# Development of a Classical Potential for $PbTiO_3$

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The use of ferroelectric perovskite oxides in a variety of technological applications has prompted extensive investigations of their structure and dynamics. First-principles density functional theory (DFT) calculations have played an important role in enhancing microscopic understanding of the relationships between composition, structure and properties [1–3]. Despite the success of first-principles methods, the great computational expense and restriction to stud ying zero-temperature properties have driven the development of more efficient atomistic and effective Hamiltonian potentials suitable for large-scale molecular dynamics (MD) simulations.

We present a modified bond-valence model of $PbTiO_3$ based on the principles of bond-valence [4] and bond-valence vector conservation [5]. The relationship between bond-valence energy and bond-order potential is derived analytically in the framework of a tight-binding model [6]. A new energy term, bond-valence vector energy, is introduced into the atomistic model and the potential parameters are re-optimized. The new model potential can be applied to both canonical ensemble ($NVT$) and isobaric-isothermal ensemble ($NPT$) molecular dynamics (MD) simulations. This model reproduces the experimental phase transition temperature in $NVT$ MD simulations and also exhibits the experimental sequence of temperature-driven and pressure-driven phase transitions in $NPT$ simulations. We expect that this improved bond-valence model can be applied to a broad range of inorganic materials.

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