

Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Itinerant magnetism in metallic CuFe_2Ge_2 ¹ K. V. SHANAVAS, D. J. SINGH, Oak Ridge National Laboratory — Discovery of superconductivity in iron pnictides and chalcogenides has generated interest in the coexistence and interplay of superconductivity and magnetism. Antiferromagnetic spin fluctuations are believed to be mediating superconductivity in these systems. The large spin-fluctuations may arise as a consequence of nearness to a quantum critical point (QCP), which can also lead to non-Fermi liquid behavior, unusual transport and novel ground states. Thus, it is of interest to look for other materials that share similar characteristics. Using density functional theory based calculations we have studied the electronic structure and magnetic properties of CuFe_2Ge_2 based on its structural similarities with recently discovered YFe_2Ge_2 . We find large density of states at the Fermi level [$N(E_F)$], consistent with itinerant character. Fermi surfaces in this system have a sheet like structure amenable to nesting and consequently to magnetic instabilities. Our results suggest that CuFe_2Ge_2 is an antiferromagnetic metal, with similarities to the Fe-based superconductors; such as magnetism with substantial itinerant character and coupling between magnetic order and electrons at the Fermi energy.

¹This research was supported by the US Department of Energy, Basic Energy Sciences, Office of Science, Materials Sciences and Engineering Division

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Date submitted: 13 Nov 2014

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