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Effective Hamiltonian Approach to Ferroelectric Ordering in Oxide Superlattices JUN HEE LEE, Seoul National University, Seoul, Korea, UMESH V. WAGHMARE, Jawaharlal Nehru Center for Advanced Scientific Research, Bangalore, India, JAEJUN YU, Seoul National University, Seoul, Korea —
We developed an effective Hamiltonian approach to the ferroelectric ordering in oxide superlattices. Despite that recent experiments have made a huge progress in making layer-by- layer heterostructures of ferroelectric superlattices, direct first-principles calculations are so far limited to the finite- size calculations, and electrostatic models are too simple to reflect intricate interactions of superlattices in atomic scale. We took the effective Hamiltonian method as one of candidates for the calculations of ferroelectric superlattices not only because it has enough degrees-of-freedom of energy terms to reflect complex interactions such as dipole-dipole interaction and short-range repulsion, but because it needs small amount of computational load compared with first- principles. All the parameters in the effective Hamiltonian are predetermined from the first-principles of constituent bulk components. As an application of the model parameters, we calculated the polarization of $(BaTiO_3)_n/(SrTiO_3)_m$, the results of which are in good agreement with those of previous first-principles calculations for not only of average polarizations but also of local polarizations. This effective Hamiltonian procedure can provide for developing a model for other kinds of oxide superlattices.

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