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Magnetic entropy change calculated from first principles based statistical sampling technique: Ni2MnGa KHORGOLKHUU ODBADRAKH, DON NICHOLSON, MARKUS EISENBACH, ORNL, GREGORY BROWN, Florida State University, AURELIAN RUSANU, ORNL, MATERIALS THEORY GROUP TEAM — Magnetic entropy change in Magneto-caloric Effect materials is one of the key parameters in choosing materials appropriate for magnetic cooling and offers insight into the coupling between the materials' thermodynamic and magnetic degrees of freedoms. We present computational workflow to calculate the change of magnetic entropy due to a magnetic field using the DFT based statistical sampling of the energy landscape of Ni2MnGa. The statistical density of magnetic states is calculated with Wang-Landau sampling, and energies are calculated with the Locally Self-consistent Multiple Scattering technique. The high computational cost of calculating energies of each state from first principles is tempered by exploiting a model Hamiltonian fitted to the DFT based sampling. The workflow is described and justified. The magnetic adiabatic temperature change calculated from the statistical density of states agrees with the experimentally obtained value in the absence of structural transformation. The study also reveals that the magnetic subsystem alone cannot explain the large MCE observed in Ni2MnGa alloys. This work was performed at the ORNL, which is managed by UT-Batelle for the U.S. DOE. It was sponsored by the Division of Material Sciences and Engineering, OBES. This research used resources of the OLCF at ORNL, which is supported by the Office of Science of the U.S. DOE under Contract DE-AC05-00OR22725.

Khorgolkhuu Odbadrakh
ORNL

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