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Domain formation and dielectric response in $PbTiO_3$: A first-principles free energy landscape analysis ANIL KUMAR, KARIN RABE, Dept of Physics and Astronomy, Rutgers University, UMESH V. WAGHMARE, Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore, India —
We determine the relative thermodynamic stability of competing homogeneously and inhomogeneously ordered ferroelectric phases of $PbTiO_3$ using its free energy landscape, obtained from a newly developed method based on a combination of constrained polarization molecular dynamics simulations with a first-principles effective Hamiltonian and thermodynamic integration. While we find that the tetragonal structure is thermodynamical ly most stable at temperatures below the ferroelectric transition temperature ($T_0 = 660K$), free energy of an "orthorhombic-like" 90° domain phase relative to the tetragonal phase almost vanishes at $T = 540K$, and remains small at all temperatures below T_0. In contrast to $BaTiO_3$, 90° domain walls are an order of magnitude lower in energy than 180° domain walls. We show that the computed dielectric response of the "orthorhombic-like" phase includes contributions from domain walls, and thus is significantly larger than that of the unifor mly polarized tetragonal phase of $PbTiO_3$.

Anil Kumar
Rutgers University

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