FIRST PRINCIPLE CALCULATION ON ELASTIC AND ELECTRONIC PROPERTIES OF CUBIC $PBTIO_3$

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ABSTRACT

FIRST PRINCIPLE CALCULATION ON ELASTIC AND ELECTRONIC PROPERTIES OF CUBIC $PbTiO_3$

The elastic constant, electronic band structure and density of state (DOS) $PbTiO_3$ (PT) are investigated through first principle calculation using the Density Functional Theory (DFT) within local density approximation (LDA). All the calculations are performed using the Cambridge Serial Total Energy Package computer code. The elastic constants and their pressure dependence are calculated up to 30 GPa. The independent elastic constants (C_{11}, C_{12}, and C_{44}) and bulk modules, B^0 are obtained and analyzed. The results show that PT has a mechanical stability in cubic phase. From the calculation along the higher symmetry direction in the Brillouin zone, the direct band gap of PT is 1.564 eV at point (X-X), and DOS shows the covalancy between Ti 3d and O 2p. The effects of pressure on volume of cubic are explained using equation of state. The fundamental band gaps (G-G) are also investigated with the external pressure applied. The results were compared and found to be in good agreement with other calculated values using different methods.

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