Total energy calculation of perovskite, $BaTiO_3$, by self-consistent tight binding method

Cong B.T., Huy P.N.A., Schelling P.K., Halley J.W.

Faculty of Physics, Hanoi University of Science, 334 Nguyen Trai Street, Hanoi, Viet Nam; Argonne National Laboratory, Argonne, IL, United States

Abstract: We present results of numerical computation on some characteristics of $BaTiO_3$ such as total energy, rgy, lattice constant, density of states, band structure etc using self-consistent tight binding method. Besides strong Ti-O bond between 3d on titanium and 2p orbital on oxygen states, we also include weak hybridization between the Ba 6s and O 2p states. The results are compared with those of other more sophisticated methods.

Author Keywords: $BaTiO_3$; Perovskite; Tight binding

Index Keywords: Band structure; Barium; Calculations; Chemical bonds; Electronic density of states; Ferroelectric materials; Integral equations; Lattice constants; Oxygen; Perovskite; Titanium; Self consistent tight binding method; Total energy; Weak hybridization; Barium titanate

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Correspondence Address: Cong, B.T.; Faculty of Physics, Hanoi University of Science, 334 Nguyen Trai Street, Hanoi, Viet Nam

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Authors with affiliations:

1. Cong, B.T., Faculty of Physics, Hanoi University of Science, 334 Nguyen Trai Street, Hanoi, Viet Nam
2. Huy, P.N.A., Faculty of Physics, Hanoi University of Science, 334 Nguyen Trai Street, Hanoi, Viet Nam
3. Schelling, P.K., Argonne National Laboratory, Argonne, IL, United States
4. Halley, J.W.

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