

Abstract Submitted
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First-principles study of the Kondo physics of a Pu impurity in a Th host¹ JIAN-XIN ZHU, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, K. HAULE, Rutgers University, Piscataway, New Jersey 08854, R.C. ALBERS, J.M. WILLS, Los Alamos National Laboratory, Los Alamos, New Mexico 87545 — From the viewpoint of condensed matter physics properties, crystal structure, and metallurgy, plutonium is the most complicated element in the Periodic Table, including a phase diagram with six allotropic phases. Its anomalous properties are related to the special position of Pu in the Periodic Table, which is at the boundary of the light actinides that have itinerant $5f$ electrons and the heavy actinides with localized $5f$ electrons, indicative of a very strongly correlated state. To reveal the role of electronic correlations in Pu, we investigate the electronic structure of a Pu atom embedded in a Th host by combining density functional theory within the local density approximation with the continuous-time quantum Monte Carlo simulation of a Pu impurity. As a hallmark of electronic correlations, the Kondo resonance peak around the Fermi energy is obtained in the local density of states on the Pu impurity. Furthermore, we show that the resonance peak width is narrower for Pu atoms that are at the surface of Th than when compared to those in the bulk, due to a weakened Pu $5f$ -ligand hybridization in the former geometry.

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