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FACULTY OF APPLIED SCIENCES

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**Preface**

The Scientific Project Colloquium offers a platform for publishing Diploma Science final year projects (FYP). The objective is to effectively distribute research findings throughout all scientific disciplines. The primary objective of including final year projects into the course curriculum is to encourage students to put their theoretical knowledge into practical applications.

We would like to express our gratitude to our primary establishment, the Faculty of Applied Sciences and Universiti Teknologi MARA, Perak Branch, for their invaluable assistance.

Lastly, we would like to express our gratitude to all of the authors for the tremendous help in preparing the articles, without which this undertaking would not have been completed.

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# PHOTOCATALYTIC BEHAVIOR OF $LiNbO_3$: A DFT-BASED INVESTIGATION OF ELECTRONIC AND OPTICAL PROPERTIES

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**Abstract:** This study employs Density Functional Theory (DFT) to explain the photocatalytic mechanisms of Lithium Niobate ($LiNbO_3$), a promising material for environmental and energy applications. The exchange correlation for this study is based on modified Perdew-Burke-Ernzerhof generalized gradient approximation for solids (GGA-PBEsol). The structural properties and electronic properties of $LiNbO_3$ are comprehensively analyzed to understand its photocatalytic potential. From the band structure, calculations shows that $LiNbO_3$ the band gap energy using GGA-PBEsol is 3.48 eV. The optical absorption spectrum indicates strong absorption in the UV region which is agree the band gap value. The photocatalytic approach shows the theoretical process happend in the process.

***Keywords:*** *$LiNbO_3$, DFT, photocatalysis, electronic properties, optical properties*

## INTRODUCTION

Using Czochralski technique, Ballman is successfully produce a $LiNbO_3$ crystal and lead to the growth of investigation of $LiNbO_3$ in 1965 (Jackson & Szaller, 2020). Since then, a variety of techniques have been employed to generate $LiNbO_3$ crystals such as spin coating, nuclear method, sol-gel, liquid phase epitaxy route and others (Shih et al., 2008)(Fadil et al., 2011)(Yu & Liu, 2007). $LiNbO_3$ is a primitive unit cell that is either rhombohedral or hexagonal in shape and is a member of the trigonal crystal system. This substance exhibits two distinct phases based on temperature. $LiNbO_3$ features a paraelectric phase with a space group of R$\underline{3}$c above 1480K and a ferroelectric phase with a space group of R3c at ambient temperature (Mamoun et al., 2013)(J. Yang et al., 2013)(Hsu et al., 1997). $LiNbO_3$ possess variety of physical characteristics like high birefringence, photo-elastic, pyroelectric, and piezoelectric properties (Sanna & Schmidt, 2012). Furthermore, $LiNbO_3$ also has a high melting point and a high Curie temperature of 1480 K. It also exhibits a significant spontaneous polarisation of roughly 0.70 $C/m^2$ (Zhang et al., 2019)(Wang et al., 2019) and a broad band gap energy of 3.78 eV (Thierfelder et al., 2010).

Photocatalysis is a process that uses a semiconductor material to accelerate a photoreaction in the presence of light. When the photocatalyst absorbs light energy, typically from ultraviolet or visible light, it generates electron-hole pairs that can drive chemical reactions at its surface (Saravanan et al., 2017)(X. Yang & Wang, 2018). This technology has significant implications for environmental and energy applications, including the degradation of pollutants in water and air, the disinfection of harmful microorganisms, and the production of clean energy through water splitting to generate hydrogen. By harnessing the power of light, photocatalysis offers a sustainable and efficient method for addressing pressing environmental challenges and advancing renewable energy solutions.

Recently, computational methods have become a crucial component of materials research as it can effectively analyse and explain the structural, electrical, and optical properties of materials. The investigation of the structural, electrical, and optical characteristics of $LiNbO_3$ has been conducted utilising the generalise gradient approximation (GGA) and local density approximation (LDA) techniques, as reported in previous studies (J. Yang et al., 2013)(Hossain, 2019)(Tripathy & Sahu, 2015). As reported in these study, the band gap energy of $LiNbO_3$ falls between the range of 3.5 eV to 5.0 eV (Tripathy & Sahu, 2015)(Hossain, 2019)(Raturi & Mittal, 2020)(Husin et al., 2019) which is slightly different from the experimental work, 3.78 eV(Thierfelder et al., 2010). The discrepancy between experimental measurements and first-principles values may arise from the self-interaction and derivative discontinuity of the exchange correlation energy in theoretical calculations. Since Density Functional Theory (DFT) offers a powerful computational tool for investigating the fundamental electronic and optical properties of materials, this method can be used to gain a deep insights into the behaviour of electron-hole pairs, band structure, and surface reactivity, all of which are crucial for optimizing the photocatalysis.

This study aims to explore the photocatalytic behaviour of $LiNbO_3$ through a DFT-based analysis, focusing on its electronic and optical properties. By examining the band structure, density of states, and optical absorption characteristics, this investigation seeks to elucidate the properties of $LiNbO_3$ as a photocatalyst. The findings of this research not only contribute to the theoretical understanding of $LiNbO_3$ as a photocatalyst but also provide valuable insights for the design and development of more efficient photocatalytic systems.

## COMPUTATIONAL METHODOLOGY

The ground state properties of any material can be computed using the density functional theory (DFT). In this paper, the plane wave DFT is used to optimize the geometry and calculate the properties of $LiNbO_3$. The first-principles calculations performed in this work are based on DFT within exchange-correlation functional from modified Perdew-Burke-Ernzerhof generalized gradient approximation for solids (GGA-PBEsol) using Cambridge Serial Total Energy Package (CASTEP) computer code. The experimental for structural $LiNbO_3$ is a=b= 5.1502 Å and c= 13.8636 Å as reported by Redfield and Burke using X-ray crystallography method was used as a reference in this work (Redfield & Burke, 1974). Geometrical optimization is first performed using GGA-PBEsol method on $LiNbO_3$ unit cell and followed by its electronic and optical properties. In GGA-PBEsol functional, the cutoff energy used in this work is 380 eV with k-point grid of 3x3x2. Geometrical optimization was set at $5.0 \times 10^{-6}$ eV/atom for total energy, 0.01 eV/Å for maximum force, 0.02 GPa for maximum stress and $5.0 \times 10^{-4}$ Å for maximum displacement.

## RESULTS AND DISCUSSION

*Computational Approach (DFT)*

The crystal structure of $LiNbO_3$ possesses a space group number of R3c with hexagonal symmetry. The experimental and theoretical lattice parameters are summarized in Table 1. According to the table, the lattice parameters optimized using the GGA-PBEsol functional yields lattice parameters with a deviation of only 0.12% for the lattice a=b and 0.13% for the lattice c. Additionally, the calculated volume using the GGA-PBEsol method is slightly overestimated by 0.25% from the experimental data. These findings indicate that the GGA-PBEsol method provides a closer match to the experimental lattice parameters. Furthermore, the results obtained in this study are consistent with other theoretical studies, confirming the reliability and accuracy of the findings

Table 1: Comparison between the experimental lattice parameters and volume of $LiNbO_3$ with other first principles result from standard DFT.

| Method | a (Å) | b (Å) | c (Å) | Volume (Å$^3$) |
|---|---|---|---|---|
| GGA-PBEsol *(this work)* | 5.160 | 5.160 | 13.846 | 319.258 |
| GGA-PBE (L. W. Zainuddin et al., 2022) | 5.159 | 5.159 | 13.869 | 320.180 |
| GGA-PBEsol (Saleev et al., 2018) | 5.118 | 5.118 | 13.958 | 316.632 |
| Experimental work (Redfield & Burke, 1974) | 5.150 | 5.150 | 13.864 | 318.460 |

Table 2 presents the band gap energy in this study in comparison to other theoretical and experimental findings. The experimental band gap energy, as reported, is 3.78 eV. The band gap result from standard GGA-PBEsol were 3.483 eV and percentage difference as compared to experimental works is 7.92%.

Table 2: Comparison of the band gap energy of $LiNbO_3$ from this work before and after Hubbard U correction with the experimental result and other theoretical work.

| Method | Band gap energy (eV) |
|---|---|
| GGA-PBEsol *(this work)* | 3.483 |
| GGA-PBE (L. W. Zainuddin et al., 2022) | 3.590 |
| Experimental work (Redfield & Burke, 1974) | 3.780 |

Figure 1 (a) shows the band structure and (b) density of state (DOS) for $LiNbO_3$. From the band structure, the energy difference between the valence band maximum (VBM) and the conduction band minimum (CBM) can be reveals.

This band gap is critical for determining whether a material behaves as a conductor, semiconductor, or insulator. For semiconductors and insulators, the size of the band gap directly affects the material's optical and electronic properties. Meanwhile, the density of states (DOS) also plays an important role in analysing the physical properties of materials. The density of state of a material is defined as the electronic energy states per unit energy at each level that are occupied by the electrons. The partial density of state for $LiNbO_3$ using GGA-PBEsol. The vertical line represents the Fermi level marked at the maximum valance band. At energy from -20 eV to -10 eV, the band is mainly derived from the O 2s state. From -5 eV to 0 eV, the highest density at the maximum valance band is mainly derived from the O 2p state flowed by Nb 4d state. It is shown an overlapping between Nb 4d and O 2p states from this energy band thus demonstrating a covalent bond between Nb and O. Meanwhile, the highest density at the lowest conduction band is mainly derived from Nb 4d state.

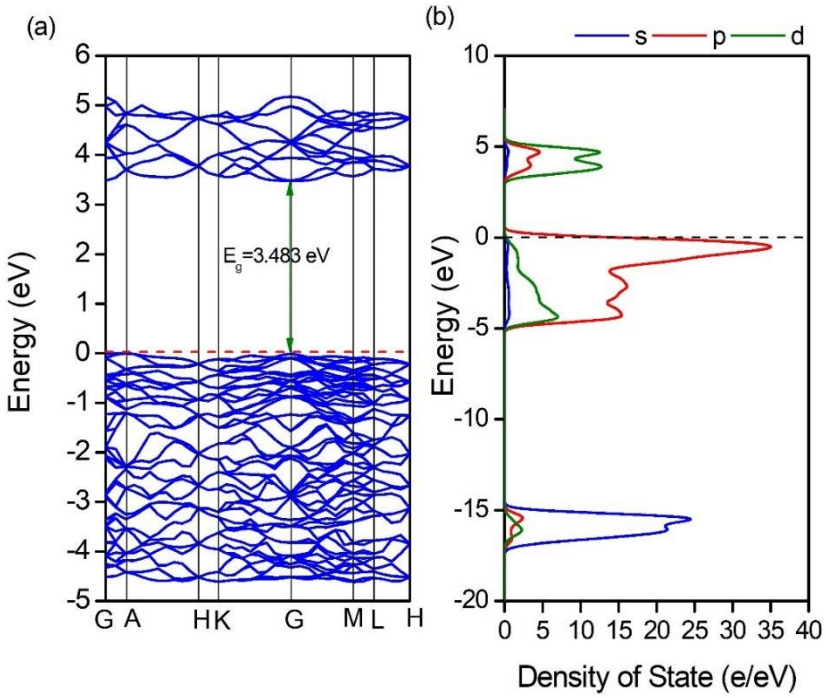


Figure 1. (a) Band structure and (b) density of states (DOS) of $LiNbO_3$ using GGA-PBEsol.

The absorption coefficient is a critical parameter in determining the efficiency of solar energy conversion, as it directly influences how deeply light of a specific wavelength can penetrate a material before being absorbed. A higher absorption coefficient indicates that the material is more effective at capturing light, which is essential for applications like photovoltaics and photocatalysis. Figure 2 shows the (a) energy-dependent absorption coefficients and (b) wavelength-dependent absorption coefficients of $LiNbO_3$ using GGA-PBEsol. The absorption edge is observed around ~3.30 eV. The optical spectrum for GGA-PBEsol was observed around ~354 nm. Based on prediction properties, it may be concluded that the study can be applied in optical applications and other potential applications such as photocatalysts and photovoltaics.

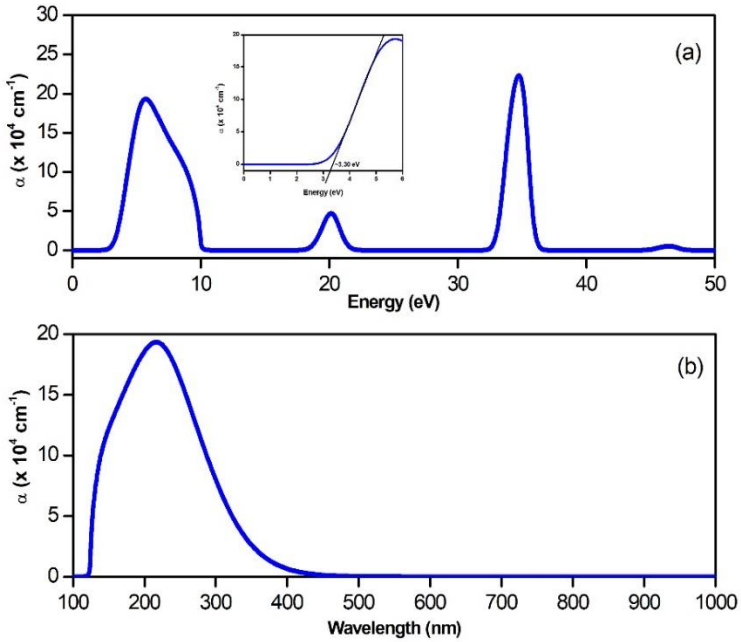


Figure 2. (a) energy-dependent absorption coefficients (b) wavelength-dependent absorption coefficients of $LiNbO_3$ using GGA-PBEsol

*Theoretical approach for photocatalysis*

Photocatalytic reactions take place at the interface between the catalyst and the reaction medium when irradiated with electromagnetic waves in the UV or visible spectrum. Photocatalysts are semiconductors characterized by a band gap ranging from 1.4 to 3.8 eV (S. S. Shinde et al., 2011). When photons with energy greater than the band gap are absorbed, electrons are excited from the valence band to the conduction band, leading to the formation of electron-hole pairs (Ranjit K. Nath et al., 2012). These electron-hole pairs possess oxidative and reductive properties, enabling redox reactions. The photocatalytic process involves several key steps as followed:

1. Photo-excitation: The semiconductor is excited by electromagnetic energy that is equal to or greater than its band gap energy.
2. Electron-Hole Pair Generation: The absorbed energy results in the generation of electron-hole pairs.
3. Separation of Charge Carriers: Electrons and holes must separate at a rate that exceeds their recombination rate; otherwise, the photocatalyst becomes deactivated.
4. Pollutant Adsorption: Pollutants adsorb onto the catalyst's surface.
5. Surface Redox Reactions: Redox reactions occur at the surface of the photocatalyst, involving electrons, holes, and the adsorbed molecules, which are critical for determining the final products.
6. Product Desorption: The reaction products desorb from the catalyst surface.

The efficiency of photocatalysis is influenced by how effectively electromagnetic energy is utilized and by minimizing the rate of recombination processes. The type, structure, and morphology of the photocatalyst are crucial factors that influence the degradation of organic pollutants, the destruction of bacteria and viruses, the decomposition of dyes, and the synthesis of specific compounds.

## CONCLUSIONS

Based on the photocatalysis and DFT approaches, it shows that $LiNbO_3$ can be a potential material for photocatalyst. The results shows that the band gap energy of 3.483 eV and the optical absorption at the edge of 330 nm. However, this shows that $LiNbO_3$ can be a good photocatalyst in the UV region. To enhance the properties of $LiNbO_3$ as the photocatalysis in visible region, $LiNbO_3$ can be doped with metal or non-metal dopants in future works.

## COMPLIANCE OF ETHICAL STANDARDS

*Not applicable.*

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*nar*