

Tuesday Evening, November 8, 2022

Actinides and Rare Earths Focus Topic

Room Ballroom A - Session AC-TuP

Actinides and Rare Earths Poster Session

AC-TuP-1 The Underlying Simplicity of 5f Unoccupied Electronic Structure, *JG Tobin*, U. Wisconsin-Oshkosh; *S. Nowak*, SLAC National Accelerator Laboratory; *S. Yu*, LLNL; *P. Roussel*, AWE, UK; *R. Alonso-Mori*, *T. Kroll*, *D. Nordlund*, *T. Weng*, *D. Sokaras*, SLAC National Accelerator Laboratory

Using a simple empirical model based upon the bremsstrahlung isochromat spectroscopy of elemental Th, it is possible to explain the recent high energy resolution fluorescence detection measurements of UF_4 ($n = 2$) and UCd_{11} ($n = 3$) as well as the new inverse photoelectron spectroscopy of Pu_2O_3 ($n = 5$), where n is the 5f occupation number. A critical issue in this analysis is the assumption that the Th 5f states are essentially empty, which will be confirmed both experimentally and computationally. Thus, for 5f systems, this simple model provides a unified and consistent picture of 5f unoccupied density of states in simple, localized systems, as the 5f occupation varies in the early part of the series, for $n = 0, \frac{1}{2}, 2, 3$, and 5. See References 1 and 2 for further detail.

[1] J. G. Tobin, et al., *J. Vac. Sci. Tech. A* 39, 043205 (2021), <https://doi.org/10.1116/6.0001007>

[2] J. G. Tobin, et al., *J. Vac. Sci. Tech. A* 39, 066001 (2021), <https://doi.org/10.1116/6.0001315>

AC-TuP-4 Epitaxial Actinide Heterostructures: Synthesis and Characterization, *Kevin Vallejo*, *B. May*, *F. Kabir*, *C. Dennett*, Idaho National Laboratory; *P. Simmonds*, Boise State University; *D. Hurley*, *K. Gofryk*, Idaho National Laboratory

Actinide-based materials possess unique physics due to the presence of 5f electrons. Their study has been mainly focused on their nuclear fuel applications, leaving plenty of fundamental physics aspects open for investigation. The effective examination of the unique quantum phenomena in these materials requires high purity monocrystalline samples. However, thin film synthesis of actinide compounds is particularly underexplored relative to other material systems because of limited source availability and safety regulations due to their radioactive nature. The promises, challenges, and synthesis routes for these actinide-bearing heterostructures is discussed. Molecular beam epitaxy (MBE) presents an attractive avenue for the study of actinide heterostructures because of the high degree of control over dimensionality, strain, and interfaces. Idaho National Laboratory has recently installed an MBE chamber with the specific goal of studying uranium, cesium, and thorium containing compounds. To facilitate deposition of these low vapor-pressure elements, the chamber is outfitted with a quad-pocket electron beam source, several high temperature cells, and a nitrogen plasma source. Additional studies on transition metals with complex oxidation states (Zr, Nb, Mn, Ni, and Cr) will function as surrogates for the actinide-based nitride compounds. These new capabilities will provide unrivaled opportunities for exploration of functional and energy materials with complex electron correlations, together with important experiments for model validation in computational studies.

Author Index

Bold page numbers indicate presenter

— A —

Alonso-Mori, R.: AC-TuP-1, **1**

— D —

Dennett, C.: AC-TuP-4, **1**

— G —

Gofryk, K.: AC-TuP-4, **1**

— H —

Hurley, D.: AC-TuP-4, **1**

— K —

Kabir, F.: AC-TuP-4, **1**

Kroll, T.: AC-TuP-1, **1**

— M —

May, B.: AC-TuP-4, **1**

— N —

Nordlund, D.: AC-TuP-1, **1**

Nowak, S.: AC-TuP-1, **1**

— R —

Roussel, P.: AC-TuP-1, **1**

— S —

Simmonds, P.: AC-TuP-4, **1**

Sokaras, D.: AC-TuP-1, **1**

— T —

Tobin, J.: AC-TuP-1, **1**

— V —

Vallejo, K.: AC-TuP-4, **1**

— W —

Weng, T.: AC-TuP-1, **1**

— Y —

Yu, S.: AC-TuP-1, **1**