

**FIRST PRINCIPLE CALCULATION ON ELASTIC AND
ELECTRONIC PROPERTIES OF CUBIC PBTIO₃**

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

JUNE 2012

This Final Year Project entitled “**First Principle Calculation on Elastic and Electronic Properties of Cubic PbTiO₃**” was submitted by Fadhlul Wafi Bin Badrudin, in partial fulfillment of the requirements for the Degree of Bachelor of Sciences (Hons.) Physics, in the Faculty of Applied Sciences, and was approved by

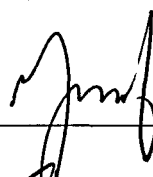


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ACKNOWLEDGMENT

Assalamualaikum, first and foremost, praise be to Allah, the most beneficent and most merciful. I wish to express my great appreciation to Professor Dr Muhd Zu Azhan Yahya and Assoc. Professor Dr Ab Malik Marwan Ali for their promptness and effort in providing me with not only the knowledge and experience, but also their believeness and encouragement.

My mentor (PhD candidates) Mr Mohamad Fariz Mohamad Taib and Mr Muhamiad Kamil Bin Yaakob who always help me in understanding this research and provide me a lot of tasks in order to complete this thesis. There is absolutely no word other than thank you, to describe their dedication through this work. Thanks for your time and kindness.

I would also like to wish the deepest thanks especially to my research mate, Muhd Sazwan Affendi Bin Rasiman who always sharing his knowledge and accompanied me in completing this thesis.

Also to all IMADE members, thanks for your kindness and great hospitality during carrying out the research in IMADE lab.

Last but not least to my family, especially to my beloved mother, Rohani Binti Hj Ali and my father Badrudin Bin Md Rejab for their prayers, patient and encouragement that strengthens my spirit in completing this thesis. To my entire sibling, Kak Long, Abang, Kak and Kak Cik, thanks for your moral and some financial supports.

ABSTRACT

FIRST PRINCIPLE CALCULATION ON ELASTIC AND ELECTRONIC PROPERTIES OF CUBIC PbTiO_3

The elastic constant, electronic band structure and density of state (DOS) PbTiO_3 (PT) are investigated through first principle calculation using the Density Functional Theory (DFT) within local density approximation (LDA). All the calculations are performed using the Cambridge Serial Total Energy Package computer code. The elastic constants and their pressure dependence are calculated up to 30 GPa. The independent elastic constants (C_{11} , C_{12} , and C_{44}) and bulk modulus, B^0 are obtained and analyzed. The results show that PT has a mechanical stability in cubic phase. From the calculation along the higher symmetry direction in the Brillouin zone, the direct band gap of PT is 1.564 eV at point (X-X), and DOS shows the covalency between Ti 3d and O 2p. The effects of pressure on volume of cubic are explained using equation of state. The fundamental band gaps (G-G) are also investigated with the external pressure applied. The results were compared and found to be in good agreement with other calculated values using different methods.

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