

**AB-INITIO STUDIES ON THE ELECTRONIC PROPERTIES OF NEW
FERROELECTRIC MATERIALS BASED ON BULK SnBO_3 (B=Ti, Zr) AND
SUPERLATTICE $\text{SnZrO}_3/\text{SnTiO}_3$ WITH USING DENSITY FUNCTIONAL
THEORY (DFT).**

MUHAMAD KAMIL BIN YAAKOB

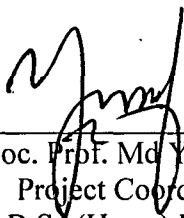
**Final Year Project Report Submitted in
Partial Fulfillment of the Requirements for the
Degree of Bachelor of Science (Hons.) Physics
In the Faculty of Applied Sciences
Universiti Tekonologi MARA**

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 $\text{SnZrO}_3/\text{SnTiO}_3$ 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:



Assoc. Prof. Dr Muhd Zu Azhan Yahya
Supervisor
B.Sc (Hons.) Physics
Faculty of Applied Sciences
Universiti Teknologi MARA
40450 Shah Alam
Selangor



Assoc. Prof. Md Yusoff Theeran
Project Coordinator
B.Sc (Hons.) Physics
Faculty of Applied Sciences
Universiti Teknologi MARA
40450 Shah Alam
Selangor



Dr. Ab Malik Marwan Ali
Head of Programme
B.Sc (Hons.) Physics
Faculty of Applied Sciences
Universiti Teknologi MARA
40450 Shah Alam
Selangor

Date: 30 NOV 2010

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 *iMade* 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 $\text{SnZrO}_3/\text{SnTiO}_3$ 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 $\text{SnZrO}_3/\text{SnTiO}_3$ 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 $\text{SnZrO}_3/\text{SnTiO}_3$ 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 $\text{SnZrO}_3/\text{SnTiO}_3$ 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 (T_c). 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

TABLE OF CONTENTS

	Pages
ACKNOWLEDGEMENT	iii
TABLE OF CONTENTS	iv
LIST OF TABLES	vi
LIST OF FIGURES	vii
LIST OF ABBREVIATIONS	ix
ABSTRACT	x
ABSTRAK	xi
CHAPTER 1 INTRODUCTION	
1.1 Background	1
1.2 Problem statements	5
1.3 Objectives of study	6
1.4 Limitation and Scope	6
1.5 Significant of study	7
CHAPTER 2 LITERATURE REVIEW	
2.1 Ferroelectricity	8
2.2 Born Effective Charges	9
2.3 Density of states and band structure for bulk single lattice	10