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Electric field-induced structural transition in rare-earth substituted $BiFeO_3$ from first principles LUCIA PALOVA, Rutgers University, DAISUKE KAN, ICHIRO TAKEUCHI, University of Maryland, KARIN M. RABE, Rutgers University — Using first principles calculations for $BiFeO_3$, we have identified an orthorhombic Pnma phase, lying only 14 meV per formula unit above the rhombohedral R3c ground state structure, as a low-energy alternative structure. We have constructed a model for the energy landscape in which rare-earth substitution on the Bi site favors the orthorhombic structure, so that it becomes the equilibrium phase about a critical rare-earth concentration (x=0.14 for Sm), resulting in the experimentally-observed morphotropic phase boundary (S. Fujino et al., APL 92, 202904 (2008)). For concentrations slightly above the critical concentration, we interpret the observed antiferroelectric-like double hysteresis loops as being produced by an electric-field-induced transition from the nonpolar orthorhombic phase back to the polar rhombohedral phase. By including the electric-field coupling through a linear $P \cdot E$ term in the energy, we have computed the magnitude and concentration dependence of the critical electric field and estimated the enhancement of the piezoelectric coefficient at the phase boundary, obtaining good agreement with the values obtained from experiment.

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