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Correlated Electronic Structures of Actinide Compounds QUAN YIN, SERGEY SAVRASOV, WARREN PICKETT, University of California, Davis — Most modern nuclear fuels are actinides compounds, such as UO2 and PuO2 (mixed oxide fuel). First-principle study of these materials is challenging because of the electron correlation. In this work we present a systematic study of AcC, AcN and AcO2 (where Ac=U, Np, Pu, Am, Cm). In order to estimate the correlation strength, we calculate the effective U by constrained-DFT, and the charge-transfer energy. In early actinides compounds such as UC, 5f electrons are mostly itinerant (LSDA works fine), while in late actinide compounds such as CmN, 5f electrons are fully localized (LDA+U) . In the intermediate region, they show competition between localization and delocalization, thus for them LDA+DMFT is used to calculate the electronic structures. The results are compared with photoemission experiments where available.

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