Calculation of the Curie temperature of Ni using first principles based Wang-Landau Monte-Carlo MARKUS EISENBACH, Oak Ridge National Lab, JUNQI YIN, Univerity of Tennessee, YING WAI LI, Oak Ridge National Lab, DON NICHOLSON, University of North Carolina, Asheville — We combine constrained first principles density functional with a Wang-Landau Monte Carlo algorithm to calculate the Curie temperature of Ni. Mapping the magnetic interactions in Ni onto a Heisenberg like model to underestimates the Curie temperature. Using a model we show that the addition of the magnitude of the local magnetic moments can account for the difference in the calculated Curie temperature. For ab initio calculations, we have extended our Locally Selfconsistent Multiple Scattering (LSMS) code to constrain the magnitude of the local moments in addition to their direction and apply the Replica Exchange Wang-Landau method to sample the larger phase space efficiently to investigate Ni where the fluctuation in the magnitude of the local magnetic moments is of importance equal to their directional fluctuations. We will present our results for Ni where we compare calculations that consider only the moment directions and those including fluctuations of the magnetic moment magnitude on the Curie temperature. This research was sponsored by the Department of Energy, Offices of Basic Energy Science and Advanced Computing. We used Oak Ridge Leadership Computing Facility resources at Oak Ridge National Laboratory, supported by US DOE under contract DE-AC05-00OR22725.

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