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).

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

Early Career and Rising Stars

Moderators: Krzysztof Gofryk, Idaho National Laboratory, **Evgeniya Tereshina-Chitrova**, Charles University, Prague, Czech Republic, **Itzhak Halevy**, Ben Gurion Uni. Be'er Sheva, **Edgar Buck**, PNNL

2:15pm **AC+MI-ThA-1 Combinatorically Estimating the Orbital Occupancy of Actinides using an Entropic Approach**, ***Miles Beaux***, *Benjamin Heiner,* Los Alamos National Laboratory **INVITED**

Predicting material properties in *f*-block elements, especially actinides, is complicated by their complex electronic structures, such as multiconfigurational ground states and strong correlation effects. These structures arise from large electron degrees of freedom, posing challenges in modelling their behavior. A non-integer orbital occupancy representation describes the superposition mixing of multiple near-energy degenerate configurations. This representation generalizes by approximation to established ground states in elements with simpler electronic structures and enables an over-approximation of entropy for multiconfigurational ground state structures. A complementary combinatorial approach applies Hund's rule constraints to establish an under-approximation of entropy. Together, these methods bracket entropy limits, providing insights into electronic configurations that most significantly contribute to the multiconfigurational ground states of actinide elements to a low order approximation. Under an energy degeneracy assumption weighted by configuration permutations, calculations iteratively refine the contributing configurations, yielding low-order orbital occupancy estimates that align with experimental data and theoretical models. (LA-UR-25-22711)

2:45pm **AC+MI-ThA-3 Applications of Scanning Tunneling Microscopy in Heavy Element Studies**, ***Benjamin Heiner***[1], *Miles Beaux,* Los Alamos National Laboratory

Scanning Tunneling Microscopy and Spectroscopy (STM/S) are powerful techniques for investigating atomic, molecular, and surface properties. At Los Alamos National Laboratory, a specialized instrument designed to contain and probe samples containing heavy elements (i.e. actinides) allows us to study of the most uncharacterized elements on the periodic table. This capability has facilitated new insights into the electronic structure of plutonium oxides, intermetallics, and complexes. Using temperature-resolved STS, we can directly and continuously measure the total density of states of these materials across the Fermi energy, addressing a critical gap in experimental plutonium data. These advancements provide valuable information for understanding the electronic behavior of plutonium, with implications for fundamental science and nuclear materials research. Additionally, our ongoing efforts aim to apply these techniques to molecular complexes containing a single actinide atom, enabling both STM imaging and localized STS probing of individual actinide atoms.LA-UR-25-22710

3:00pm **AC+MI-ThA-4 Electronic Structure of Uranium-Based Ferromagnet UPS**, ***Sabin Regmi***, Idaho National Laboratory*; Alexei Fedorov,* Lawrence Berkeley National Laboratory*; Dariusz Kaczorowski,* Polish Academy of Sciences, Poland*; Peter Oppeneer,* Uppsala University, Sweden*; Krzysztof Gofryk,* Idaho National Laboratory

Strongly correlated *f*-electron systems often exhibit intriguing properties such as unconventional superconductivity and heavy fermion behaviors. Particularly in 5*f*-electron systems, the understanding of the relation between *f* electrons and observed physical properties has been a challenge due to their duality. Here, we present an angle-resolved photoemissions spectroscopy (ARPES) study of uranium-based ferromagnet UPS, supported by density-functional theory calculations. Measurements carried out at on and off-resonant photon energies suggest strong contribution from U 5*f* in the vicinity of the Fermi level and c-*f* hybridization. The results reveal the Fermi surface, underlying electronic structure in this system, and the nature of the 5*f* electrons in this ferromagnetic material. This work provides a valuable platform to advance the fundamental understanding of the 5*f* electronic structure in uranium-based and actinide materials in general.

***This work is supported by Idaho National Laboratory's laboratory directed research and development (LDRD) program and the US Department of energy (DOE) Basic Energy Sciences, Materials Sciences and Engineering Division.*

3:15pm **AC+MI-ThA-5 The Plutonium Auto-reduction Reaction, Predicting Kinetics, and Assessing Impacts to Surface Science Measurements**, ***Timothy Gorey***, *Daniel Rodriguez, Sarah Hernandez,* Los Alamos National Laboratory

Plutonium is a fascinating and difficult material to measure in vacuum systems due to its auto-catalytic reduction of higher oxides into plutonium sesquioxide (Pu_2O_3). This "auto-reduction" reaction complicates surface science measurements aiming to understand higher oxides, because these layers, when exposed to vacuum as is required for many surface-sensitive techniques (e.g. X-ray Photoelectron and Auger Electron spectroscopies (XPS and AES), and Secondary Ion Mass Spectrometry (SIMS)) spontaneously converts into sesquioxide. This presentation will discuss an XPS-focused study into the nuances of high oxide (PuO_2) surface analysis and propose likely mechanistic origins for the auto-reduction reaction as well as methods to predict the chemical progression of the surface.

3:30pm **AC+MI-ThA-6 Magnetic Properties of UP_2 Probed by High-Magnetic Field**, ***Volodymyr Buturllim***[2], *Sabin Regmi,* Idaho National Laboratory*; Rubi KM,* High Magnetic Field Laboratory, Los Alamos National Laboratory*; Dariusz Kaczorowski,* Polish Academy of Sciences, Poland*; Neil Harrison,* Los Alamos National Laboratory*; Krzysztof Gofryk,* Idaho National Laboratory

Due to its complex tetragonal crystal structure, with three distinct uranium sites, UP_2 stands out among other uranium dipnictides such as UAs_2, USb_2, and UBi_2. UP2 exhibits antiferromagnetic ordering at ambient pressure with T_N = 204 K and an effective moment of μ_{eff} = 2.29 μ_B/U. The neutron scattering experiment indicates that the ordered moment is parallel to the [0 0 1] direction and equals 2.0 μ_B/U. There is, however, a lack of information regarding the magnetic properties of UP_2 in high magnetic fields, particularly concerning its magnetic phase diagram. Here we present detailed experimental and theoretical studies of the magnetic properties of oriented high-quality single crystals of UP_2. The measurements were performed at the High Magnetic Field Laboratory, Los Alamos National Laboratory, using pulsed magnetic fields up to 60 T. We will discuss details of the obtained phase diagram and its relationships to the localization/delocalization of 5f-electrons in this material.

3:45pm **AC+MI-ThA-7 Properties of Carbon-Related Point Defects in Plutonium Oxides**, ***Andrew Rowberg***, *Kyoung Eun Kweon, Scott Donald,* Lawrence Livermore National Laboratory

Carbon is a ubiquitous impurity; therefore, investigating how it incorporates in materials is vital for understanding their properties, stability, and performance. Here, we evaluate the formation of carbon impurities in the most common stoichiometric plutonium oxides, PuO_2 and Pu_2O_3, which has not been systematically studied to date. We use hybrid density functional theory calculations to compute formation energies and other relevant properties of carbon species in various configurations. We find the stability of carbon defects to be strongly dependent on charge state and oxygen coordination environments. Accordingly, these properties can influence the phase evolution between PuO_2 and Pu_2O_3. We also evaluate the interactions between carbon and other defects present in these oxides.

4:00pm **AC+MI-ThA-8 Vacancy-mediated Conduction Tunability in Epitaxial SmN**, ***Kevin Vallejo***, *Volodymyr Buturlim, Zachery Cresswell, Brelon May, Brooke Campbell,* Idaho National Laboratory*; Bobby Duersch,* University of Utah*; Krzysztof Gofryk,* Idaho National Laboratory

We establish the relationship between native N vacancies, introduced through varying growth parameters, and electronic properties of SmN thin films grown via molecular beam epitaxy grown on MgO(001). We show substrate temperature having a larger impact on V$_N$ formation during growth than the ratio of Sm to N atoms. We observe a transition from insulating to conducting behavior of the film over a range of two orders of magnitude, from highly resistive to highly conductive. X-ray photoelectron spectroscopy and room temperature electrical transport results confirm the rapid degradation of the film despite the presence of capping layers. A ferromagnetic feature in the film is shown through low-temperature resistivity measurements to be the onset of ferromagnetic behavior. These promising results indicate a path forward in the epitaxy of versatile materials able to provide monolithic integration of different electronic behaviors without the associated strain brought about by heteroepitaxial integration of dissimilar materials. The integration between SmN and

[1] **JVST Highlighted Talk**

[2] **JVST Highlighted Talk**

several transition metal nitride compounds has the potential to unlock new electronic and spintronic device architectures with low strain barriers.

Actinides and Rare Earths
Room Ballroom BC - Session AC-ThP

Actinides and Rare Earths Poster Session

AC-ThP-2 Deep Fission Track Analysis for Nuclear Forensics, *Noam Elgad,* Ben Gurion University Be'er Sheva, Israel*;* ***Itzhak Halevy****, Rami Babayew,* Ben Gurion Uni. Be'er Sheva, Israel*; Mark Last, Itzhak Orion,* ben Gurion Uni. Be'er Sheva, Israel*; Jan Lorincik,* research centre rez, Czechia*; Yaakov Yehuda-Zada, Galit Katarivas Levy,* ben Gurion Uni. Be'er Sheva, Israel*; Aryeh Weiss,* bar-ilan university, israel*; Erez Gilad,* ben Gurion Uni. Be'er Sheva, Israel

Abstract Summary:
Fission Track Analysis (FTA) is a key method in nuclear forensics for detecting fissile materials. This study proposes a novel deep learning approach to automate the segmentation and classification of star-shaped patterns in microscopic images, reducing the need for manual analysis.

Methodology:
Using a U-Net fully convolutional neural network, the research focuses on identifying star-like features in microscopy. A custom simulation tool generated artificial star shapes for training, alongside a new, diverse image database. Models were trained separately for small stars (under 60µm, fewer than 10 branches, no black center) and larger, more complex patterns. An adaptive thresholding method was introduced to improve data labeling and background noise filtering.

Key Findings:
The model reached 92.04% accuracy for small star classification and an ROC AUC of 0.84. For multi-class tasks, it achieved 86.3% accuracy in distinguishing star quality and 82.63% accuracy in recognizing stars with varying numbers of branches. Advanced classification models reached an AUC of 0.90.

Conclusion:
This study shows that deep learning can significantly enhance FTA by automating star pattern detection and classification, offering a more efficient and accurate tool for nuclear forensic analysis.

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

Spectroscopy, Spectrometry, 5f Behavior and Forensics

Moderators: Ladislav Havela, Charles University, Czech Republic, **Gertrud Zwicknagl**, Technical University Brauschweig, **Alison Pugmire**, LANL

8:15am **AC+MI-FrM-1 Exploring the Surface Chemistry of Plutonium using ToF-SIMS**, ***Sarah Hernandez,*** Los Alamos National Laboratory **INVITED**

Plutonium metal is highly reactive by immediately forming an oxide layer when exposed to air and quickly forming a hydride when exposed to hydrogen. The fundamental understanding of the impact of impurities and defects on the effect of oxidation and corrosion of Pu is limited in both experimental and theoretical studies. Time-of-Flight Secondary Ion Mass Spectroscopy (ToF-SIMS) is a unique surface science technique that is highly sensitive to the first 1-2 monolayers of the surface (<1nm) and can detect all isotopes (including hydrogen) at parts-per-million levels, which gives a comprehensive survey of surface constituents. This technique also provides a structural and reactivity, chemisorption versus physisorption, information and complements other surface science techniques, such as X-ray photoelectron spectroscopy (XPS). In general, ToF-SIMS may provide a more in-depth analysis of surface constituents that otherwise might not be detected or deconvolute from a complex XPS spectra. A newly installed ToF-SIMS nanoToF 3 at LANL uses a 30 kV Bi_3^{++} liquid metal ion gun as the primary ion source and has a mass resolution of 12,000 (Δm/m), thus providing a new level of mass resolution and sensitivity on Pu surfaces that was not previously achieved. I will show recently collected ToF-SIMS results of hydrogen and oxygen gas reactions on alpha-Pu and 2 at. % Ga stabilized δ-Pu surfaces and how they compare with other.

8:45am **AC+MI-FrM-3 HERFD vs XAS: The Case for Equivalence**, ***J G Tobin,*** U. Wisconsin - Oshkosh

The advent of new, powerful, highly efficient, multi-component, X-ray monochromators used in the detection of tender x-rays has revolutionized spectroscopic investigations of the 5f electronic structure. All of the new experiments are, in essence, variants of X-ray Emission Spectroscopy (XES), where the improved monochromatized detection, applied to novel specific decay pathways, plays a key role. In HERFD (High Energy Resolution Fluorescence Detection) a type of Resonant Inelastic X-Ray Scattering (RIXS), the monochromatized XES detection allows the performance of a scattering experiment with vastly improved resolution.It is argued here that HERFD devolves into a higher resolution version of X-Ray Absorption Spectroscopy (XAS). It has been shown that the M_4 and M_5 spectra are essentially direct measurements of the j-specific ($5f_{5/2}$ and $5f_{7/2}$) Unoccupied Density of States (UDOS), which can be directly correlated with the UDOS from Inverse Photoelectron Spectroscopy (IPES) and Bremsstrahlung Isochromat Spectroscopy (BIS). [1-3] Furthermore, a remarkable level of agreement is achieved between a model based upon the UDOS of Th and a series of HERFD and IPES/BIS results with various 5f occupation levels. [4-6] Finally, the historical record of XAS will be examined, demonstrating the success of various resonant decay schemes as measures of the underlying XAS.

1. J.G. Tobin, H. Ramanantoanina, C. Daul, P. Roussel, S.-W. Yu, D. Sokaras and A. Kutepov, "Isolating Multiplet Structure in 5f Inverse Photoemission, " Solid State Sciences 160, 107779 (2025).
2. J. G. Tobin, H. Ramanantoanina, C. Daul, S.-W. Yu, P. Roussel, S. Nowak, R. Alonso-Mori, T. Kroll, D. Nordlund, T.-C. Weng, D. Sokaras, "The Unoccupied Electronic Structure of Actinide Dioxides," Phys. Rev. B 105, 125129 (2022)
3. J. G. Tobin, S. Nowak, C.H. Booth, E.D. Bauer, S.-W. Yu, R. Alonso-Mori, T. Kroll, D. Nordlund, T.-C. Weng, D.Sokaras, "Separate Measurement of the 5f5/2 and 5f7/2 Unoccupied Density of States of UO2," J. El. Spect. Rel. Phen. 232, 100 (2019).
4. J. G. Tobin, S. Nowak, S.-W. Yu, P. Roussel, R. Alonso-Mori, T. Kroll, D. Nordlund, T.-C. Weng, D. Sokaras, "The Underlying Simplicity of 5f Unoccupied Electronic Structure," J. Vac. Sci. Tech. A 39, 043205 (2021).
5. J. G. Tobin, S. Nowak, S.-W. Yu, P. Roussel, R. Alonso-Mori, T. Kroll, D. Nordlund, T.-C. Weng, D. Sokaras, "Comment on The Underlying Simplicity of 5f Unoccupied Electronic Structure," J. Vac. Sci. Tech. A 39, 066001 (2021).
6. J. G. Tobin, S. Nowak, S.-W. Yu, P. Roussel, R. Alonso-Mori, T. Kroll, D. Nordlund, T.-C. Weng, D. Sokaras, "The Thorium Model and Weak 5f Delocalization," J. Vac. Sci. Tech. A 40, 033205 (2022).

9:00am **AC+MI-FrM-4 Room Temperature H_2 Dosing on Polished α-Pu Surfaces with XPS**, ***Daniel Rodriguez***[1], *Timothy Gorey, William Ponder, Alessandro Mazza, Raymond Atta-Fynn, Sarah Hernandez,* Los Alamos National Laboratory

Plutonium (Pu) is a complex element with an interesting electronic structure, and it is also a material of great importance for both nuclear energy and security. To better understand its interaction with gases, surface analysis of the alpha (α) variant provides valuable insight when coupled with a technique such as X-ray photoelectron spectroscopy (XPS). Different core electron orbitals may be probed, and binding energies from emitted electrons provide information on the local chemical state, i.e., degree of oxidation, reduction, or carbonization within the α-Pu.

Here we investigated the effect of hydrogen (H_2) gas dosing of α-Pu surfaces, which reacts and forms plutonium hydride (PuH_2) at temperatures >100 °C. By slowing the kinetics at room temperature, we may witness H_2 dynamics on native α-Pu surfaces, and view how Pu materials such as oxidized and carbonized forms evolve with H_2 exposure. In addition, we present our findings from density functional theory (DFT) validating experimental observation. To provide an example, **Fig. 1** shows a plot of various Pu 4f spectra. In red, metal α-Pu is observed after having been sputtered to remove both surface contaminants and the native oxide layer. The defining metal feature in the $4f_{7/2}$ peak is seen at ~422.2 eV. Next, the sample was dosed with H_2 gas for 198 Langmuir (L) (blue line), and then the exposure was increased (green line) until reaching 396 L. A clear reduction in the signal's intensity is seen in both the 5/2 and 7/2 metal peaks. Secondly, the 7/2 satellite shows an increase in signal, which is indicative of surface passivation. Clearly, more is needed to know what these H_2 induced changes signify, and this presentation will show additional spectra from the O 1s, C 1s, and the Pu valence band, along with DFT to contextualize the on-going mechanisms of H_2 with the α-Pu surface.

9:15am **AC+MI-FrM-5 Ab Initio Modeling of Hydrogen Interaction with the Surface of α-Pu**, ***Raymond Atta-Fynn,*** *Sarah Hernandez,* Los Alamos National Laboratory

Hydrogen (H) reacts strongly with plutonium (Pu) metal, with the reaction primarily initiated on the metal surface. However very little is known theoretically about H dynamics on the surface of the ambient temperature phase of Pu, namely α-Pu. In this regard, we carried out calculations on H interactions with the α-Pu(020) surface using density functional theory-based geometry optimizations and *ab initio* molecular dynamics at 300 K. Molecular H_2 dissociated spontaneously on the metal surface at room temperature, resulting in atomic H chemisorption. The energy barriers to diffusion of the chemisorbed H from the surface into the subsurface and bulk layers were modeled using accelerated *ab initio* molecular dynamics. The magnitudes of the energy barriers to H diffusion in relation to hydride formation will be discussed.

9:30am **AC+MI-FrM-6 A Novel Lexan-Aerogel Detector for Fission Track Analysis for Advancing Nuclear Forensics**, ***Itzhak Halevy,*** *Rami Babayew, Yaacov Yehuda-Zada,* Ben Gurion University Be'er Sheva, Israel*; Galit Bar,* Soreq Nuclear Research Center, Israel*; Noam Elgad, Mark Last,* Ben Gurion University Be'er Sheva, Israel*; Jan Lorincik,* Research Centre Řež, Czechia*; Itzhak Orion,* Ben Gurion University Be'er Sheva, Israel*; Shay Dadon,* Nuclear Research Center Negev, Israel*; Aryeh M. Weiss,* Bar Ilan University, Israel*; Galit Katarivas Levy,* Ben Gurion University Be'er Sheva, Israel

Fission track analysis is a technique employed in nuclear forensics to identify and examine fission isotopes. This technique is specific for small samples in the range of a few picograms or to analyze bigger samples and check for homogeneity.

In the old Lexan detector, the tracks are pretty close, and that limits much the ability to count the tracks and analyze the length of the tracks. The main target of the fission track is to locate the fission ions in between a lot of other isotopes. The located fission ions could be transferred to other techniques like ICP-MS for further analysis. Better separation between tracks and analysis could lead to showing the yield of fission products, which is specific to every fission isotope. The yield fission products are two humps on the graph that are equal in area. One hump is around A=95, 135; in the length of the track histogram, the two humps look different due to

[1] **JVST Highlighted Talk**

the difference in dE/dx of the different energies. The light elements hump looks narrow, and the heavy elements hump looks wide; still, the area of those humps is equal. We created a novel detector for fission track analysis with the Lexan-modified detector.

This innovative detector exhibits more dispersion of fission tracks. In this innovative approach, we adhered aerogel to the Lexan. The aerogel has a low absorption coefficient; hence, it does not substantially obstruct the fission products in the detector. The incorporation of aerogel modifies the geometric configuration, enlarges the dimensions of the fission track stars, and increases the separation between individual tracks, as seen in Fig. 1 in the supplement. A fission track star of a size of 150 microns can reach 350 microns with the aerogel configuration. Given that the fission products are distributed isotopically while the aerogel is two-dimensional, it is necessary to employ stereoscopic projection to facilitate their integration. An illustration of this enhancement of the fission track star is seen in Fig. 1, where the dimensions of the fission track star are greater and the tracks are widely spread. The newly developed analytical program, **Finder**, may utilize a 2D representation of the fission track star. Whether an actual star or a simulated star, of a fission track to conduct analysis and provide 3D evaluations, therefore illustrating the fission yield of the fission isotope. The analysis of the fission track star is shown in Fig. 2, supp. The fission track analysis of ^{235}U star in that software is depicted in Fig. 3 supp.

Fission track length before the detector and in it are shown in that figure of the fission track analysis of ^{235}U star.

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