Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Thermodynamics of magnetic systems from first principles: gWL-LSMS[1] MARKUS EISENBACH, G. MALCOLM STOCKS, DON M. NICHOLSON, THOMAS SCHULTHESS, Oak Ridge National Laboratory — Density Functional Calculations have proven to be a useful tool to study the ground state of many materials. For finite temperatures the situation is less ideal an one is often forced to rely on models with parameters either fitted to first principles or experimental results. This approach is especially unsatisfactory in inhomogeneous systems, nano particles or other systems where the model parameters should vary significantly from one site to another. Here we describe a possible solution to this problem by combining classical thermodynamic Monte Carlo calculations - The Wang-Landau method in this case [F Wang and DP Landau, PRL 86, 2050 (2001)] - with a first principles electronic structure calculation, specifically our locally selfconsistent multiple scattering code. The combined code shows superb scaling behavior on massively parallel computers and first tests on Fe systems provide a proof of principle.

[1]Research sponsored by the Laboratory Directed Research and Development Program of Oak Ridge National Laboratory, managed by UT-Battelle, LLC, for the U. S. Department of Energy.

Markus Eisenbach
Oak Ridge National Laboratory

Date submitted: 20 Nov 2008 Electronic form version 1.4