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Accidental degeneracy leads to increased An(5f)-O(2p) hybridization in PuO₂ and AmO₂

Enrique R. Batista, Richard L. Martin, and Xiaodong Wen

Illustrated energy levels for Th, Pa, U, Np, Pu, Am and O

While the actinide contraction suggests that the 5f electrons should become more localized as one moves to the right in the row, our calculations show that the 5f orbital energy decreases steadily across the row, becoming nearly degenerate with the O2p band beginning with Pu. This proximity in energy drives a significant orbital mixing and increased dispersion in PuO₂ and AmO₂. This prediction of “unexpected covalency” has recently been confirmed by angle-resolved photoemission experiments.

Hybrid-DFT prediction of strongly correlated metal, UN

Enrique R. Batista, Richard L. Martin, and Xiaodong Wen

Calculated density of states (DOS) and band structure for AFM UN by PBE, PBE+U and HSE.

Energy as a function of volume using HSE, PBE and PBE+U with experiment denoted by arrow.

Screened hybrid DFT is not so effective for the strongly correlated metals. Here we study UN with HSE, GGA, and GGA+U approximations. HSE yields a much stiffer lattice and larger lattice constant. A comparison of the DOS as compared to angle resolved photoemission also shows that the hybrids are inferior to a simple GGA (PBE), and suggests that we must consider the dynamic screening of the Hartree-Fock exchange term if hybrids are to be effective for metals.

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