Thermag VIII – International Conference on Caloric Cooling

Plenary Talk

Caloric effects around phase transitions in magnetic materials described by ab-initio theory

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When a metal goes through a change of magnetic order, the complex electronic fluid with its emergent magnetic 'local moments' transforms. The coupled itinerant electron and more localized spin degrees of freedom have a profound effect on structure, electronic transport, and so on which can be particularly dramatic around first-order phase transitions. An ab-initio treatment of temperature dependent spin-polarised electronic structure can therefore provide the means to locate and characterize magnetic phase transitions and describe quantitatively caloric effects in their vicinity triggered by application of magnetic field, pressure or strain. In this context the Density Functional Theory (DFT)-based Disordered Local Moment Theory (DLM) of magnetic materials will be discussed [1-4]. The theory can be applied to materials with quenched static compositional disorder traversing first-order magnetic phase transitions such as nearly stoichiometric Fe-Rh alloys [2], describe tricritical metamagnetism in antiferromagnets [5] and for the Mn-antiperovskites [6] highlight the potential for rich magnetic-strain phase diagrams and associated caloric effects. Relativistic effects such as spin-orbit coupling can be included and results will also be presented for the magnetic properties of rare earth - transition metal permanent magnets such as SmCo5 [4] focussing on their ferrimagnetism and how to describe their intrinsic temperature dependent magnetic anisotropy using DFT-DLM.

This work forms part of the PRETAMAG project, funded by the UK Engineering and Physical Sciences Research Council (EPSRC), Grant no. EP/M028941/1.

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