Electronic property of $ThSn_3$ in comparison with uranium and transuranium compounds

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Recent rapid expansion of the research frontier of condensed matter physics from uranium to transuranium compounds has stimulated renewed attention and much interest on exotic properties of actinides and related compounds. It is a challenge to modern electronic-structure theory to understand the appearance of a large number of exceptionally complicated crystal structures of actinide metal. It is important to clarify electronic structure of actinide compounds which exhibit exotic magnetism and unconventional superconductivity.
By using a relativistic linear augmented-plane-wave (RLAPW) method with the one-electron potential in the local-density approximation, we investigate energy band structures and the Fermi surfaces of transuranium compounds $ThSn_3$, USn_3, $NpSn_3$ and $PuSn_3$. It is found in common that the energy bands in the vicinity of the Fermi level are mainly due to the large hybridization between $5f$ and Sn $5p$ electrons. Thorium contains no occupied $5f$ states, thorium compounds provide good comparative systems for investigating the role of $5f$ electrons. In the presentation, we try to understand what the key issues are to construct the energy band structures around the Fermi energy for $ThSn_3$, USn_3, $NpSn_3$ and $PuSn_3$, we attempt to unveil $5f$ electron properties purely originating from actinide atoms.