

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

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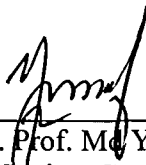
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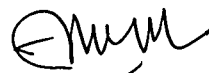
This Final Year Project Report entitled “Ab initio study on ferroelectric oxide $ATiO_3$ ($A=Sr, Ba, Sn, Pb$) by using Density Functional Theory” was submitted by Khairul Helmy Kamalul Arifin, in partial fulfilment for the degree of Bachelor of Science (Hons.) Physics, in the Faculty of Applied Sciences, and was approved by:



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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 $ATiO_3$ ($A= Sr, Ba, Sn, Pb$). 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).