Fermi liquid behavior, with a change from metallic to semiconductor-upon applying magnetic field. In contrast, $UFe_{0.7}Sb_2$ (and, in a minor scale, $UFeSb_2$), shows an increase in electrical resistivity with decreasing temperature under zero magnetic field, but for high magnetic fields a metallic behavior is established. First principles calculations indicated that in $UFeSb_2$ some bands cross the Fermi level, but they are relatively steep and, as a result, the density of states at Fermi level is low, which supports the semi-metallic character of this composition. In the case of $UFe_{0.5}Sb_2$, a higher concentration of bands at the Fermi level, some of them relatively flat, exist, which cause a sudden step-shaped drop of density of states just above Fermi level. The magnetic field application can raise the Fermi level into the pseudo-gap, which is probably the reason for the change from a metallic-like to a semiconductor-like behavior.

11:00am **AC+LS+MI-WeM-10 Uranium Hydrides Revisited***, **Ladislav Havela,*** Charles University, Faculty of Mathematics and Physics, Czechia*; D. Legut,* VSB Technical University Ostrava, Czechia*; J. Kolorenc,* Institute of Physics, Czech Academy of Sciences, Czechia

Uranium hydrides are not only materials important for understanding of fundamental aspects of actinides. They are also relevant for nuclear technologies as well as for specific hydrogen storage tasks, as e.g. storing of tritium in nuclear fusion devices. Electronic structure of uranium hydrides (α- and β-UH_3, UH_2) reflects two contradictory tendencies. One is a charge transfer from U towards H, the other is a stability of the *f* shell. The latter is illustrated also on the case of rare earth hydrides with anomalous rare earth elements, such as Yb or Eu, which surprisingly retain their lower valence state, i.e. with a higher *f*-occupancy. The transfer is thus realized in U by the 6*d* and 7*s* electrons, which become noticeably depleted, but the 5*f* occupancies remain high. The concomitant reduction of the 5*f*-6*d* hybridization contributes, together with the volume expansion, to pronounced ferromagnetism of the U hydrides with Curie temperatures far above 100 K. We compare individual hydrides described by the GGA+*U* calculations, yielding numbers on the charge transfer or spin and orbital moments, with relevant experimental data. Interesting feature obtained from calculations is that the two different U sites in β-UH_3 have the respective magnetizations non-collinear. The same calculations yield also phonon dispersion relations, which are used to determine the temperature dependence of phonon contribution to heat capacity. The agreement in the paramagnetic range is so good that it allows to determine both the magnetic entropy and changes of the Sommerfeld coefficient between the ground state and paramagnetic state, the latter being twice higher. The position of the U hydrides on the map of localization-delocalization dichotomy will be discussed.

The work was supported by the Czech Science Foundation under the grant No. 21-09766S.

11:20am **AC+LS+MI-WeM-11 Towards a Better Understanding of the Rkky Interaction in Ce- and Yb-Based Compounds: Anisotropies from Cef Effects and Fermi Surfaces***, **Gertrud Zwicknagel,*** Institut für Mathematische Physik, Germany*; V. Zevin,* The Racah Institute of Physics, Israel

We calculate the influence of Crystalline Electric Field (CEF) effects and the Fermi surface topology on the indirect Ruderman-Kittel-Kasuya-Yoshida (RKKY) exchange interaction between local 4f moments in Ce- and Yb-compounds. Starting from a periodic Anderson model, we show that the anisotropy of the CEF ground state manifests itself in the anisotropy of the effective exchange coupling constant J(R,R’) between two moments at sites R and R’. If spin-orbit effects among the conduction states can be neglected, the interaction between two Kramers doublets is isotropic in pseudo-spin space. Adopting the Stationary Phase approach, we derive the asymptotic form of the exchange constant for arbitrary Fermi surfaces. We evaluate the anisotropy of the RKKY interaction in tetragonal Ce- and Yb-122 compounds for realistic model bands. The influence of spin-orbit interaction among the conduction electrons is discussed.

11:40am **AC+LS+MI-WeM-12 Mechanically Forced Tuning of Interactions in Tetragonal 221 Intermetallics*, Petr Král,*** *J. Prchal,* Charles University, Czech Republic*; J. Kaštil,* Czech Academy of Sciences, Czech Republic*; D. Daisenberger,* Diamond Light Source, UK*; D. Staško,* Charles University, Czech Republic

Family of R_2T_2X intermetallics adopting the tetragonal Mo_2FeB_2-type crystal structure represents the group of anisotropic systems with potential to exhibit geometrical frustration effects due to the Shastry-Sutherland-like arrangement of *R*-atoms in the aa-planes alternated by usually non-magnetic *T-X* planes along the crystallographic *c*-axis. Crucial for resulting magnetic behavior are the interatomic distances affecting the exchange interactions between individual ions. Especially interesting may be the compounds close to the empirical boundary of crystal structure stability since, based on available data, the lowest observed unit-cell volume among Mo_2FeB_2-type materials is about $V_{\mathrm{f.u.,crit}}$ = 200 Å^3.

The unique tool allowing to act directly on the interatomic distances without changes of chemical composition is mechanical pressure. Employing the high-pressure techniques, it is possible to influence all lattice-related physical properties including e.g. the magnetic interactions and electronic structure. Especially in the strongly anisotropic compounds, the hydrostatic pressure effect depends on the compressibility of individual lattice parameters. This is the case, when the uniaxial pressure may represent the opportunity to act selectively in chosen crystallographic directions and thus to provide the insight into the layout of interactions within the crystal lattice.

Herewith, we are presenting the results of systematical study of pressure impact on the R_2T_2X compounds. Special attention is paid to Ce_2Pd_2In considered to be one of the most interesting systems among R_2T_2X family. It represents the rare example of Ce-based ferromagnet, however the ground state is reached through the antiferromagnetic interphase. High sensitivity of magnetic behavior to hydrostatic pressure has been revealed showing the preference of antiferromagnetic phase at lower pressures followed by the Kondo-like anomaly formation and suppression of magnetic ordering at pressures around 4 GPa. Based on the results of high-pressure XRD experiment, the hydrostatic pressure acts more significantly within the basal plane. Indeed, different response to the uniaxial pressure applied along the *c*-axis was observed.

Compounds with the unit-cell volume closest to $V_{\mathrm{f.u.,crit}}$ belongs to the series R_2Cu_2In. Among them the ferromagnets Dy_2Cu_2In (exhibiting the signs of spin-reorientation at lower temperatures) and Tm_2Cu_2In (with signs of spin-glass behavior) were investigated. Concerning the later one, the pressure was found to support the frustration effects responsible for the spin-glass properties as the unit-cell volume tends to reach the $V_{\mathrm{f.u.,crit}}$.

12:00pm **AC+LS+MI-WeM-13 Effects of O_2 Growth Pressure on the Magnetization of $LaMnO_3$-$SrTiO_3$ Thin Films*, Ghadendra Bhandari,*** West Virginia University*; R. Trappen,* University of Waterloo*; N. Mottaghi, M. Holcomb,* West Virginia University

Magnetic properties of epitaxial $LaMnO_3$ thin films grown on $SrTiO_3$ substrate have been studied. Thin films are grown at various oxygen pressure using pulsed laser deposition and deposition has been monitored by reflection high energy electron diffraction (RHEED) to verify layer-by-layer growth. Bulk stoichiometric $LaMnO_3$ exhibits A-type antiferromagnetic order, whereas thin films show a ferromagnetic FM phase. Structure and magnetic properties have been characterized by X-ray diffractometry (XRD), X-ray reflectivity (XRR) and vibration sample magnetometry (VSM). The thin films are showing ferromagnetic (FM) phase. Depth dependent magnetization studied by polarized neutron beam reflectivity found that magnetization is higher near interfacial region and a magnetically dead region lies at the surface. We have observed c-lattice correlated magnetization, which is minimized at 30mTorr O_2 pressure.

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