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Latent heat of magnetization for MnFeSi0.33P0.66[1] PRASENJIT ROY, ROBERT A. DE GROOT, Radboud University Nijmegen, THEORETICAL CHEMISTRY TEAM — Magnetic refrigeration is a very promising environmental-friendly method to encounter the energy shortage of the world by implementing the magnetocaloric effect. MnFeSiP series of materials are distinguishable magnetocaloric meterial for the use of non-toxic, inexpensive elements as well as high efficiency. There are several ways to measure the efficiency of the MCE, viz.- measuring the adiabatic temperature change or measuring the entropy change at the transition. MnFeSiP materials show a first order magneto-elastic phase transition at the Curie temperature (T_C). This simultaneous occourance of the magnetic and elastic transition in this material account for a higher ΔT_{ad} (or high entropy change), which is linearly proportional to the Latent heat (L) of magnetization. Experimentally L can be determined with techniques such as Differential Scanning Calorimetry. In our study we use VASP in addition to the Phonopy package, to determine the finite temperature properties of the system. Quasi Harmonic Approximation was applied successfully to determine the Gibbs free energy of $MnFeSi_{0.33}$ $P_{0.66}$. Hence we show a phase transition around 425 K. From the temperature derivative of G , the specific heat was obtained and finally the latent heat was obtained.

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