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Electronic Structure of Pu and Pu Compounds

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We report the electronic structure of Pu metal and several Pu compounds including materials with magnetic (PuSb2, Pu2RhGa8) and superconducting (PuCoGa5) transitions. The materials are experimentally determined by photoelectron spectroscopy and computationally by the mixed level model. The photoemission measurements are generally conducted at low temperatures 10-80 K and experimental resolutions between 35 to 75 meV. The electronic structure calculations are a mixed level model which is an extension of the generalized gradient approximation (GGA) within density functional theory. As determined both experimentally and computationally, the 5f electrons of plutonium exhibit two different configurations, one localized and the other hybridized. The dual nature of the Pu 5f electrons clearly indicates the boundary between localized and itinerant in the actinide series. Interestingly, the Pu 5f electrons exhibit this dual behavior over a wide ligand and crystal structure range. Limiting cases are observed on the localized side of 5f characteristics and some attribute the characteristics of alpha phase Pu metal to nearly itinerant 5f electrons. The successes and limitations of this Pu research will be discussed.

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