Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Electronic Structure Calculations of Filled Skutterudites $\mathbf{RGe_4Pt_{16}}$[1] KHANDKER QUADER, Department of Physics, Kent State University, Kent, OH 44242, MICHAEL WIDOM, Department of Physics, Carnegie-Mellon University, Pittsburgh, PA 15213, LUCIAN PASCUT, Department of Physics Astronomy, Rutgers University, Piscataway, NJ 08854 — We present a comparative study of the filled skutterudites RGe_4Pt_{16} (R=La, Ce, Pr), based on T=0 density functional theory (DFT) calculations. To elicit possible role of the lanthanide f-electrons and f-f interaction U, we calculate band structures, Fermi surfaces and density of states (DOS) for different scenarios: (a) frozen f-electron GGA; (b) unfrozen f-electron GGA + U with spin-orbitcoupling;(c) unfrozen f-electron GGA with spin-orbitcoupling. Comparison of our DFT DOS with experimental electronic heat capacity suggest a modest values of m^*/m_{band}. Our calculated Fermi surface topology near Fermi energy may provide clues into the occurrence of superconductivity in the La and Pr compounds and the non-occurrence in the Ce one. Our T=0 calculations of magnetism at zero doping and pressure show that Pr has a large moment and is ferrimagnetic; Ce has a very weak moment and marginally favors antiferromagnetism. We explore if the experimentally observed variation of superconducting T_C with pressure in the Pr compound can be accounted for in terms of the variation of DOS with pressure.

[1]Work supported in part by DOE grant DE-SC0014506 (Widom)

Khandker Quader
Department of Physics, Kent State University, Kent, OH 44242

Date submitted: 07 Nov 2016 Electronic form version 1.4