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Delocalization and occupancy effects of 5f orbitals in plutonium intermetallics using L3-edge resonant x-ray emission spectroscopy

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Although actinide (An) L3-edge x-ray absorption near-edge structure

(XANES) spectroscopy has been very effective in determining An oxidation states in insulating, ionicallybonded materials, such as in certain coordination compounds and mineral systems, the technique fails in systems featuring more delocalized 5f orbitals, especially in metals. Recently, actinide L3-edge resonant x-ray emission spectroscopy (RXES) has been shown to be an effective alternative. This technique is further demonstrated here using a parametrized partial unoccupied density of states method to quantify both occupancy and delocalization of the 5f orbital in alpha-Pu, delta-Pu, PuCoGa5, PuCoIn5, and PuSb2. These new results, supported by FEFF calculations, highlight the effects of strong correlations on RXES spectra and the technique's ability to differentiate between f-orbital occupation and delocalization.

Primary author: BOOTH, C. H. (LBNL)

Co-authors: VEIRS, D. K. (Los Alamos National Laboratory); NORDLUND, D. (Stanford Synchrotron Radiation Lightsource); SOKARAS, D. (Stanford Synchrotron Radiation Lightsource); BAUER, E. D. (Los Alamos National Laboratory); KAS, J. J. (University of Washington); MITCHELL, J. N. (Los Alamos National Laboratory); WALL, M. A. (Lawrence Livermore National Laboratory); ALLEN, P. G. (Lawrence Livermore National Laboratory); TOBASH, P. H. (Los Alamos National Laboratory); MEDLING, S. A. (Lawrence Berkeley National Laboratory); WEND, T.-C. (Stanford Synchrotron Radiation Lightsource); JAING, Yu (Lawrence Berkeley National Laboratory)

Presenter: BOOTH, C. H. (LBNL)

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