AB-INITIO STUDIES ON THE ELECTRONIC PROPERTIES OF NEW FERROELECTRIC MATERIALS BASED ON BULK $SnBO_3$ (B=Ti, Zr) AND SUPERLATTICE $SnZrO_3/SnTiO_3$ WITH USING DENSITY FUNCTIONAL THEORY (DFT).

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Final Year Project Report Submitted in
Partial Fulfillment of the Requirements for the
Degree of Bachelor of Science (Hons.) Physics
In the Faculty of Applied Sciences
Universiti Teknologi MARA

NOVEMBER 2010

This Final Year Project Report entitled "**Ab-initio studies on the electronic properties of new ferroelectric materials based on bulk $SnBO_3$ (B=Ti, Zr) and superlattice $SnZrO_3$ /$SnTiO_3$ with using density functional theory (DFT)**" was submitted by Muhamad Kamil Bin Yaakob, 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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ACKNOWLEDGEMENT

First of all, I am really grateful to the greatest Allah s.w.t for the blessing, strength and ability given to me to complete this thesis.

This thesis would not have been completed without support and guidance of several people. I would like to sincerely thank Assoc. Prof. Dr. Muhd Zu Azhan Yahya for his contribution, valuable advices, constructive comments and continuous guidance during completing this work.

Also, I would like to acknowledge Mohamad Fariz Mohamad Taib and Khairul Helmy Kamalul Arifin for their taught and guidance during the completion of this thesis.

Also, I would like to thank all of the students in *i*Made laboratory for their support and motivation in order to accomplish this thesis.

I am deeply grateful to my parents for their prayers, support and encouragement during my study. In addition, a thank you to all the lectures, my friends and everybody who had contributed for this thesis directly or indirectly with or without my concern their contributions are gratefully acknowledge.

ABSTRACT

AB-INITIO STUDIES ON THE ELECTRONIC PROPERTIES OF NEW FERROELECTRIC MATERIALS BASED ON BULK $SnBO_3$ (B=Ti, Zr) AND SUPERLATTICE $SnZrO_3/SnTiO_3$ WITH USING DENSITY FUNCTIONAL THEORY (DFT).

The electronic band structure, density of states (DOS) and phonon vibration of perovskite $SnBO_3$ (B=Ti, Zr) and superlattice $SnZrO_3/SnTiO_3$ investigated from first principles calculation using Density Functional Theory (DFT) within Local-density Approximation (LDA). Full geometry optimization of $SnTiO_3$, $SnZrO_3$ and superlattice $SnZrO_3/SnTiO_3$ provides a stable tetragonal structure relative to cubic one. The calculated energy gap in the band structure of $SnTiO_3$ and $SnZrO_3$ and superlattice $SnZrO_3/SnTiO_3$ is 0.966 eV, 1.691 eV and 1.089 eV respectively. Phonon dispersion curves and lattice dynamic of bulk $SnTiO_3$ and $SnZrO_3$ 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 (Tc). The born effective charges shows large charges between Sn-O bond refers the strong electronic interaction (Coulomb interaction) along the bond and is also a factor that resulting ferroelectricities in the compound

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