

First-principles-guided design of classical interatomic potential for oxides

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We developed a new type of interatomic potential for oxides based on the principles of bond-valence and bond-valence vector conservation. [1] The relationship between the bond-valence model and the bond-order potential is derived analytically in the framework of a tight-binding model. We showed that the bond-valence energy can be rewritten into the form of the well-known Finnis-Sinclair potential. The model potentials for two ferroelectric materials, PbTiO_3 and BiFeO_3 , have been parametrized based on first-principles results. [2,3] The optimized potential is accurate for both canonical ensemble and grand canonical ensemble molecular dynamics (MD) simulations and sufficiently efficient for studying large systems ($\sim 1,000,000$ atoms). We expect that this bond-valence model can be applied to a broad range of inorganic materials.

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- [2] S. Liu, H. Takenaka, T. Qi, I. Grinberg, and A. M. Rappe, arXiv:1211.5166 (2012).
- [3] S. Liu, I. Grinberg, and A. M. Rappe, *J. Phys. Cond. Matt.* **25**, 102202 (1-6) (2013).