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First principles calculations of magnetic properties of Fe and Fe₃C at finite temperature MARKUS EISENBACH, GREGORY BROWN, AURELIAN RUSANU, DON M. NICHOLSON, Oak Ridge National Laboratory — We demonstrate a method to investigate finite temperature magnetism from first principles that harnesses massively parallel computers to obtain the free energy, specific heat, magnetization, susceptibility, and other quantities as function of temperature by combining classical Wang-Landau Monte-Carlo calculations with a first principles electronic structure code that allows the energy calculation of constrained magnetic states. Here we will present our calculations of finite temperature properties such as specific heat, magnetization and susceptibility of Fe and Fe₃C using this approach where we find the Curie temperatures to be in good agreement with experiment at 980K and 425K respectively. This work was conducted at Oak Ridge National Laboratory (ORNL), which is managed by UT-Battelle for the U.S. Department of Energy (US DOE) under contract DE-AC05-00OR22725 and sponsored in parts by the Center for Nanophase Material Sciences, Scientific User Facilities Division, the Center for Defect Physics, an Energy Frontier Research Center funded by the US DOE Office of Basic Energy Sciences and by the US DOE Office of Energy Efficiency and Renewable Energy, Industrial Technologies Program. This research used resources of the Oak Ridge Leadership Computing Facility at ORNL, which is supported by the US DOE, Office of Science.

Markus Eisenbach
Oak Ridge National Laboratory

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