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Electrocaloric effect in ferroelectric alloys from atomistic simulations[1] SERGEY LISENKOV, INNA PONOMAREVA, University of South Florida — Caloric effects, such as magnetocaloric and electrocaloric effects, have attracted a lot of attention recently in the context of increasing interest in energy conversion and renewable energy materials and devices. Here we develop and use accurate first-principles-based simulations to study electrocaloric effect (ECE) from an atomistic point of view. In particular, we develop a computational technique that allows both direct and indirect simulations of ECE within the *same* atomistic framework. We then use such a tool to provide first systematic comparison between ECE estimates obtained from direct and indirect approach which will allow us to bridge the macroscopic and atomistic description of ECE. The results of our direct atomistic simulations are then used to explore the intrinsic features of ECE in ferroelectrics with multiple transitions.

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