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COMPUTATIONAL SEARCH FOR GIANT MAGNETOCALORIC MATERIALS: APPLICATION TO MNAS

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Current high-performance magnetic refrigerants are the result of years of extensive experimental work, after thousands of samples were prepared and characterized in laboratories around the world. Computational tools to assist the search for new and optimized magnetocaloric materials would be welcome, but the challenges for their development are considerable. The approach must be predictive and not merely descriptive, to be of use. In other words, using experimental results as inputs to a computational approach that is intended to look for new materials somewhat defeats the purpose. While Density Functional Theory (DFT) allows the ab-initio determination of microscopic parameters, these need to be fed to a thermodynamic model to make predictions of performance parameters such as Tc and entropy change. This model must be able to describe first-order phase transitions to allow the search of giant magnetocaloric materials. We here report on the combined use of DFT and Monte Carlo simulations of a compressible Heisenberg-like model, applied to describe the giant magnetocaloric effect of MnAs. Our DFT calculations follow previous reports, estimating the magnetic exchange parameters as a function of structural distortion between the ordered (FM) phase, where the total magnetic and structural energy is minimized, and the disordered (PM) phase, where only the structural energy is minimized. Our estimates of structural and magnetic phase transition temperatures and magnetocaloric effect show good agreement with experimental data, highlighting the entropy change contribution of the structural phase transition. The generalization of this approach to other magnetic systems is discussed.

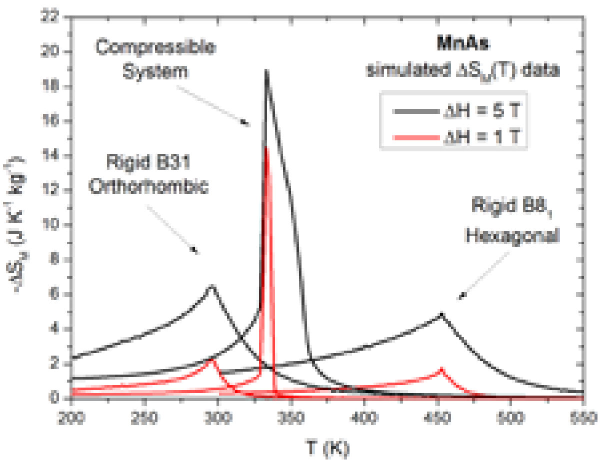

Figure.1: Simulated magnetocaloric effect of MnAs, considering rigid hexagonal and orthorhombic lattices, together with the compressible system,which shows a giant magnetocaloric effect.