NanoSaclay
Laboratoire d'Excellence en Nanosciences et Nanotechnologies

Séminaire Labex NanoSaclay

Le 9 juillet à 14h, au C2N

Modeling of Electrocaloric Materials for Waste Heat Recovery

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Abstract:

There is a need for the development of comprehensive, multi-scale theoretical tools in the search for better materials. This is essentially at the core of the recent "materials genomics/informatics" initiatives that seek to accelerate materials discovery through the use of computations across length and time scales, supported by judicious experimental work. In this talk we will apply these principles to understand pyroelectric, electrocaloric, elastocaloric, and flexocaloric properties of ferroelectric materials. Pyroelectrics can convert heat into electricity by cycling around thermally- and electrically-induced polarization changes, where the energy density scales with the product of the polarization change and applied field. The challenges in realizing caloric energy conversion system are multi-scale and multi-faceted, requiring a combination of first principles computations, phenomenological theory, classical thermodynamics, materials synthesis, and eventually system design [1]. We will discuss our successes and challenges with relating modeled to measured material properties for bulk and epitaxial thin film ferroelectrics. We will provide specific examples related to electrocaloric, elastocaloric, and flexocaloric properties of ferroelectrics [2,3].

1. S. P. Alpay, J. V. Mantese, S. Trolier-McKinstry, Q. M. Zhang, and R. W. Whatmore, "Next Generation Electrocaloric and Pyroelectric Materials for Solid State Electrothermal Energy Interconversion," MRS Bulletin 39, 1099 (2014).
2. H. Khassaf, T. Patel, S. P. Alpay, "Combined Intrinsic Elastocaloric and Electrocaloric Properties of Ferroelectrics," J. Appl. Phys. 121, 144102 (2017).
3. H. Khassaf, T. Patel, R. J. Hebert, and S. P. Alpay, "Flexocaloric Response of Epitaxial Ferroelectric Films," J. Appl. Phys. 123, 024102 (2018).

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