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Finite Temperature Properties of $KTaO_3$ Thin Films from First-Principles ALIREZA AKBARZADEH, LAURENT BELLAICHE, University of Arkansas, KEVIN LEUNG, Sandia Laboratories, NM, JORGE ÍÑIGUEZ, NIST Center for Neutron Research, DAVID VANDERBILT, Rutgers University,NJ, LAURENT BELLAICHE TEAM, KEVIN LEUNG COLLABORATION, JORGE ÍÑIGUEZ COLLABORATION, DAVID VANDERBILT COLLABORATION — Thin films made of the incipient ferroelectric $KTaO_3$ are studied using a parameterized effective Hamiltonian, H_{eff}. Quantum effects are turned off and on by performing classical Monte Carlo and, path integral quantum Monte Carlo simulations respectively. The films are simulated to be grown along the [001] pseudo-cubic direction. Different electrical and mechanical boundary conditions are investigated. Particular striking predictions are (1) that, unlike in the bulk, quantum effects are unable to suppress ferroelectricity in $KTaO_3$ thin films and, (2) the formation of complex ferroelectric nanodomains, depending on the boundary conditions.
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