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Molecular dynamics simulations of ferroelectric perovskites (BaTiO3 , BiFeO3) based on the effective Hamiltonian approach

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The theoretical description of ferroelectric perovskite materials at finite temperatures is commonly analyzed using Landau-Ginzburg type phenomenological models, and Monte-Carlo [MC] or molecular dynamics [MD] simulations. The parametrization of the phenomenological potentials originates from experimental data or from first principal calculations [1]. The MC and MD simulations use as bases the zero-temperature energy potentials determined from ab-initio calculations. There are commonly used two main approaches, the effective Hamiltonian method [2] and core-shell atomic-level simulations [3].

In this work, we address the structural and polar properties, the phase transition sequence of BiFeO3 and BaTiO3 at finite temperatures using molecular dynamic simulations based on the effective Hamiltonian, which was determined from ab-initio calculations, with strain, polarization, and oxygen octahedra tilt degrees of freedom [4]. The ground state energy landscape of the effective Hamiltonian is parametrized up to high orders at degrees of freedom. Such parametrization can precisely characterize the ordered phase and domain wall properties. To characterize the ferroelectric phase transitions we perform the simulations for various temperatures and compare them with outcomes of the core-shell approach [5].

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Summary

Topic

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