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First-principles study of electronic structure and local moment interactions in PuAm alloy MYUNG JOON HAN, XIANGANG WAN, SERGEJ Y. SAVRASOV, Department of Physics, University of California, Davis — Expected to provide a clue about the origin of zero moment in the bulk phase of Plutonium, $Pu_{1-x}Am_x$ alloy has attracted a great attention, in which as Am ratio, x, increases, Pu approaches from bulk to atomic limit. To understand the electronic structure and the magnetic properties of Pu in different crystal environments, we perform fully self-consistent first-principles calculations of the PuAm system based on the density functional theory. Electronic structure strongly depends on the level of approximation for correlation effects. The exchange interactions between Pu 5f electrons and the Kondo screening strength were estimated and compared, which provide a new insight to Pu magnetism.

Myung Joon Han
UC Davis

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