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Theoretical Study of Structural and Electronics Properties of Lithium Niobate $LiNbO_3$

Nadia Hadjila[1], Faiza Bouamra[1], Michel Rérat[2]

[1]Department of physic, LASICOM Laboratory, University of Blida 1, Algeria.

[2]E2S UPPA, CNRS, IPREM, Université de Pau et des Pays de l'Adour, France

*Corresponding author

ABSTRACT

The main objective of this work is to study the structural and electronic properties of Lithium niobite in his ferroelectric phase. Calculations are released using the periodic LCAO-DFT-B3LYP approximation with the program CRYSTAL17[3]. Analysis of band structure and density of state diagram shows that lithium niobate is an insulator.

INTRODUCTION

At the last decade, Lithium niobate (LiNbO3, LN) materials, has attracted a great interest as a future functional material due to their excellent ferroelectric, photorefractive, electro-optic, piezoelectric, nonlinear-optical, photocatalytic, and ion conductive properties[1,2]. These various properties of LN open the way to various technological applications. The aim of this study is to release a calculation with Density Functional Theory (DFT) of structural and electronics properties of lithium niobate.

THEORETICAL STUDY

In the present work, structurals and electronics properties of lithium niobate (LiNbO3) have been studied using density functional theory (DFT). Exchange and correlation functional were taken using the B3LYP approximation. The LiNbO3 crystallizes in trigonal structure of hexagonal symmetry with ten atoms per unit cell. with space group R3c (no. 161) and change into para-electric phase (R3c) above 1480K temperature[1]. Atomic positions are: Li (0, 0, 0.21956); Nb (0,0,0) and O(0.0376, 0.32347,0.1028)[2]. The atomic configurations used are: Li $2s^1$, Nb $4d^4$ $5s^1$ and O $2s^2$ $2p^4$. Integration in the 1BZ use k-point mesh 9*9 of Monkhorst-Pack scheme.

RESULTS AND DISCUSSION

The unit cell structure of LiNbO3 is shown in Fig.1. The optimized lattice parameters and related cell volume are presented in Table 1.

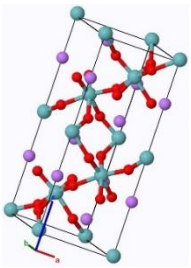

Fig 1 : Unit cell structure of $LiNbO_3$

a=b	c	volume	References
5.148	13.863	318.17	This work
5.159	13.869	320.18	Theor[3]
5.147	13.849	317.73	Expt[4]

Table 1 : Optimized lattice parameters and volume of unit cell of $LiNbO_3$

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It is noted that the values of the structural parameters obtained are in good agreement and very close with the parameters of the literature.

Electronic properties

The energy bands of LiNbO3 are along the high symmetry direction, (G-M-K) of the Brillouin zone. The Fermi level is chosen at zero value of energy Fig.2.a.

Total and local electronic density of states of LiNbO3 are shown in Fig2. The value of the gap energy obtained is 11eV, which means that our system is an insulator. Analysis of diagram of DOS and LDOS, show that the conduction and valence band are essentially composed of the participation of niobium (Nb) and oxygen (O) atoms simultaneously. We note that the Li element has a weak participation at the CBM and VBM.

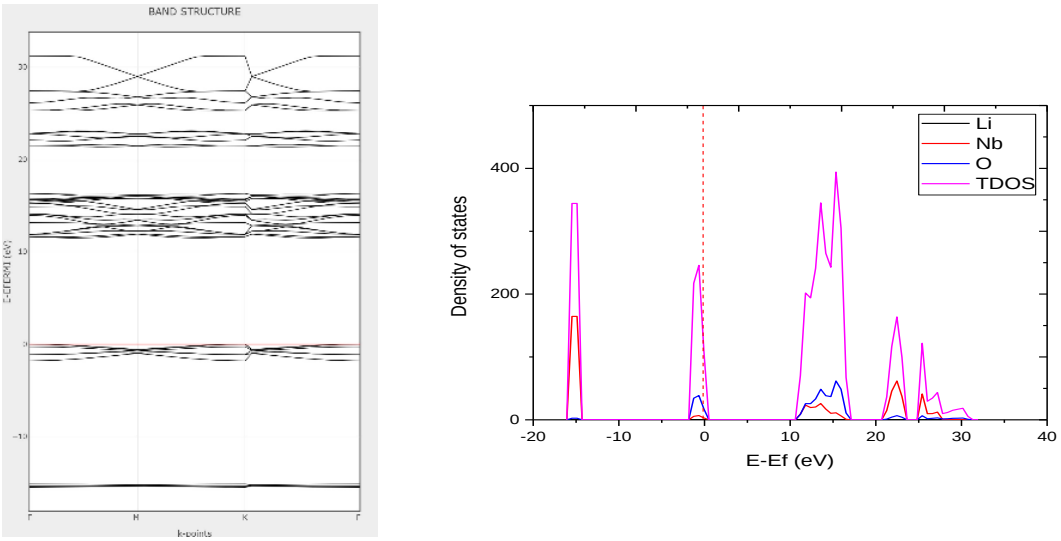

Fig.2: (a) Band Structure diagram of LiNbO3, (b) Total and partial density of states (DOS) of $LiNbO_3$

CONCLUSION

Structural and electronic properties of $LiNbO_3$ have been studied by using SCF-LCAO-DFT-B3LYP approximation. The band gap of LN is calculated to be 11eV.

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REFERENCES

[1]K. Toyoura, M. Ohta, A. Nakamura, K. Matsunaga, J. Appl. Phys. 118 (6) (2015), 064103.

[2]S.C. Abrahams, E. Buehler, W.C. Hamilton, S.J. Lapaca, J. Phys. Chem. Solids 34 (3)(1973) 521e532.

[3] R. Dovesi et al., "User's Manual of CRYSTAL17", code available from http://www.crystal.unito.it

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