Electronic structure and Fermi surface topology in PuIn3 and PuSn3

CHENG-CHING WANG, Theoretical Division, Los Alamos National Laboratory, MATTHEW JONES, University at Buffalo, SUNY, JIAN-XIN ZHU, Theoretical Division, Los Alamos National Laboratory — The itinerant-to-localized crossover of the 5f electrons that occurs near plutonium in the actinide series is one of the most challenging issues in condensed matter physics, while the highest superconductivity across the whole f-electron systems emerges in PuCoGa5. These novel behaviors are indicative of strong electronic correlations effects. Electronic band structure calculations serve as the first step for better understanding of these correlation effects. The compounds PuIn3 and PuSn3 crystallize into cubic AuCu3-type structure and have an actinide-actinide distance far above the Hill limit, making the 5f-ligand hybridization the dominant mechanism for Pu 5f-electron delocalization. With their simple crystallographic structure and rich magnetic and electronic properties, these two compounds provide a particularly convenient and systematic way to study the delocalization-localization crossover of Pu 5f electrons. It is particularly encouraging that PuIn3 is the first Pu-based compound in which the de-Haas van-Alphen effect has been observed. In this talk, we present a systematic study of electronic structure calculations on PuIn3 and PuSn3 in the framework of density functional theory with the generalized gradient approximation.

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