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First-principles determination of free energies of ferroelectric phase transitions and domains in $BaTiO_3$ and $PbTiO_3$ ANIL KUMAR, UMESH V. WAGHMARE, Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore, India — We present a powerful method based on a combination of (a) constrained polarization molecular dynamics and (b) thermodynamic integration to determine the free energy landscape relevant to structural phase transitions and related phenomena in ferroelectric materials, bridging the gap between first-principles calculations and phenomenological Landau-like theories. We illustrate it using first-principles effective Hamiltonians of $BaTiO_3$ and $PbTiO_3$ to (a) uncover the quantitative features of the free energy function that are responsible for its first-order ferroelectric transitions, and (b) calculate the minimum free energy pathway for the polarization switching and (c) evaluate temperature dependent domain wall free energy and pathways of the formation of domains. Our method can be readily generalized to any classical microscopic Hamiltonian and ensembles characterized with a given constraint. We show that certain terms have to be added to the phenomenological Landau-Devonshire free energy functions to capture the physics of ferroelectric materials.

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