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Shell Model of $BaTiO_3$ derived from *ab-initio* DFT Calculations
JASON VIELMA, GUENTER SCHNEIDER, Oregon State University — A shell model for ferroelectric perovskites fitted to properties of first-principles density functional theory (DFT) is strongly affected by approximations made in the exchange-correlation functional within DFT and in general not as accurate as a shell model derived from experimental data. We have developed an isotropic shell model for $BaTiO_3$ based on the PBEsol exchange-correlation functional, which was specifically designed for solids and gives overall good agreement for the lattice parameters of all $BaTiO_3$ phases. Our shell model reproduces the sequence of phases of $BaTiO_3$ (rhombohedral, orthorhombic, tetragonal, cubic) and shows good agreement with experimental lattice constants at all temperatures, however the phase transition temperatures are too low. The energy scale can be improved by a simple scaling of the *ab-initio* potential energy surface. The polarization in the shell model is qualitatively correct but too small by approximately 30% compared to the experimental value.

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