Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

First principles statistical mechanics of alloys and magnetism[1]
MARKUS EISENBACH, SUFFIAN N. KHAN, YING WAI LI, Oak Ridge National Lab — Modern high performance computing resources are enabling the exploration of the statistical physics of phase spaces with increasing size and higher fidelity of the Hamiltonian of the systems. For selected systems, this now allows the combination of Density Functional based first principles calculations with classical Monte Carlo methods for parameter free, predictive thermodynamics of materials. We combine our locally selfconsistent real space multiple scattering method for solving the Kohn-Sham equation with Wang-Landau Monte-Carlo calculations (WL-LSMS). In the past we have applied this method to the calculation of Curie temperatures in magnetic materials. Here we will present direct calculations of the chemical order disorder transitions in alloys. We present our calculated transition temperature for the chemical ordering in CuZn and the temperature dependence of the short-range order parameter and specific heat. Finally we will present the extension of the WL-LSMS method to magnetic alloys, thus allowing the investigation of the interplay of magnetism, structure and chemical order in ferrous alloys.

[1]This research was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Science and Engineering Division and it used Oak Ridge Leadership Computing Facility resources at Oak Ridge National Laboratory.

Markus Eisenbach
Oak Ridge National Lab

Date submitted: 06 Nov 2015 Electronic form version 1.4