# DF 5: SYCE: Caloric effects in ferroic materials (MM with MA, DF)

Time: Monday 15:00–17:45 Location: H1

**Invited Talk** DF 5.1 Mon 15:00 H1
**Multicaloric effects in metamagnetic Heusler materials** — •Antoni Planes — Departament d'Estructura i Constituents de la Matèria. Facultat de Física. Universitat de Barcelona. Diagonal 647. 08028 Barcelona. Catalonia.

The talk is aimed at presenting a general thermodynamic framework to deal with multicaloric effects in multiferroic materials. After discussing a number of recently reported examples showing that various caloric effects may occur in the same material interdependently, the formalism will be applied to the study of mulicaloric effects taking place near the magnetostructural transition in metamagnetic Heusler shape-memory materials. This class of metamagnetic materials will be modelled by means of a Landau free energy expansion with appropriate interplay between the corresponding structural and magnetic order parameters. Caloric effects will be quantified by the isothermal entropy changes and the adiabatic temperature changes induced by application of the fields thermodynamically conjugated to the order parameters. It will be shown that multicaloric effects comprise the corresponding contributions from the effects associated with each ferroic property and the cross-contribution arising from the interplay between these properties. Finally, the obtained results will be compared with available experimental data.

**Invited Talk** DF 5.2 Mon 15:30 H1
**Multicaloric effect in biological systems: a case of nerve action** — •Matjaz Valant[1], Lawrence J. Dunne[2], Anna-Karin Axelsson[2], Florian Le Goupil[3], and George Manos[4] — [1]University of Nova Gorica — [2]London South Bank University, UK — [3]Imperial College London, UK — [4]University College London, UK

In the recent decades the "caloric community" has demonstrated the technological value of different types of reversible caloric effects induced by pulsing external fields that trigger changes in materials* order parameters. The applied research continues towards first prototypes of refrigeration systems. In addition, we have gained much better understanding of the microscopic processes related to the caloric effects, which enabled us also to recognize their occurrence and role in biological systems. We will discuss a model of nerve action, which is a natural continuation of the soliton model that considers a solitonic type pressure/density pulse propagating along the long axis of the nerve. A special emphasis has been placed on a reversible caloric response during the nerve action, which can be described as a multicaloric effect. We have calculated changes in membrane temperature, thickness, entropy and trans-membrane voltage. All of these calculated parameters are in striking agreement with experimental results. The temperature change is explained with the solitonic propagation that is iso-entropic. This observation is an important biological manifestation of the multicaloric effect, which has hitherto not being described in these terms.

**Invited Talk** DF 5.3 Mon 16:00 H1
**Optimizing the electrocaloric effect by first-principles simulations: The role of strain and defects** — •Anna Grünebohm — University of Duisburg-Essen and Cenide, Germany

The electrocaloric effect (ECE) is the adiabatic tempearture change of a material in a varying external electrical field. The ECE is promising for novel cooling devices [1]. However, in many ferroelectrics the large ECE is restricted to a narrow temperature interval.

To model modifications of the ferroelectric and electrocaloric properties of $BaTiO_3$ by defects and epitaxial strain we have combined *ab initio*-based molecular dynamics simulations with a simple model for defects [2]. For polar defects the temperature range of the large caloric response is broadened. Still more striking, a giant inverse caloric effect has been observed for the first time.

Additionally, epitaxial strain can be used to enhance the caloric response and shift the operation range [3,4]. In particular tensile strain is promising to enhance the ECE of $BaTiO_3$ around room temperature.

[1] X. Moya, *et al.*, Nature Mater. **13**,439 (2014)
[2] A. Grünebohm, *et al.*, arXiv:1502.05201
[3] M. Marathe, *et al.*, APL **104**, 212902 (2014)
[4] A. Grünebohm, *et al.*, APL **107**, 102901 (2015).

**15 min. coffee break**

**Invited Talk** DF 5.4 Mon 16:45 H1
**Giant inverse barocaloric effects in ferrielectric ammonium sulphate** — Pol Lloveras[1], Enric Stern-Taulats[2], Maria Barrio[1], Josep Lluis Tamarit[1], Sam Crossley[3], Wei Li[3], Vladimir Pomjakushin[4], Antoni Planes[2], Lluis Mañosa[2], Neil Mathur[3], and •Xavier Moya[3] — [1]Departament de Física i Enginyeria Nuclear, ETSEIB, Universitat Politècnica de Catalunya, Diagonal 647, Barcelona, 08028 Catalonia, Spain — [2]Facultat de Física, Departament d'Estructura i Constituents de la Matèria, Universitat de Barcelona, Martí i Franquès 1, 08028 Barcelona, Catalonia, Spain — [3]Department of Materials Science, University of Cambridge, Cambridge, CB3 0FS, UK — [4]Paul Scherrer Institute, WHGA/133, 5232 Villigen - PSI, Switzerland

Giant barocaloric effects driven by hydrostatic pressure have been suggested for cooling applications, but they are only seen in a small range of magnetic materials that are relatively expensive. Here I will present pressure-dependent calorimetry data to demonstrate giant inverse barocaloric effects in ferrielectric ammonium sulphate, which is made of cheap abundant elements [Lloveras et al., Nature Communications, in press].

**Invited Talk** DF 5.5 Mon 17:15 H1
**TiNiCu-based thin films for elastocaloric cooling** — •Eckhard Quandt and Christoph Chluba — Chair of Inorganic Functional Materials, Institute for Materials Science, Faculty of Engineering, University of Kiel, Germany

The elastocaloric effect is a promising alternative for the replacement of conventional vapor compression cooling which suffers from a high environmental impact and limited efficiency improvement possibilities. Instead of a vapor-liquid transition in a conventional cooling, the elastocaloric effect is based on a stress induced structural phase transition usually from a high symmetry to a low symmetry phase. At adiabatic conditions this results in a temperature change of the material. For a continuous use of this effect in a cooling cycle, several requirements have to be fulfilled. Transformation temperatures, effect size and efficiency have to be suitable, but most importantly a high functional and structural fatigue resistance is necessary.

Highly fatigue resistant Ti-rich TiNiCu compositions prepared by thin film technology have been found that can withstand 10 million transformation cycles without functional degradation [1]. Within this talk the reasons for the fatigue resistance will be discussed. In situ synchrotron and TEM investigations have been conducted to investigate the underlying microstructural mechanisms that ensure the reversible transformation. Cobalt and iron addition is used to adjust the transformation temperature to a suitable range to enable the use of this compositions at room temperature. The compositional influence on the elastocaloric parameters is investigated by temperature dependent tensile tests, infrared (IR) thermography and differential scanning calorimetry. Due to the small hysteresis of TiNiCu-based compositions an improved elastocaloric cooling efficiency is found in comparison to binary NiTi thin films. Considering also the high fatigue resistance, this class of materials is promising for future elastocaloric cooling applications.

[1] Chluba, C.; Ge, W.; Lima de Miranda, R.; Strobel, J.; Kienle, L.; Quandt, E.; Wuttig, M.: Ultralow-fatigue shape memory alloy films, Science 348 (2015), 1004-1007.