NAPLES, ITALY 23-27 JUNE
DSL2025 NAPLES
21st International Conference on Diffusion in Solids and Liquids

ABSTRACT

Conventional and Inverse Electrocaloric Effects in Perovskites: Insights from ab initio based Modelling

A. Grünebohm[1], L.-T. Hsu[1], M. Namisi[1], M. Marathe[2]

Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Ruhr-University Bochum, Universitätsstr. 150, 44801 Bochum, Germany
[2]KTH Royal Institute of Technology, SE-100 44 Stockholm, Sweden

The electrocaloric effect (ECE), where a material undergoes a temperature change under an applied electric field, is a promising candidate for sustainable and scalable cooling technologies. Unlike traditional refrigeration, the ECE involves no moving parts and large temperature changes have been predicted at phase transitions in idealized materials. However, there are significant gaps in the understanding of the factors determining reversibility and temperature stability of the response as well as on the impact of the microstructure. Since even the sign of the response can change with temperature or time (conventional ECE : cooling under field removal and inverse ECE: cooling under field application [1]), these gaps challenge the implementation of electrocaloric devices. To address these gaps, we simulate the ECE in oxidic and halide perovskites combining density functional theory and coarse-grained molecular dynamics simulations [2]. We find that the predicted maximal ECE values cannot be realized without careful control of the relative orientation between the applied electric field and the local polarization. Even the sign of ΔT depends on this orientation [3], and the responses of domains exhibiting conventional and inverse ECE can compensate each other [4].

[1] A. Grünebohm et al, *Origins of the inverse electrocaloric effect*, Energy. Techn. 6, 1491 (2018)
[2] T. Nishimatsu et al, *Fast molecular-dynamics simulation for ferroelectric thin-film capacitors using a first-principles effective Hamiltonian*, Phys. Rev. B 78, 104104 (2008)
[3] L.-T. Hsu, F. Wendler and A. Grünebohm, *Electric field direction dependence of the electrocaloric effect in $BaTiO_3$*, Phys. Rev. Mater. 8, 094408 (2024)
[4] A. Grünebohm, S.-H. Teng and M. Marathe, *Influence of domain walls and defects on the electrocaloric effect*, J. Phys. Energy 5, 034010 (2023)