Actinides and Rare Earths
Room 207 A W - Session AC+MI-ThM

Superconductivity, Magnetism, Electron Correlation and Complex Behavior

Moderators: Krzysztof Gofryk, Idaho National Laboratory, **James G. Tobin**, University of Wisconsin-Oshkosh

8:00am **AC+MI-ThM-1 Phase Transition and Magnetism in UTe_2, *Dominik Legut,*** VSB - Technical University of Ostrava, Czechia*; Alexander Shick,* Institute of Physics CAS, Prague, Czechia*; Urszula Wdowik,* VSB - Technical University of Ostrava, Czechia **INVITED**

For the magnetic properties of UTe_2 the correlated band theory implemented as a combination of the relativistic density functional theory with exact diagonalization [DFT+U(ED)] of the Anderson impurity term with Coulomb repulsion U in the 5*f* shell needs to be applied. This allows us to determine the orbital to spin ration as well as number of the uranium valence states in close correspondance with recent experiment (XANES, XMCD). The uranium atom 5*f* -shell ground state with 33% of f^2 and 58% of f^3 configurations is determined[1]. In contrast to the above, for the bonding in UTe_2 it is satisfactory to be modelled by DFT+U methodology. We theoretically determined the lattice contribution to the specific heat of UTe_2 over the measured temperatures ranging from 30 to 400 K as well as the the orthorhombic-to-tetragonal phase transition pressure of 3.8 GPa at room temperature in very good agreement with the recent experimental studies. Last, but not least we determined the Raman spectra that were compared with recent Raman scattering experiments as well.

[1] A. B. Shick, U. D. Wdovik, I. Halevy, and D. Legut, Spin and Orbital Magnetic Moments of UTe_2 induced by the external magnetic field, Scientific Reports **14**, 25337 (2024), https://doi.org/10.1038/s41598-024-75321-4.

[2] U. D. Wdowik, M. Valiska, A. Cabala, F. Borodavka, E. Samolova, and D. Legut, Raman spectroscopy and pressure-induced structural phase transition in UTe_2, Frontiers of Physics, **20**, 014204 (2025), https://doi.org/10.15302/frontphys.2025.014204.

8:30am **AC+MI-ThM-3 Single-ion Anisotropy Controls Magnetic Excitations in $REMn_6Sn_6$ (RE = Tb, Dy, Ho) Ferimagnetic Kagome Metals**, ***Kelsey Collins,*** *Michael Susner, Michael Newburger,* Air Force Research Laboratory, Materials and Manufacturing Directorate, USA

The $REMn_6Sn_6$ family of materials, where RE is a generic rare earth trivalent cation, have attracted much interest due to their complex electronic and magnetic structures. This complexity arises from the coupling of highly anisotropic lanthanide ions spins with large spin-orbit couplings to the spins of the Mn atoms, which are arrayed in a kagome lattice, a lattice topology known to give rise to exotic topological phenomena. This interplay of magnetic anisotropy and electronic topology motivates investigation into the magnetic excitations of these materials, which unlike the ground state magnetic structures of this family have not been extensively studied. Herein, we use Brillouin light scattering to measure the magnon spectra of $TbMn_6Sn_6$, $DyMn_6Sn_6$, and $HoMn_6Sn_6$, measuring the magnon frequency, lifetime, and intensity as a function of applied magnetic field and sample temperature. We find that the identity of the lanthanide effectively tunes the frequency of the magnon over a range from ~18 GHz (Tb) to ~5 GHz (Ho) at zero applied field. Despite the difference in the magnetic ground states between a canted easy-axis (Tb) and easy-cone (Dy, Ho) spin orientation, these three congeners respond remarkably similarly to a magnetic field. Quantitative fitting of the three magnon dispersions reveals that the tuning of the magnon frequencies stems primarily from the differing magnetic anisotropies of the lanthanide ions. This work demonstrates that the anisotropy of the trivalent ion controls not only the magnetic ground state, but also the magnetic excitations, in this family of topological magnets.

8:45am **AC+MI-ThM-4 Suppression of the CDW State in UPt_2Si_2 by Ir Substitution; 5*f* States Into Bonding**, ***Ladislav Havela,*** Charles University, Faculty of Mathematics and Physics, Czechia*; Volodymyr Buturlim,* Idaho National Laboratory*; Silvie Cerna, Oleksandra Koloskova,* Charles University, Faculty of Mathematics and Physics, Czechia*; Daniel Chaney,* ESRF, Grenoble, France*; Peter Minarik,* Charles University, Faculty of Mathematics and Physics, Czechia*; Mayerling Martinez Celis,* CRISMAT, University of Caen, France*; Dominik Legut,* Charles University, Faculty of Mathematics and Physics, Czechia

5*f* states in light actinides adopt either an itinerant, i.e. bonding, nature, or they preserve their localized atomic character similar to free ions and they stand aside from bonding. The large pool of known U intermetallics comprises mainly compounds with itinerant 5*f* states. One of exceptions is arguably UPt_2Si_2, at which some features of 5*f* localization were identified [1,2]. One of its interesting features is the Charge Density Wave (CDW) with a propagation vector (0.42,0,0), developing below T = 320 K [3]. Importantly, practically identical CDW appears also in multiple rare-earth isotypes $REPt_2Si_2$ with localized (or empty) 4*f* states, all crystallizing in the tetragonal structure type $CaBe_2Ge_2$[4]. While the CDW phenomenon is very interesting per se (one can discuss whether it is primarily due to phonon softening of Fermi surface nesting), one can also assume it as a sensitive indicator of the 5*f* localization. The only U-based sibling, UIr_2Si_2, is undoubtedly an itinerant antiferromagnet and no CDW has been reported.

Here we describe results of the study of the pseudo-ternary system $U(Pt_{1-x}Ir_x)_2Si_2$. The γ coefficient of 32 mJ/mol K^2 of UPt_2Si_2 starts to increase for $x > 0.05$, reaching 100 mJ/mol K^2 for 20% Ir, which indicates that the localization with 5*f* states out of the Fermi level is suppressed already for low Ir concentrations. Variations of lattice parameters *a*,*c* are non-monotonous, but the unit cell volume tends to decrease, which is compatible with the progress in 5*f* bonding. The Néel temperature T_N of the AF order decreases towards 6 K in UIr_2Si_2. The diffuse X-ray scattering experiment at ESRF, ID28 beamline, reveals that the CDW state, developing gradually below 400 K, is still present for x = 0.05, where γ is still rather low, 33 mJ/mol K^2. Further CDW development will be revealed at a forthcoming experiment.

This work was supported by the Czech Science Foundation under the grant # 25-16339S.

[1] R.A. Steeman et al., J. Phys.: Condens. Matter **2**, 4059 (1990).

[2] R.A. Steeman et al.,J. Magn. Magn. Mater. **76&77**, 435 (1988).

[3] J. Lee et al., Phys. Rev. B **102**, 041112(R) (2020).

[4] M. Falkowski et al., Phys. Rev. B **101**, 174110 (2020).

9:00am **AC+MI-ThM-5 Revisiting Unconventional Superconductivity in Thorium-Doped UBe13**, ***Yusei Shimizu,*** The University of Tokyo, Japan*; Mitja Krnel, Andreas Leithe-Jasper, Markus König, Ulrich Burkhardt, Nazar Zaremba, Thomas Lühmann, Manuel Brando, Eteri Svanidze,* Max Planck Institute for Chemical Physics of Solids, Germany **INVITED**

The uranium-based superconductors have attracted considerable interest because of their unusual superconducting (SC) and normal-state properties. Among them, UBe_{13} (cubic O_h^6, space group #226) has attracted much attention as a promising candidate for spin triplet superconductivity since the early stage [1]. The strong sample dependence of this superconductivity [2,3] and the lack of understanding of its 5f electronic state make the unraveling of superconductivity in UBe_{13} even more difficult. In particular, the non-monotonic Th concentration dependence of T_{sc} in $U_{1-x}Th_xBe_{13}$ and occurrence of SC double transition of heat capacity with a small amount of thorium ($0.019 < x < 0.045$) [4-8] are quite anomalous properties, and understanding this multiple SC phase diagram is important for elucidating the true nature of uranium spin triplet superconductors.

In this study, we focus on the low-temperature physics on thorium-doped UBe_{13} and we revisit their unusual SC and normal-state properties. We have fabricated polycrystals of $U_{1-x}Th_xBe_{13}$ (x = 0.01, 0.015, 0.02, 0.03, 0.04, 0.05, 0.07) in an arc furnace. We determined their lattice constants from x-ray powder diffraction. Previous studies have found double transition of superconductivity at $0.019 < x < 0.045$ in heat capacity [5-8]. In order to clarify whether this double SC transition is intrinsic, we have performed detailed EDS (Energy Dispersive X-ray Spectroscopy), low-temperature heat-capacity and electrical resistivity measurements for $U_{1-x}Th_xBe_{13}$. The EDS results show that the distribution of Th is uniform within the crystals and that there is no heterogeneous $U_{1-x}Th_xBe_{13}$ composition within the experimental accuracy. Furthermore, the low-temperature heat capacity results for $U_{1-x}Th_xBe_{13}$ show that for x = 0.02, 0.03, 0.04 a second transition occurs in the SC state, while for x = 0.015, 0.05 only one SC transition is

observed, which is consistent with previous studies. In our presentation, we will discuss the detail of SC *H-T-x* phase diagram and non-Fermi-liquid behavior in $U_{1-x}Th_xBe_{13}$.

[1] H. R. Ott *et al*., Phys. Rev. Lett. **50**, 1595 (1983).; H. R. Ott *et al*., Phys. Rev. Lett. **52**, 1915 (1984). [2] A. Amon *et al*., Sci. Rep. **8**, 10654 (2018). [3]H. M. Voltz *et al*., Philos. Mag. **98**, 2003 (2018). [4] J. L. Smith *et al*., Physica B **135**, 3 (1985). [5] H. R. Ott *et al*., Phys. Rev. B **31**, 1651(R) (1985). [6] R. H. Heffner *et al*., Phys. Rev. Lett. **65**, 2816 (1990). [7] F. Kromer *et al*., Phys. Rev. Lett.**81**, 4476 (1998).F. Kromer *et al*., Phys. Rev. B **62**, 12477 (2000). [8] Y. Shimizu *et al*., Phys. Rev. B **96**, 100505(R) (2017).

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