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6a) FIRST PRINCIPLES STUDY OF ELECTRONIC PROPERTIES OF PBTIO$_3$ PARAELECTRIC AND FERROELECTRIC PHASES

S. M. Hosseini, T. Movlarooy* and A. Kompany**
**Department of Physics, materials and Electroceramics laboratory*
Ferdowsi University of Mashhad, Iran

The electronic structure, energy gap, total and partial density of states of $PbTiO_3$ in cubic and tetragonal phases have been studied using full potential linearized augmented plane wave method (FP-LAPW). The calculations have been made within the framework of density functional theory (DFT), with local density approximation (LDA) and generalized gradient approximation (GGA). In the tetragonal phase, it is found that the bond between Pb and O is ionic while there is a strong hybridization between Ti-*3d* and O-2p, which is necessary for ferroelectricity in $PbTiO_3$. It is also indicated that shallow Pb-6s semicore hybridize with the O-2p state. The results also show an indirect band gap of 1.7eV at X-□ points in the Brillouin zone for the cubic phase and an indirect band gap of 2.0eV at X-Γ point for the tetragonal phase, in the absence of the scissors operation. These results are in better agreement with the published theoretical and experimental data.