# Investigation of electronic and optical properties of barium titanate using calculations of the basics

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**In this project we have studied theoretically the structural, electronic and optical properties of BaTiO3 in two phases, cubic and tetragonal. In this work we have used full potential linearized augmented plane waves in the framework of density functional theory and by local density approximation (LDA) ,and generalized gradient approximation (GGA) , Engle Vosko (EV). The results of calculations for cubic and tetragonal phasesof PbTiO3 show that there is a direct band gap in Γ direction in the first brillouin zone. The results of calculation for LDA , GGA and EV method give the band gap about 2-2.3 eV. Electronic density around each atom (Ti, Pb and O) have been calculated. Different Optical parameter of cubic and tetragonal phases ofBaTiO3 ( JDOS, Dielectric function, Refraction coefficient, Conductivity and Electron Energy Loss Spectroscopy) have been calculated. The refraction coefficient for two phases is in good agreement with experiment.**

**Keywords : Electronic-Optical Properties - Barium Titanate**

Islamic Azad University, Rasht Branch - Thesis Database
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