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

Superconductivity, Magnetism, Electron Correlation and Complex Behavior

Moderators: James G. Tobin, University of Wisconsin-Oshkosh, **David Shuh**, Lawrence Berkeley National Laboratory, **Tomasz Durakiewicz**, Idaho National Laboratory, **Paul Roussel**, AWE

8:00am **AC+MI-ThM-1 Unconventional Superconductivity and Magnetism in Strongly Correlated U- Based Compounds**, ***Shinsaku Kambe,*** Japan Atomic Energy Agency, Japan **INVITED**

Exotic magnetism and superconductivity have been observed in uranium-based compounds, including spin-triplet superconductivity in UTe_2 and a hidden order(likely a high-rank multipole ordering never been observed before) in URu_2Si_2. These phenomena may arise from the strong correlations and the unique characteristics at the boundary between itinerant and localized states of U 5f electrons. Recent advancements in the physics of strongly correlated materials in uranium-based compounds will be discussed.

8:30am **AC+MI-ThM-3 Superconductivity in High Entropy Actinide Alloys**, *Wojciech Nowak, Piotr Sobota, Rafal Topolnicki, Tomasz Ossowski,* Institute of Experimental Physics, University of Wroclaw, Poland*; Tomasz Pikula,* Institute of Electronics and Information Technology, Lublin University of Technology, Poland*; Daniel Gnida,* Institute of Low Temperature and Structure Research, Polish Academy of Sciences, Poland*; Rafal Idczak,* Institute of Experimental Physics, University of Wroclaw, Poland*;* ***Adam Pikul,*** Institute of Low Temperature and Structure Research, Polish Academy of Sciences, Poland **INVITED**

There is a growing interest in high entropy alloys (HEAs), which are solid solutions of five or more elements, at least 5 at.% each, that crystallize in simple structures and are characterized by high configurational entropy during solidification [1]. Known for their exceptional mechanical properties, thermal stability, and corrosion resistance [2–4], they are considered materials with high potential for applications such as durable mechanical devices, magnets, or, more recently, superconductors [5].

Currently, the study of HEA with uranium or thorium is mainly focused on the development of advanced high-strength materials. However, a superconducting state has also been discovered in one of the alloys, namely $(TaNb)_{0.31}(TiUHf)_{0.69}$ [6]. Here we present the crystal structure and physical properties of two other high-entropy alloys, namely $(NbTa)_{0.67}(MoWTh)_{0.33}$ [7] and UNbTiVZr [8], which exhibit BCS superconductivity with the critical temperature of about 5.6-7.5 K in the case of the thorium-based alloy and 2.1 K in the case of uranium-based system. Their upper critical magnetic field is of about 0.7 T and 5 T, respectively. In addition, we present the results of a numerical study of the electron structure of the alloy using the DFT formalism.

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References

[1] J.-W. Yeh et al., *Advanced Engineering Materials* **6**, 299 (2004).

[2] K. M. Youssef et al. *Materials Research Letters* **3**, 95 (2015).

[3] B. Gludovatz, *Science* **345**, 1153 (2014).

[4] Y. Y. Chen et al. *Scripta Materialia* **54**, 1997 (2006).

[5] P. Koželj et al., *Phys. Rev. Lett.* **113**, 107001 (2014).

[6] W. L. Nelson et al., *Scientific Reports* **10**, 4717 (2020).

[7] P. Sobota et al., *Scientific Reports* **13**, 16317 (2023).

[8] W. Nowak et al., unpublished.

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).

9:30am **AC+MI-ThM-7 Field-Induced Lifshitz Transitions: Probe of Heavy Fermion Band Structure**, *Evrard-Ouicem Eljaouhari,* Institut f. Mathemat. Physik, TU Braunschweig, Germany*;* ***Gertrud Zwicknagl,*** Institut f. Mathemat. Physik, TU Braunschweig, Max-Planck-Institute for Chemical Physics of Solids, 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 Fermi surface sheets changes abruptly under the influence of external parameters like chemical doping, pressure, or magnetic field.Lifshitz transitions 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 chemical potential is of the order of the bandwidth, the critical points hardly affect the low temperature behavior of “conventional” metals. In heavy-fermion materials, however, the widths of the quasi-particle bands are strongly reduced by electronic correlations and, consequently, magnetic fields can drive Lifshitz transitions. The characteristic anomalies in the equilibrium and transport properties provide a method to test the quasi-particle dispersion away from the Fermi surface. The values of the field at which the transitions occur reflects the microscopic mechanism leading to the formation of the heavy quasi-particles.

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 chemical potential but also on the effective mass tensor, i. e.,the quasi-particle dispersion in the vicinity of the critical points. For lanthanide-based HFS, the theoretical analysis is based on Renormalized Band (RB) structure calculations assuming that the heavy quasi-particles result from a Kondo effect. For U-based HFS, on the other hand, we adopt the fully microscopic model which emphasizes the role of intra-atomic Hund's rule-type correlations for

appearance of heavy quasi-particle masses. The calculations reproduce the observed positions of the anomalies very well.

9:45am **AC+MI-ThM-8 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

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.

11:00am **AC+MI-ThM-13 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.

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[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).

11:15am **AC+MI-ThM-14 Topology in Uranium-Based Materials, *Eteri Svanidze,*** MPI CPfS, Germany

Unique bonding, observed in uranium-based materials, is not only fundamentally fascinating, but also gives rise to unusual physical and chemical properties. For instance, coexistence of superconductivity and magnetism, complex magnetic configurations, singlet magnetism, hidden and multipolar order, heavy fermion and non-Fermi-liquid behaviors, quantum criticality and, more recently, spin-triplet superconductivity have so far been observed in uranium-based compounds. These unprecedented phenomena – many of which are present in the same system albeit under various conditions – are driven by strong correlations and the duality of f-electrons, which are an ideal playground for studying topological properties of interacting electrons. Deviations from theoretical predictions are often observed in the vicinity of such emergent ground states and could serve as the basis for the discovery of uncharted electronic states, transitions, and functionalities – potentially leading to novel paradigms and applications of the future. Surprisingly, the possibility of robust quantum states, as promised by topological features of certain band structures, remains largely understudied in uranium-based materials. In this talk, I will examine several systems which host non-trivial topological states and their behavior under various tuning conditions.

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