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OPTIMIZED CRYSTALLINE STRUCTURE AND PROPERTIES OF CUBIC AND TETRAGONAL $BaFeO_3$

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Abstract:
The ab-initio Hartree Fock, DFT-LDA, DFT-PWGGA, DFT-PBE and hybrid B3LYP potentials are employed to compute the optimized cubic and tetragonal crystalline structures by employing BILLY script and CRYSTAL09 code. ELASTCON and EOS algorithms are employed to compute the elastic constants and bulk moduli of the cubic phase. The equation of state bulk moduli of tetragonal phase is computed.

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