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First Principles Approach to $BaTiO_3$

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Abstract: We present state of art first-principles study on the static and dynamic properties of $BaTiO_3$, a typical ferroelectric material. Here, structure, equation of state, phase stability, and phase transformations of $BaTiO_3$ studied in Generalized Gradient Approximation. Furthermore, properties such as, Born effective charges, optical dielectric constant and phonon spectra are calculated from Density Functional Perturbation Theory.

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