Thesis Project Offer

Joint Research and Education Programme "Palestinian-German Science Bridge PGSB"
Forschungszentrum Jülich GmbH & Palestine Academy for Science and Technology

Thesis type*

☐ BSc	☒ MSc	☐ PhD	Intended starting date (approx.): October-December 2023

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Project description*

Effect of deuteration on caloric effects in spin-crossover compounds

In view of global warming, there is rising demand of energy-efficient and environmentally friendly cooling technologies (e.g. for household fridges). In contrast to the conventional vapour compression cycle, ferroic cooling technologies promise higher device efficiencies and do not rely on gaseous refrigerants with high global warming potential (like e.g. hydrofluorocarbons) [1]. In caloric materials, which form the basis for ferroic cooling technologies, the adiabatic application of a field results in a temperature change ΔT_{ad}, which is closely related to a change in entropy ΔS upon isothermal field application. Ferroic cooling effects can by driven by a magnetic field (magnetocaloric effect, MCE), an electric field (electrocaloric, ECE), uniaxial stress (elastocaloric, eCE) or by hydrostatic pressure (barocaloric, BCE). They are particularly large close to an appropriate phase transition where the applied field can suppress fluctuations and hence decreases the entropy. Multicaloric effects arise through a coupling between different degrees of freedom [2].

Recently spin-crossover (SCO) compounds have been identified as potentially very interesting candidate materials for ferroic cooling [3]. Typical spin-crossover compounds are octahedrally coordinated complexes of Fe with Fe in d^5 or d^6 electronic configurations

[4]. In these compounds, a transition from a low spin (LS) state to a high spin (HS) state can occur as a function of e.g. temperature. The transition is accompanied by a significant change in entropy ΔS and can be either of first or second order. The most effective way of influencing the transition temperature is elastic strain or pressure (both stabilize the LS state, leading to negative ΔS) [3].

We are investigating the changes of the crystal structure at the spin crossover and are particularly interested in the dynamics in these materials close to the phase transition. In this context, neutron scattering investigations play a major role. Due to the large incoherent scattering cross section of hydrogen, this requires deuteration of the organic ligands.

Deuteration leads to an expansion of the crystal lattice due to the larger size of deuterium when compared to hydrogen, and can thus be considered as exerting *"negative pressures*". As a consequence, in particular intermolecular interactions are expected to change on deuteration. This in turn should lead to a change not only of the transition temperatures, but also of the nature of the transition (whether gradual or sharp) and the caloric properties.

Within this project - which will be performed at the Jülich Centre of Neutron Science-2 - the fellow will investigate the changes on deuteration in selected SCO compounds using magnetization and powder diffraction measurements as a function of temperature.

The results from these investigations will then be complemented by x-ray single crystal diffraction, vibrational spectroscopy and inelastic neutron scattering investigations, which will be realized in parallel by our group.

References

[1] I. Takeuchi & K. Sandeman, *Solid-state cooling with caloric materials*, Physics Today 68, 48 (2015).
[2] M. M. Vopson, *The multicaloric effect in multiferroic materials*, Solid State Comm. 152, 2067 (2012)
[3] K. G. Sandemann, *Research Update: The mechanocaloric potential of spin crossover compounds,* APL Materials 4, 111102 (2016).

Date*	**Signature***
31.01.2023	

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