ISETC2025

UNIVERSITI TEKNOLOGI MARA

ISETC2025

2 ND INTERNATIONAL SCIENCE, ENGINEERING AND TECHNOLOGY COLLOQUIUM



THE POWER OF SCIENTIFIC INNOVATION

INTELLIGENT SOLUTIONS FOR A SUSTAINABLE WORLD

ORGANIZED BY:
FACULTY OF APPLIED SCIENCES
UNIVERSITI TEKNOLOGI MARA
PERAK BRANCH, TAPAH CAMPUS
MALAYSIA

CO-ORGANIZED BY:

三重大学
MIE UNIVERSITY

2nd International Science, Engineering and Technology Colloquium

(ISETC 2025)

Faculty of Applied Sciences,
Universiti Teknologi MARA,
Perak Branch, Tapah Campus,
35400 Tapah Road, Perak, Malaysia.

Colloquium date: 9th July 2025
Publication date: 9th September 2025

Proceedings of Extended Abstracts

EDITORS

Dr. Emi Norzehan Mohamad Mahbob
Dr. Saiyidah Nafisah Hashim
Ms. Lili Widarti Zainuddin
Ms. Nurul Nazwa Mohammad
Ms. Rozaina Saleh

e-ISBN: 978-629-97630-5-5

Copyright © 2025 ISETC
Published by Faculty of Applied Sciences, Universiti Teknologi MARA,
Perak Branch, Tapah Campus, 35400 Tapah Road, Perak, Malaysia.

All rights reserved. No part of this publication may be reproduced, stored in a retrieval system, or transmitted in any form or by any means, electronic, mechanical, photocopying, recording, or otherwise, without the prior written permission of the Faculty of Applied Sciences, Universiti Teknologi MARA, Perak Branch, Tapah Campus, 35400 Tapah Road, Perak, Malaysia.

PREFACE

Welcome to the 2nd International Science, Engineering and Technology Colloquium 2025 (ISETC 2025)!

It is with great pleasure that we present this year's colloquium, a distinguished gathering of scholars, researchers, and professionals dedicated to the advancement of applied sciences. Held virtually on 9th July 2025, ISETC 2025 serves as a platform to highlight cutting-edge research, foster meaningful networking, encourage collaborations, and explore innovative solutions to global challenges.

This year's theme, "The Power of Scientific Innovation: Intelligent Solutions for a Sustainable World" highlights our shared goal to solve global challenges through applied science. It celebrates innovation as a key to building a more sustainable and resilient future. We're proud to feature keynote speakers and presenters who bring fresh insights, bold ideas, and breakthroughs shaping tomorrow's world.

We would like to extend our heartfelt appreciation to the Faculty of Applied Sciences, Universiti Teknologi MARA, Perak Branch, Tapah Campus, for their outstanding support and assistance throughout the planning and execution of the event. Their dedication has been instrumental to the success of this colloquium. We would like to sincerely thank all participants and researchers for their valuable contributions. We also appreciate the reviewers for their careful evaluations and helpful feedback. Your hard work and support mean a lot to us.

As editors, we are proud to present this collection of proceedings. It is an honour to bring together the interesting and meaningful work of our speakers and authors. We hope the ideas shared will lead to new discoveries, encourage more research, and help solve global challenges through science and innovation.

Warm regards,

Dr. Emi Norzehan Mohamad Mahbob
Dr. Saiyidah Nafisah Hashim
Ms. Lili Widarti Zainuddin
Ms. Nurul Nazwa Mohammad
Ms. Rozaina Saleh

ISETC 2025 Proceedings Editors

IMPACT OF HUBBARD U CORRECTION ON THE BAND GAP ENERGY OF $LiNbO_3$

Lili Widarti Zainuddin[1,2*], Mohd Hazrie Samat[3], Nur Hafiz.Husin[4], Oskar Hasdinor Hassan[5,6], Mohammad Fariz Mohd Taib[2,5*]

[1]*Faculty of Applied Sciences, Universiti Teknologi MARA, Perak Branch, Tapah Campus, Tapah Road, 35400 Perak, Malaysia*
[2]*Faculty of Applied Sciences, Universiti Teknologi MARA, 40450 Shah Alam, Selangor, Malaysia*
[3]*School of Distance Education, Universiti Sains Malaysia, 11800 Penang, Malaysia*
[4]*Faculty of Applied Sciences, Universiti Teknologi MARA, Jengka Campus, 26400, Jengka, Pahang, Malaysia*
[5]*Ionic Materials and Devices (iMADE), Institute of Science, Universiti Teknologi MARA, 40450 Shah Alam, Selangor, Malaysia*
[6]*Department of Industrial Ceramic, Faculty of Art and Design, Universiti Teknologi MARA, 40450 Shah Alam, Selangor, Malaysia*

**Corresponding authors: liliwidarti@uitm.edu.my, mfariz@uitm.edu.my*

Abstract: The electronic properties of lithium niobate ($LiNbO_3$) were investigated using first-principles calculations based on density functional theory (DFT). The simulations were carried out using the CASTEP code with the LDA-CAPZ functional, both with and without the inclusion of Hubbard U correction (LDA+U). A hexagonal $LiNbO_3$ structure with space group R3c was used. Electronic properties were analyzed through band structure and density of states calculations. The Hubbard U value was varied from 0 to 14 eV, and its impact on the band gap was studied. The calculated band gap energies were 3.506 eV (LDA) and 3.751 eV (LDA+U), with the closest agreement to the experimental band gap observed at U = 13 eV. The application of DFT+U improved the description of electronic structure and optical transitions. The computed values were in good agreement with available experimental data and previous reports, validating the effectiveness of the DFT+U approach for modelling $LiNbO_3$.

Keywords**:** *First-principle, $LiNbO_3$, DFT+U, structural properties, band gap*

INTRODUCTION

Lithium niobate ($LiNbO_3$) is a man-made dielectric material that does not occur naturally. In 1965, Ballman successfully grew large single crystals of $LiNbO_3$ using the Czochralski method (Nassau, 1984). Following this achievement, significant progress was made at Bell Laboratories, leading to the publication of five pioneering papers in 1966. Since then, various techniques have been employed for the preparation of $LiNbO_3$ crystals, including the Czochralski method for single crystals and sol-gel and liquid-phase epitaxy routes for thin films. Extensive experimental studies have explored the structural and physical properties of $LiNbO_3$ (Kuo et al., 2011; Maldonado-Orozco et al., 2015; Masloboeva et al., 2020; Yu & Liu, 2007).

$LiNbO_3$ belongs to the trigonal crystal system and can be described using either hexagonal or rhombohedral primitive unit cells. It exhibits two distinct phases depending on temperature. At room temperature, $LiNbO_3$ is ferroelectric with a space group of R3c and undergoes a phase transition to a paraelectric state ($R\bar{3}c$) at a high Curie temperature of 1230 °C (Jackson & Szaller, 2020; Sanna & Schmidt, 2012). The spontaneous polarization in the ferroelectric phase is about 0.70 C/m², which originates from the displacement of Li and Nb atoms along the c-axis due to internal elastic forces. Above the Curie temperature, these atoms return to centrosymmetric positions relative to the oxygen layers, making the structure non-polar (Sanna & Schmidt, 2017; Wang et al., 2019). $LiNbO_3$ also possesses a wide band gap of approximately 3.78 eV (Thierfelder et al., 2010), resulting in a low absorption coefficient in the visible light range. Its unique combination of properties has made it an essential material in optoelectronics, including applications such as transducers, amplitude and phase modulators, second-harmonic generators, and holographic devices.

In the past two decades, computational methods have emerged as indispensable tools in materials science, enabling high-accuracy predictions of various properties including structural, electronic, and optical characteristics. Through first-principles studies, researchers have investigated the origin of ferroelectricity and related phenomena in $LiNbO_3$. In this study, we present a comprehensive first-principles investigation of the structural, electronic, and optical properties of $LiNbO_3$ using the CASTEP computational package. To improve the accuracy of the band gap prediction, we employ the DFT+U approach, which is known for its improved treatment of electron correlation effects in transition-metal oxides. Optical properties are also explored to assess the material's potential in photonic applications.

MATERIALS AND METHODS

The first-principles calculations performed in this work are based on DFT within exchange-correlation functional from LDA-CAPZ for solids using CASTEP computer code. Geometrical optimization is first performed using standard DFT method on $LiNbO_3$ unit cell and followed by its electronic and optical properties. Hubbard U was introduced to the d-orbitals of Nb atoms ranging from U=1 eV until U=14 eV. In this study, the effect of Hubbard U to Nb d-orbitals towards the electronic properties was investigated. For exchange correlation of LDA-CAPZ, the cutoff energy used in this work is 380 eV with k-point grid of 3x3x2. Geometrical optimization was set at 5.0×10^{-6} eV/atom for total energy, 0.01 eV/Å for maximum force, 0.02 GPa for maximum stress and 5.0×10^{-4} Å for maximum displacement.

RESULTS AND DISCUSSION

To investigate the electronic properties of $LiNbO_3$, electronic band structure calculations were performed. The resulting band gap energies, along with values from other theoretical and experimental studies, are summarized in Table 1. The band gap obtained using the LDA-CAPZ functional shows a deviation of 7.14% from the experimental value and is in good agreement with previously reported theoretical result.

Table 1. Comparison the band gap energy of $LiNbO_3$ from this work with experimental result and others theoretical work

		Band gap energy (eV)
LDA-CAPZ	This work	3.506
	(Hossain, 2019)	3.54
	(Tripathy & Sahu, 2015)	3.59
Experimental	(Dhar & Mansingh, 1990)	3.78

In general, standard LDA and GGA functionals are insufficient to accurately describe the strong electron correlation effects in materials containing d and f orbitals (Kirchner-Hall et al., 2021). To overcome this limitation, a Hubbard U correction was applied to the Nb atoms. In this study, the valence electron configurations considered were Li ($2s^1$), Nb ($4p^6$ $4d^4$ $5s^1$), and O ($2s^2$ $2p^4$). The variation in the band gap with respect to the U value primarily arises from changes in the Nb 4d orbital. The electronic band structure of $LiNbO_3$ at U = 11 eV is shown in Figure 1. The calculated band gap at the Γ point along the high-symmetry directions of the Brillouin zone is 3.751 eV, which shows a deviation of only 0.77% from the experimental value. Therefore, U = 11 eV is considered the optimal Hubbard U value for accurately reproducing the experimental band gap of $LiNbO_3$.

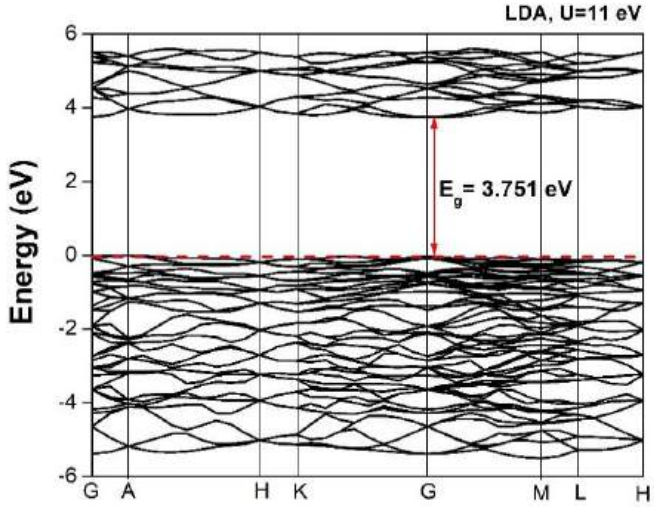


Figure 1. Band structure of $LiNbO_3$ at U=11 eV

CONCLUSIONS

In this study, the electronic properties of $LiNbO_3$ were systematically investigated using first-principles calculations. The inclusion of Hubbard U correction in the electronic structure calculations significantly improved the accuracy of the predicted band gap. Specifically, the band gap value increased from 3.506 eV (without U) to 3.751 eV (with LDA+U), which closely matches the experimental value. These results demonstrate that the DFT+U approach is essential for accurately describing the electronic behavior of $LiNbO_3$, particularly due to the presence of strongly correlated Nb 4d electrons. The insights gained from this work can provide a reliable theoretical foundation for future studies and potential applications of $LiNbO_3$ in optoelectronic and ferroelectric devices.

REFERENCES

Dhar, A., & Mansingh, A. (1990). Optical properties of reduced lithium niobate single crystals. *Journal of Applied Physics*, *68*(11), 5804–5809. https://doi.org/10.1063/1.346951

Hossain, M. M. (2019). First-principles study on the structural, elastic, electronic and optical properties of $LiNbO_3$. *Heliyon*, *5*(4), e01436. https://doi.org/10.1016/j.heliyon.2019.e01436

Jackson, R. A., & Szaller, Z. (2020). Recent progress in lithium niobate. In *Crystals* (Vol. 10, Issue 9). https://doi.org/10.3390/cryst10090780

Kirchner-Hall, N. E., Zhao, W., Xiong, Y., Timrov, I., & Dabo, I. (2021). Extensive benchmarking of DFT+U calculations for predicting band gaps. *Applied Sciences (Switzerland)*, *11*(5). https://doi.org/10.3390/app11052395

Kuo, C., Chang, Y., Chang, Y., & Hwang, W. (2011). *Synthesis of nanocrystalline lithium niobate powders via a fast chemical route*. *37*, 951–955. https://doi.org/10.1016/j.ceramint.2010.11.008

Maldonado-Orozco, M. C., Ochoa-Lara, M. T., Sosa-Márquez, J. E., Olive-Méndez, S. F., & Espinosa-Magaña, F. (2015). Synthesis and characterization of electrospun $LiNbO_3$ nanofibers. *Ceramics International, 41*, 14886–14889. https://doi.org/10.1016/j.ceramint.2015.08.013

Masloboeva, S. M., Smirnov, M. V., & Palatnikov, M. N. (2020). Sol-gel synthesis of lithium niobate doped by zinc and boron and study of the luminescent properties of ceramics LiNbO3: Zn: B. *Russian Chemical Bulletin*, *69*(5), 947–951. https://doi.org/10.1007/s11172-020-2853-0

Nassau, K. (1984). Early History of Lithium Niobate: Personal Reminiscences. *Proceedings of the SPIE*, *460*, 2–5. https://doi.org/10.1117/12.939449

Sanna, S., & Schmidt, W. (2012). Ferroelectric phase transition in $LiNbO_3$: Insights from molecular dynamics. *IEEE Transactions on Ultrasonics, Ferroelectrics, and Frequency Control*, *59*(9), 1925–1928. https://doi.org/10.1109/TUFFC.2012.2408

Sanna, S., & Schmidt, W. G. (2017). $LiNbO_3$ surfaces from a microscopic perspective. *Journal of Physics Condensed Matter*, *29*(41). https://doi.org/10.1088/1361-648X/aa818d

Thierfelder, C., Sanna, S., Schindlmayr, A., & Schmidt, W. G. (2010). Do we know the band gap of lithium niobate? *Physica Status Solidi (C) Current Topics in Solid State Physics*, *7*(2), 362–365. https://doi.org/10.1002/pssc.200982473

Tripathy, S. K., & Sahu, G. (2015). Ground state properties of $LiNbO_3$ from first-principles calculations. *Advanced Materials and Radiation Physics*, *1675*. https://doi.org/10.1063/1.4929163

Wang, W., Zheng, D., Hu, M., Saeed, S., Kong, Y., Zhang, L., & Xu, J. (2019). Effect of Defects on Spontaneous Polarization in Pure and Doped $LiNbO_3$: First-Principles Calculations. *Materials*, *12*, 1–9. https://doi.org/10.3390/ma12010100

Yu, J., & Liu, X. (2007). Hydrothermal synthesis and characterization of $LiNbO_3$ crystal. *Materials Letters*, *61*(2), 355–358. https://doi.org/10.1016/j.matlet.2006.04.087

Pejabat Perpustakaan
Library Office

Universiti Teknologi MARA
Cawangan Perak
Kampus Seri Iskandar
32610 Bandar Baru Seri Iskandar,
Perak Darul Ridzuan, MALAYSIA
Tel: (+605) 374 2093/2453 Faks: (+605) 374 2299

UNIVERSITI TEKNOLOGI MARA

Surat kami : 700-KPK (PRP.UP.1/20/1)
Tarikh : 20 Januari 2023



Prof. Madya Dr. Nur Hisham Ibrahim
Rektor
Universiti Teknologi MARA
Cawangan Perak

Tuan,

PERMOHONAN KELULUSAN MEMUAT NAIK PENERBITAN UiTM CAWANGAN PERAK MELALUI REPOSITORI INSTITUSI UiTM (IR)

Perkara di atas adalah dirujuk.

2. Adalah dimaklumkan bahawa pihak kami ingin memohon kelulusan tuan untuk mengimbas (*digitize*) dan memuat naik semua jenis penerbitan di bawah UiTM Cawangan Perak melalui Repositori Institusi UiTM, PTAR.

3. Tujuan permohonan ini adalah bagi membolehkan akses yang lebih meluas oleh pengguna perpustakaan terhadap semua maklumat yang terkandung di dalam penerbitan melalui laman Web PTAR UiTM Cawangan Perak.

Kelulusan daripada pihak tuan dalam perkara ini amat dihargai.

Sekian, terima kasih.

"BERKHIDMAT UNTUK NEGARA"

Setuju.

27.1.2023

PROF. MADYA DR. NUR HISHAM IBRAHIM
REKTOR
UNIVERSITI TEKNOLOGI MARA
CAWANGAN PERAK
KAMPUS SERI ISKANDAR

Saya yang menjalankan amanah,

SITI BASRIYAH SHAIK BAHARUDIN
Timbalan Ketua Pustakawan

nar

Powered by CamScanner