AB INITIO STUDY ON FERROELECTRIC OXIDE $ATiO_3$ (A=Sr, Ba, Sn, Pb) BY USING DENSITY FUNCTIONAL THEORY

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ABSTRACT

AB INITIO STUDY ON FERROELECTRIC OXIDE ATiO$_3$ (A=Sr, Ba, Sn, Pb) BY USING DENSITY FUNCTIONAL THEORY

The first principle study using Density Functional Theory (DFT) and Local-density Approximation (LDA) is studied to calculate electronic band structure and density of states (DOS) of ferroelectric oxide ATiO$_3$ (Sr, Ba, Sn, Pb). The calculations include its bulk, BaTiO$_3$, SrTiO$_3$, PbTiO$_3$ and SnTiO$_3$, and superlattices BaTiO$_3$/SrTiO$_3$, PbTiO$_3$/SrTiO$_3$ and SnTiO$_3$/SrTiO$_3$ with SrTiO$_3$ is treated as substrate of the superlattices. For bulk ferroelectric compounds, the calculated energy gap in the band structure of SrTiO$_3$, BaTiO$_3$, PbTiO$_3$ and SnTiO$_3$ is 1.864 eV, 1.776 eV, 1.549 eV and 0.967 eV respectively. The interaction exists in the density of states of each compounds is studied as to determine the ferroelectric behaviour in each compounds. The calculated energy gap of BaTiO$_3$/SrTiO$_3$, SnTiO$_3$/SrTiO$_3$ and PbTiO$_3$/SrTiO$_3$ superlattices is 1.895 eV, 1.467 eV and 1.958 eV respectively. Hence the difference between each superlattice compounds and bulk BaTiO$_3$, PbTiO$_3$ and SnTiO$_3$, is studied and show in good agreement. Lastly, phonon dispersion curves and lattice dynamic of bulk BaTiO$_3$, SrTiO$_3$, PbTiO$_3$ and SnTiO$_3$ is evaluated and found that these compounds having possibilities to transform into the lowest symmetry phase which are tetragonal, orthorhombic and rhombohedral below its Curie temperature (T_c).