

Abstract Submitted  
for the MAR13 Meeting of  
The American Physical Society

**First principles calculation of finite temperature magnetism in Ni** MARKUS EISENBACH, JUNQI YIN, DON M. NICHOLSON, YING WAI LI, Oak Ridge National Laboratory — We harnesses the computational power of massively parallel computers to calculate finite temperature magnetic properties by combining classical Monte-Carlo calculations with our first principles multiple scattering electronic structure code (LSMS) for constrained magnetic states. Our previous calculations of Fe and Fe<sub>3</sub>C [J. Appl. Phys. 109, 07E138 (2011)] only considered fluctuations in the local moment directions. Recent advances, both in the understanding of the Wang-Landau method used in our calculations [Phys. Rev. E 84, 065702(R) (2011)] and more powerful computing resources have enabled us to investigate Ni where the fluctuation in the magnitude of the local magnetic moments is of importance equal to their directional fluctuations. Here we will present our recent results for Ni that axpands our method to an even wider class of 3d element based ferromagnets. This research was sponsored by the Offices of Basic Energy Science (M.E. and D.M.N) and the Office of Advanced Computing Research (J.Y. and Y.W.L) of the US Department of Energy. This research used resources of the Oak Ridge Leadership Computing Facility at Oak Ridge National Laboratory, which is supported by the Office of Science of the Department of Energy under contract DE-AC05-00OR22725.

Markus Eisenbach  
Oak Ridge National Laboratory

Date submitted: 22 Jan 2013

Electronic form version 1.4