OPTIMIZED CRYSTALLINE STRUCTURE AND PROPERTIES OF CUBIC AND TETRAGONAL BaFeO$_3$

Author(s): Ghous Bakhsh Narejo, Warren Perger

Volume: Thematic Issue on Energy

Pages: 91-98

Date: January 2012

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.

For full paper, contact:
Prof Muhammad Masood Rafi
Editor, NED University Journal of Research
Ph: +92 (21) 99052413; Fax: +92 (21) 99261255
Email: NED-Journal@neduet.edu.pk
Website: http://www.neduet.edu.pk/NED-Journal