Electronic structures of Plutonium compounds with the NaCl-type monochalcogenides structure

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Some of the uranium and the transuranium compounds are characterized as strongly correlated f electron systems and have attracted particular interest because of rich variety of anomalous physical phenomena such as the valence fluctuation, the Kondo lattice, exotic magnetism, unconventional superconductivity, etc. Among such compounds, the plutonium monochalcogenides display a variety of anomalous physical properties. For PuX (X=S, Se, Te) have been studied intensively both theoretically and experimentally.[1] [2] To understand the electronic properties of these materials, the features of the ground state should be first clarified.

The calculations for the energy band structure have been done by using the relativistic linear augmented-plane-wave (RLAPW) method. Note here that relativity should be taken into account, because of large atomic numbers of the constituent atoms.

In the presentation, we try to understand what the key issues are to construct the energy band structures around the Fermi energy for PuS, PuSe and PuTe.

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[2]P. M. Oppeneer, T. Kraft, and M. S. S. Brooks, Phys. Rev. B **61**, 12825 (2000).