Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Fist Principles Approach to the Magneto Caloric Effect: Application to Ni_2MnGa KHORGOLKHUU ODBADRAKH, DON NICHOLSON, AURELIAN RUSANU, MARKUS EISENBACH, GREGORY BROWN, BOYD EVANS III, ORNL — The magneto-caloric effect (MCE) has potential application in heating and cooling technologies. In this work, we present calculated magnetic structure of a candidate MCE material, Ni_2MnGa. The magnetic configurations of a 144 atom supercell is first explored using first-principle, the results are then used to fit exchange parameters of a Heisenberg Hamiltonian. The Wang-Landau method is used to calculate the magnetic density of states of the Heisenberg Hamiltonian. Based on this classical estimate, the magnetic density of states is calculated using the Wang Landau method with energies obtained from the first principles method. The Currie temperature and other thermodynamic properties are calculated using the density of states. The relationships between the density of magnetic states and the field induced adiabatic temperature change and isothermal entropy change are discussed. This work was sponsored by the Laboratory Directed Research and Development Program (ORNL), by the Mathematical, Information, and Computational Sciences Division; Office of Advanced Scientific Computing Research (US DOE), and by the Materials Sciences and Engineering Division; Office of Basic Energy Sciences (US DOE).

Khorgolkhuu Odbadrakh
ORNL

Date submitted: 27 Nov 2010 Electronic form version 1.4