**Quantifying the magnetocaloric effect**

**from first-principles**

Diana Iuşan1, Johan Hellsvik2, Erna K. Delczeg-Czirjak1, and Olle Eriksson1

*1 Division of Materials Theory, Department of Physics and Astronomy, Uppsala University*

*2 Nordita and the Department of Physics, KTH*

The magnetocaloric effect may be described in terms of the adiabatic temperature and entropy change during the cooling cycle: ΔT and ΔS. In order to predict theoretically new magnetocaloric materials, or improve upon the existing ones, we need to be able to quantify ΔT and ΔS. In this talk, I will present a way for estimating these quantities from first-principles. Our approach consists in a two-step procedure: The first step is the calculation of the electronic structure and magnetic properties within density functional theory and the mapping of the magnetic interactions onto a magnetic Hamiltonian. This is later used in Monte Carlo simulations at finite temperatures and/or magnetic fields, from which ΔT and ΔS is calculated. The recipe will be exemplified for the Gd, FeRh, Fe2AlB2, Fe2P, and La(Fe,Si)13 systems.



*Short figure caption.*

*The calculated magnetic entropy for Fe2AlB2. The black full (dashed) line indicate the adiabatic cooling when reducing the external magnetic field from H = 2T (5T) for a system initially at room temperature.*

**References**

[1] A.M. Tishin and Y.I. Spichkin, *The Magnetocaloric Effect and its Applications*, Institute of Physics Publishing, Bristol, United Kingdom, 2003

[2] Z. Gercsi et al., Physical Review B 88, 024417 (2013)

[3] E. K. Delczeg-Czirjak et al., Physical Review B 85, 224435 (2012)

[4] E. K. Delczeg-Czirjak et al., Physical Review B 86, 045126 (2012)

[5] E. K. Delczeg-Czirjak et al., Physical Review B 90, 214436 (2014)

[6] O. Eriksson, A. Bergman, L. Bergqvist, and J. Hellsvik, Atomistic Spin Dynamics (Oxford University Press, 2017)