Fixed Spin Moment Study of Quantum Critical Fe$_3$Mo$_3$N

BRIAN NEAL, WARREN E. PICKETT, University of California Davis — Quantum critical behavior and weak magnetism occurs in a handful of intermetallic transition metal compounds, with a recent example being Fe$_3$Mo$_3$N with the geometrically frustrated stella quadrangula lattice. Neutron scattering reveals antiferromagnetic ordering, but a 14 T magnetic field induces a ferromagnetic state as does substitution of 5% Co on the Fe site [1]. We present the energetics of a transition between these states with density functional based fixed spin moment studies. Our (mean field) ground state occurs with nearly equal Fe1 and Fe2 moments of 1.8 $\mu_B$. As the total moment is reduced, a crossover occurs until at zero total moment the Fe1 moment is -1.1 $\mu_B$ (antialigned with the strong Fe2 moment). We use these results to construct scenarios for discussing the observations.