

Abstract Submitted
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An investigation of non-superconducting PuPt₂In₇ HAHNBIDT RHEE, WARREN PICKETT, UC Davis, Dept of Physics, FILIP RONNING, Los Alamos National Lab, MPA-CMMS, JIAN-XIN ZHU, Los Alamos National Lab, Theoretical Division, ERIC BAUER, Los Alamos National Lab, MPA-CMMS — PuPt₂In₇, like the heavy-fermion 115s, is member of a family of systems that are made up of RM₃ (R=Ce, Pu, ...; M=In, Ga, ...) building blocks. Superconductivity is observed in many of these materials, and it is understood to arise from an unconventional pairing mechanism due to antiferromagnetic spin fluctuations. Experiments discover that PuPt₂In₇, however, is an enhanced Pauli paramagnet with a Sommerfeld coefficient of ~ 250 mJ/mol K². Here we present a DFT (Density Functional Theory) study of its electronic structure, with direct comparisons made to superconducting PuCoGa₅ and PuCoIn₅. Fermi surfaces, orbital decomposition of density of states, and band structures reveal many similarities between the two compounds. Our goal is to understand why we observe superconductivity in one but not the other.

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