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Modeling the electrocaloric and magnetocaloric effect in nematic liquid crystals

Caloric effects are reversible thermal changes under an applied external electric, magnetic, or mechanical field. The caloric response is expected to be largest near a phase transition where the corresponding order parameter can be manipulated by an external field. Materials with a large caloric response have a potential use in alternative cooling technology that could be more efficient and environmentally friendly compared to traditional vapor-compression technology.[1]

Liquid crystals represent an example of such promising materials due to their excellent responsivity to external fields. The orientation of anisotropic liquid crystal molecules can easily be manipulated by an applied electric or magnetic field to induce nematic or smectic order. Experimental measurements near the smectic-isotropic and nematic-isotropic phase transitions have revealed that the magnitude of the electrocaloric response is comparable to that found in solid materials.[2, 3]

Here, we present an estimation of the magnitude of the electrocaloric and magnetocaloric effect near the nematic-isotropic phase transition in liquid crystals. To obtain our estimate we rely on using the indirect approach based on Maxwell relations. We use molecular dynamics simulations to estimate the heat exchanged during an isothermal application of an external field.

References:

- [1] Y. Liu et al, Applied Physics Reviews 3: 031102 (2016)
- [2] E. Klemenčič et al, Scientific Reports 9: 1721 (2019)
- [3] M. Trček et al, Phil. Trans. R. Soc. A. 374: 20150301 (2016)

Primary authors: AUPIČ, Polona (University of Ljubljana, Faculty of Mathematics and Physics, Ljubljana, Slovenia); Dr SKAČEJ, Gregor (University of Ljubljana, Faculty of Mathematics and Physics, Ljubljana, Slovenia)

Presenter: AUPIČ, Polona (University of Ljubljana, Faculty of Mathematics and Physics, Ljubljana, Slovenia)

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