Electron Correlations in Plutonium and the Actinides Transition

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We perform first principle calculations of Pu and the other actinides using the Gutzwiller approximation (GA) in combination with density functional theory (DFT), finding good agreement with the experiments.

In particular, we discuss the zero-temperature phase diagram of Pu [PRX 5, 011008 (2015)] in relation with the so called "actinides transition", i.e., the abrupt change of density found experimentally near Pu as a function of the atomic number in the actinides.

Our analysis demonstrate that these phenomena are due to the f-electron correlations and their interplay with other physical effects, such as the spin-orbit coupling and the Peierls mechanism.