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A new type of interatomic potential for oxides and its applications to $BiFeO_3$ and $PbTiO_3$[1] SHI LIU, HIROYUKI TAKENAKA, TINGTING QI, ILYA GRINBERG, ANDREW RAPPE, Department of Chemistry, University of Pennsylvania — Conventional first-principles methods are limited due to their intense computational cost. There is therefore still a strong need to develop accurate and efficient atomistic potential that could reproduce the full dynamical behaviors of metal oxides for large-scale finite-temperature simulations. We will present a new type of interatomic potential based on principles of bond-valence conservation and bond-valence vector conservation. The physical basis is justified quantum mechanically in the framework of a tight-bonding model, demonstrating that our model is formally equivalent to the bond-order potential (BOP), but is dramatically more efficient computationally. We will present an interatomic potential for $BiFeO_3$ and $PbTiO_3$, respectively. The validity of those model potentials is tested for both constant-volume and constant-pressure molecular dynamics simulations. The ferroelectric-to-paraelectric phase transitions of $BiFeO_3$ and $PbTiO_3$ are successfully reproduced. The calculated domain-wall energies using classical potentials are in satisfying agreement with DFT values. We conclude that our model potential is a promising type of force field that can have a broad application to a wide range of inorganic materials.

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