ELECTRONIC PROPERTIES OF $LiNbO_3$ USING DENSITY FUNCTIONAL THEORY

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Abstract: Using the density functional theory, the structural and electronic properties of $LiNbO_3$ are investigated. The lattice constants and unit cell volume were calculated from the optimized unit cell, which were in well agreement with the reported theoretical as well as experimental values. Electronic band structure and density of states (DOS) demonstrated its semiconducting nature showing a band gap of 3.504 eV.

Keywords: *$LiNbO_3$, DFT, electronic properties.*

INTRODUCTION

$LiNbO_3$ were firstly synthesised in Bell Laboratories in 1966. It is an artificial dielectric substance that does not occur in nature. It was found to be ferroelectric for the first time in 1949 (Weis & Gaylord, 1985). Ferroelectric lithium niobate ($LiNbO_3$) is widely used in the field of integrated and guided-wave optics due to its advantageous optical, piezoelectric, electro-optic, elastic, photoelastic, and photorefractive characteristics(Sanna & Schmidt, 2017). The common synthesized method in producing $LiNbO_3$ crystal are Czochralski method, sol-gel method, citrate method and a few more method (Masloboeva et al., 2020)(Reza & Fray, 2014).

$LiNbO_3$ has gain researcher attention due to its unique properties. $LiNbO_3$ belongs to a trigonal crystal system and can be describe as hexagonal or rhombohedral primitive unit cell. This material exhibit in two different phases according to the temperature. $LiNbO_3$ exhibits a ferroelectric phase at room temperature with a space group of R3c and possess a paraelectric phase with a space group of R$\bar{3}$c above 1480K (Dan-dan et al., 2015)(Saleev et al., 2018). $LiNbO_3$ also owns diverse physical properties such as pyroelectric, piezoelectric, photo-elastic, electro-optic and large birefringence (Sanna & Schmidt, 2012). In addition, $LiNbO_3$ has a high Curie temperature of 1480 K with a high melting point. It also exhibit a wide band gap energy of 3.78 eV (Thierfelder et al., 2010) and a large spontaneous polarization about 0.70 C/m^2 (Sanna & Schmidt, 2012).

In the last 20 years, computational methods have become an important and necessary part of material science study and it can give a high accuracy detailed feature of materials, such as their structural, electronic, and optical properties. Kohiki et al. conducted a comparative investigation of the energy loss function using theoretical calculation and experimental measurement with X-ray photoemission spectra (Kohiki et al., 1998). Comparative structural and physical studies of the paraelectric and ferroelectric phases of $LiNbO_3$ are also available. Numerous studies on the structural, electronic, and optical properties of $LiNbO_3$ were conducted using theory (Husin et al., 2019)(L. W. Zainuddin et al., 2022)

In this paper, the structural and electronic properties of $LiNbO_3$ have been performed using density functional theory. This study is carried out using Cambridge Serial Total Energy Package (CASTEP) computer code within the exchange correlation of local density approximation (LDA) approach. The objective of this work is to investigate the density of state and band gap energy of $LiNbO_3$.

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 desired properties of $LiNbO_3$. The first-principles calculations performed in this work are based on density functional theory (DFT) within exchange-correlation functional from Local Density Approximation (LDA) using Cambridge Serial Total Energy Package (CASTEP) computer code. Geometrical optimization is first performed using the LDA method on $LiNbO_3$ and followed by its electronic properties. In LDA functional, the cutoff energy used in this work is 380 eV with k-point
grid of 3×3×2. Geometrical optimization was set at 5.0 x 10^{-6} eV/atom for total energy, 0.01 eV/Å for maximum force, 0.02 GPa for maximum stress and 5.0 x 10^{-4} Å for maximum displacement.

RESULTS AND DISCUSSION

This section analyzes the structural and electronic properties of $LiNbO_3$ crystal in details. Table 1 shows the lattice parameter for $LiNbO_3$ via experimental and theoretical values. From Table 1, the optimized lattice parameter as compared to the experimental values shows an underestimated value of 1.8% for lattice and b, 1.4% for lattice c and 4.7% for cell volume. As comparaison with others theoretival results, the lattice parameter shows a comparable and acceptable values. Figure 1 shows the band structure and partial density of states (DOS) fro $LiNbO_3$. From the band structure, the band gap energy of 3.504 eV is observed. This value indicate that $LiNbO_3$ has wide band gap energy. In the same figure, the density of state of $LiNbO_3$. At valance band (VB) from -6 eV to 0 eV was mainly derived from O 2p state meanwhile from 0 eV to 3 eV shows a gap which indicate the band gap energy similar to the band structure. From 3 eV to 6 eV, the main peak were corespond to Nb 4d state folowwed by O 2p state and Li 2s state. It clearly observed that there is overlapping between Nb 4d and O 2p states which show a strong covalent bonding between Nb and O.

Table 1. Structural Parameters of $LiNbO_3$ from Theoretical and Experimental

a (Å)	b (Å)	c (Å)	Volume ($Å^3$)	References
5.058	5.058	13.699	303.631	This work
5.057	5.057	13.942	308.58	Theoretical (Hossain, 2019)
5.186	5.186	14.009	326.289	Theoretical (Boukhtouta et al., 2020)
5.150	5.150	13.864	318.460	Experimental (Redfield & Burke, 1974)

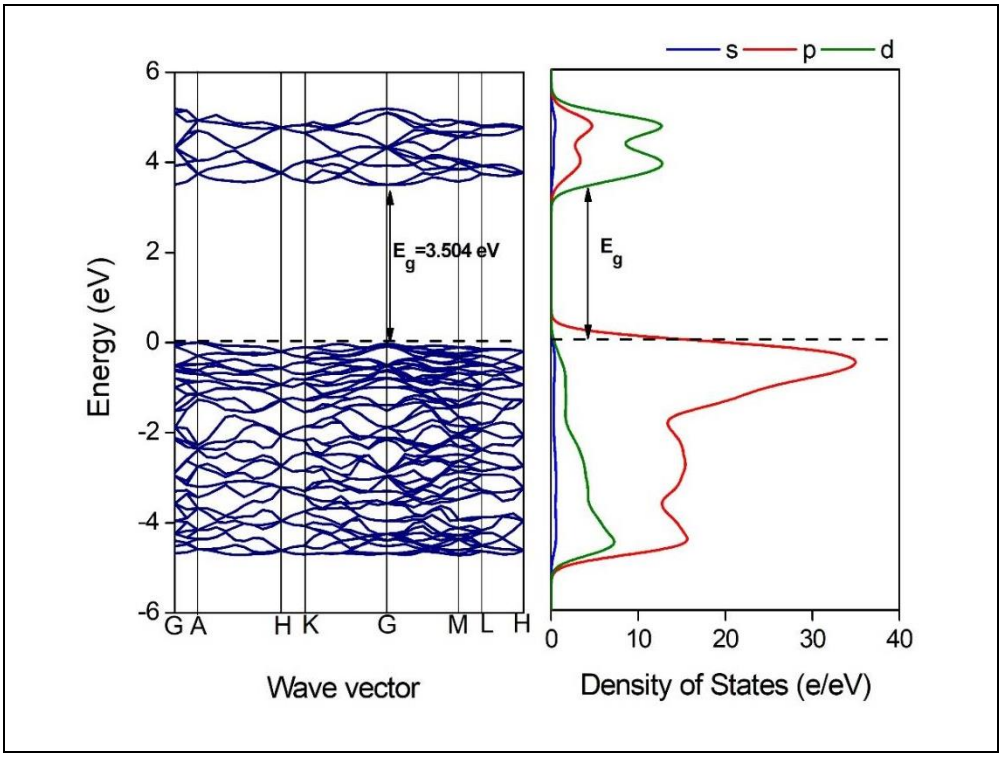

Figure 1. Band structure and density of states (DOS) of $LiNbO_3$ using LDA.

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