An investigation of non-superconducting PuPt2In7

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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 — PuPt$_2$In$_7$, like the heavy-fermion 115s, is member of a family of systems that are made up of RM$_3$ (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 PuPt$_2$In$_7$, however, is an enhanced Pauli paramagnet with a Sommerfeld coefficient of $\sim$250 mJ/mol K$^2$. Here we present a DFT (Density Functional Theory) study of its electronic structure, with direct comparisons made to superconducting PuCoGa$_5$ and PuCoIn$_5$. 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.