Actinides and Rare Earths
Room Ballroom A - Session AC-ThP
Actinides and Rare Earths Poster Session

AC-ThP-1 The Application of Occam's Razor to Bremsstrahlung Isochromat Spectroscopy, ***J G Tobin,*** University of Wisconsin - Oshkosh

In philosophy and science, Occam's Razor is the problem-solving principle that recommends searching for the simplest possible explanation, consistent with the facts. [1] As put forth by Ptolemy (circa AD 90 -180): "We consider it a good principle to explain the phenomena by the simplest hypothesis possible." [2] More colloquially, "When you hear hoofbeats, think of horses not zebras," as suggested by Theodore Woodward. [3] In the case of Bremsstrahlung Isochromat Spectroscopy (BIS), [4-9] there have been many different interpretation methods based upon different theoretical models. Here, a simple picture will be presented, founded upon one underlying principle: the 5f electrons of the actinides are a slightly perturbed jj-coupled system. [10-15] This simple picture will include (1) the demonstration that many uranium systems are 5f3-localized and (2) a model for 5f mixing and delocalization. [16 -17] ACKNOWLEDGEMENTS: JGT wishes to thank the University of Wisconsin - Oshkosh for its on-going support. It is a gem set beside the Fox River and Lake Winnebago. References1.https://en.wikipedia.org/wiki/Occam%27s_razor2.Franklin, James (2001). The Science of Conjecture: Evidence and Probability before Pascal. The Johns Hopkins University Press. Chap 9. p. 2413.Sotos, John G. (2006) [1991]. Zebra Cards: An Aid to Obscure Diagnoses. Mt. Vernon, VA: Mt. Vernon Book Systems. ISBN 978-0-9818193-0-3.4.J.K. Lang and Y. Baer, Rev. Sci. Instrum. 50, 221 (1979).5.Y. Baer and J. Schoenes, Solid State Commun. 33, 885 (1980).6.Y. Baer and J.K. Lang, Phys. Rev. B 21, 2060 (1980).7.Y. Baer, Physica 102B, 104-110 (1980).8.E. Wuilloud et al., Phys. Rev. B 29, 5228 (1984).9.Y. Baer, "Electron Spectroscopy Studies," Chapter 4, "Handbook of the Physics and Chemistry of the Actinides," eds. A.J. Freeman and G.H. Lander, North Holland, Amsterdam (1984)10.J. G. Tobin et al., Phys. Rev. B 105, 125129 (2022).11.J.G. Tobin et al., Solid State Sciences 160, 107779 (2025).12.J. G. Tobin, "An Empirical Analysis of alpha-U Bremsstrahlung Isochromat Spectroscopy," MRS Advances 7, 783-788 (2022).13.J.G. Tobin et al., Phys. Rev. B 72, 085109 (2005).14.A. L. Kutepov, J. G. Tobin, S.-W. Yu, B. W. Chung and P. Roussel, J. of Phys.: Cond. Matter, 36, 045601 (2024).15.J. G. Tobin et al., MRS Bulletin 47, 1078–1083 (2022).16.J.G. Tobin, J. Vac. Sci. Technol. A 43, 063206 (2025).17.J.G. Tobin and A. Kutepov, J. Electron Spect. Rel. Phen. 284, 147577 (2026).

AC-ThP-2 Uranium 2D Ferromagnetism at Ambient Temperatures in Layered Zintl Phase UCu_2P_2, ***Ladislav Havela,*** *Alexandre Kolomiets, Volodymyr Buturlim,* Charles University, Czechia*; Fuminori Honda,* Kyushu University, Japan*; Fabrice Wilhelm,* ESRF Grenoble, France*; Jiri Prchal,* Charles University, Czechia*; Andrei Rogalev,* ESRF Grenoble, France

Light-actinide magnetism is based on 5*f* electronic states, which are typically involved in metallic bonding, in contrast with the localized 4*f* states in lanthanides. Hence they are rather an analogy to transition-metal 3*d* materials, characterized by itinerant character. There is, however, a special ingredient in actinides, the strong spin-orbit interaction. It gives rise to orbital magnetic moments, yielding the strong anchor to the crystal lattice, providing thus new functionalities, as enormous magnetocrystalline anisotropy or giant magnetoresistance effects.

However, weaker Coulomb *U* restricts the 5*f* magnetism to the low temperature range. Combining with 3*d* metals, efficiently enhancing ordering temperatures in compounds with rare earths, does not work with actinides, as the 3*d* and 5*f* band states coexist at similar energies and hybridize between each other, suppressing typically both 3*d* and 5*f* magnetism.

There exists an alternative route of further reducing the 5*f* delocalization in compounds with large U-U spacings and weak 5*f*-ligand hybridization. The trick is to use polar bonding to reduce also the 5*f*-6*d* hybridization by withdrawing the U-6*d* states from the energy range of 5*f*'s by the bonding to an anion in Zintl phases. The most successful case is UCu_2P_2, a layered compounds with trigonal crystal structure, formed by alternating slabs of U (cation) and Cu-P (polyanion). The interactions can be further tuned by hydrostatic pressure, increasing the Curie temperature from 216 K to 296 K at pressures reaching 15 GPa. To describe variations of Curie temperature and spin and orbital moments, we applied X-ray magnetic circular dichroism at U-$M_{4,5}$ edges (ID 12 at ESRF) using perforated diamond anvil cells, minimizing the absorption in diamond. The results are in a good agreement with ab-initio calculations by means of the GGA+*U* method, which reveal other surprising features of the compound.

This work was supported by the Czech Science foundation under grant No. 25-16339S.

AC-ThP-3 Recent Studies of Actinide Materials by Soft X-Ray Synchrotron Radiation Methods, ***David Shuh,*** Lawrence Berkeley National Laboratory*; Haisley Windsor, Cambell Conour,* Department of Chemistry, University of California Berkeley*; Emma Archer, Nic Cicchetti, Olivia Gunther,* Lawrence Berkeley National Laboratory*; Jennifer Wacker,* Lawrence Berkeley National Lab*; Sergei Butorin,* Uppsala University, Sweden*; Polly Arnold,* Department of Chemistry, University of California Berkeley*; Hendrik Ohldag, Matthew Marcus,* Lawrence Berkeley National Laboratory

The capability to conduct x-ray synchrotron radiation spectroscopy on actinide materials has led to marked improvement in the fundamental understanding of *f*-electron behavior and chemistry of *f*-electron materials. Specialized beamlines and endstations capable of utilizing the unique spatial resolution, energy resolution, and intensity provided by the advent of near and third generation synchrotron radiation x-ray beams from storage ring user facilities, coupled to new sample holding techniques, has provided unmatched opportunities to characterize the chemical and physical properties for a range of actinide materials. This has been particularly evident in the soft x-ray region of synchrotron radiation where the scanning transmission x-ray microscope (STXM) has been used to determine electronic structure from the ligand perspective via ligand K-edge spectroscopy and resonant inelastic x-ray scattering (RIXS) has been employed to garner information about actinide metal centers Both have emerged as uniquely powerful tools to elucidate the electronic structure of actinide materials.

The results of recent actinide soft x-ray STXM and RIXS studies will be presented. These will include recent studies of the actinyl tris(benzoate) complexes with a range of donating/withdrawing substituents studied using scanning transmission x-ray microscopy (STXM) and time dependent density functional theory (TDDFT). The results from RIXS studies of the Am oxides will be recapped and prospects for future studies highlighted. Lastly, an update on the status of the laboratory-based x-ray absorption system used for f-element studies at LBNL will be presented.

AC-ThP-5 5f Electronic Structure of van der Waals Uranium-Tellerium Alloys, ***Jonathan Denlinger,*** Lawrence Berkeley National Laboratory*; Christopher Broyles, Justin Shotton, Sheng Ran,* Washington University, St. Louis

Low dimensionality of magnetism and of correlated f-electron physics are current high interest research topics in condensed matter. Here, we compare and contrast the properties of two layered van der Waals uranium alloys with a focus on the diversity of their U 5f electronic structures measured by angle-resolved photoemission (ARPES), and on new f-spectroscopic features not previously reported.

UOTe crystallizes in (Te-U-O-U-Te) quintuplet layers and exhibits bilayer (uddu) antiferromagnetic ordering of local moments below 165K [1]. The U 5f states are found to be well localized at ~1 eV below E_F similar to UO_2, but with an additional weak satellite peak at -0.2 eV of unexplained origin that exhibits a Kondo-like temperature dependence. Moreover, the AFM ordering has a distinct effect on the relative energy alignment of the localized f-states between the zone center and the zone boundary. ARPES of UOTe also exhibits unusual superstructure replicas of the Fermi surface that result from an exotic incommensurate structural modulation of its vdW gap between Te layers.

The UTe_3 crystal structure contains two Te square-net planes that ubiquitously promote charge density wave (CDW) formation in the rare-earth tritellurides. Here strong U 5f character near E_F with strong temperature-dependent Kondo coherence is found in a shallow electron pocket whose high density of states is consistent with its ferromagnetic ordering below 20K [2]. The strong f-scattering dominates the otherwise delicate imperfect Fermi surface nesting of light mass Te p-bands, that results in the suppression of CDW ordering. Finally, an unusual momentum-dependent 'negative' spectral weight profile for zone-folded Te p-bands is observed and discussed as an interference phenomena.

[1] C. Broyles *et al.*, Adv. Mater. **37**, 2414966 (2025).
[2] J. Shotton *et al.*, arXiv: 2603.03509 (2026).

AC-ThP-6 Development of a Novel Aerogel-Assisted Ssntd for Automated Fissile Isotope Identification

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Accurate identification of fissile isotopes is a central challenge in nuclear forensics and safeguards. Fission Track Analysis (FTA) using solid-state nuclear track detectors (SSNTDs) provides high sensitivity but is limited by manual processing and restricted isotopic discrimination. This work presents an automated, physics-informed framework for fissile isotope characterization combining Monte Carlo simulations, synthetic data generation [1], and image-based analysis.

GEANT4 simulations were performed for ^{235}U, ^{233}U, and ^{229}Th to model fission fragment transport and cluster formation in LEXAN® SSNTDs with silica aerogel spacers. Synthetic track images were generated to study the effect of aerogel thickness on cluster morphology. Results show that increasing aerogel thickness enhances cluster separation and improves signal-to-noise ratio up to an optimal range, beyond which performance saturates due to pixel-resolution constraints and track truncation effects.

An automated image-processing pipeline (FTA-Finder) was developed to identify fission sites, separate overlapping clusters, and suppress background tracks. The fraction of well-resolved clusters increases with aerogel thickness, indicating improved reconstruction robustness.

Isotopic discrimination was evaluated using reconstructed track-length histograms and double-Gaussian fits for heavy and light fission fragments. A complementary analysis based on Real Flight Path (RFP) distributions showed clear isotope-dependent peak shifts. For 0.1 µm grains embedded in 50 µm aerogel (ρ = 0.033 g/cm^3), ^{235}U exhibited higher RFP peak positions than ^{233}U, while ^{229}Th showed the lowest values due to differences in fission-fragment energy and mass distributions.

Statistical analysis over 30 synthetic realizations showed significant separation between ^{235}U and ^{229}Th at ~3σ, while discrimination between ^{235}U and ^{233}U approached the resolution limit (~1σ). Peak deviations remained below 0.69%, confirming stable reconstruction performance.

All results are based on simulation and synthetic data. Future work will focus on experimental validation using neutron irradiation in reactor environments and extension to additional detector configurations. The proposed framework provides a scalable pathway toward quantitative isotopic fingerprinting for nuclear forensic and safeguards applications.

Reference:

[1] R. Babayew, Y. Yehuda–Zada, N. Elgad, J. Lorince, I. Orion, A. Weiss, G. Katarivas Levy, I. Halevy, *Simulation tools for improvement of the fission track analysis method for nuclear forensics* (2024), JRNC, Akadémiai Kiadó, Budapest, Hungary, DOI: 10.1007/s10967-023-09313-5.

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