Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Itinerant Magnetism and the Ferromagnetic Quantum Critical Point in Fe(Ga,Ge)$_3$[1] DAVID J. SINGH, Oak Ridge National Lab — $FeGa_3$ is a tetragonal semiconductor with a band gap of $\sim$0.5 eV and interesting thermoelectric properties. It shows diamagnetic behavior but when modestly electron doped by Ge, a ferromagnetic quantum critical point emerges and the ground state becomes a ferromagnetic metal. We present first-principles calculations showing that the magnetism can be readily explained in an itinerant picture without the need for preexisting moments in the semiconducting state and without the need for correlation terms. We also present Boltzmann transport calculations of the thermopower. Itinerant magnetism implies strong coupling between the electrons at the Fermi energy that control transport and the magnetism. Thus, $FeGa_3$ may be a particularly interesting material near a quantum critical point. We find that the ferromagnetic state is half-metallic over a substantial composition range.

[1]Work supported by the Department of Energy, BES, Materials Sciences and Engineering Division

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Date submitted: 11 Oct 2013 Electronic form version 1.4