Junaid Khan

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Nationality: Pakistan

Education:

PhD (In Progress)

Department of Physics University of Peshawar, KP, Pakistan

2016-2019 M.Phil. Physics

Area of Interest (Computational Nano-Fusion Technology)

Advisor: Professor Dr. Shabeer Ahmad Main

Research Area: "Density Functional Theory Study of Copper Silicide Cu_3Si as an anode material for Secondary Lithium Ion battery".

Department of Physics University of Malakand, KP, Pakistan

2011-2015 Bachelor of Science in Physics

Area of Interest (Computational Physics)

Advisor: Assistant Professor Dr. Zahid

Co-Advisor: Professor Dr. Shabeer Ahmad Main

Research Area: 'Structural, Electronic And Optical Properties of Lithium-Selenide (Li_2se) Batteries A Density Functional Theory Study"

Allama Iqbal Open University, Islamabad, Pakistan

2016-2018 B.Ed., Bachelor of Education in Teaching of Physics

Govt Degree College Gulabad Dir Lower

2009-2011 Higher Secondary School Certificate

Faran Public High School Chakdara, KP, Pakistan

2007-2009 Secondary School Certificate

Allama Iqbal Open University, Islamabad, Pakistan

2015-2016 Certified Teaching Certificate

RESEARCH EXPERIENCE

Computationally Synthesis and investigation Advance materials for electrochemical energy storage and conversion, including electrolytes and electrodes in Lithium-ion batteries. Solid State compounds

Key Area Lithium-Ion Battery System, Sodium Ion Battery, Perovskite Solar cell

Research Field & Interest

1. *Synthesis and investigation Advance materials for electrochemical energy storage and conversion, including electrolytes and electrodes in Lithium-ion batteries.*
2. *Study materials via both Density Functional Theory (DFT) methods such win2k, materials studio, Siesta & Experimental methods via different technique.*
3. *ab-initio MD Simulation*

CONFERENCE & WORKSHOP ATTAND

1. Awarded certificate for the Oral Presentation ***1st National Conference on recent Trends in Physics & Material Science*** March 25-27 2019 Department of Physics University of Science and Technology Bannu Kp
2. Awarded certificate for the Oral Presentation ***4th invention to innovation summit*** KP 22-23 Nov 2018 at Cecose University Peshawar
3. Awarded certificate for the ***Poster Presentation 1st International Conference on "Emerging Trends in Material Science***" 27th Feb to 1st March 2018 at Islamia College Peshawar.
4. Awarded certificate for the participation ***workshop on Molecular Dynamic Simulations*** Feb 6, 2017 Institute of Chemical Science University of Peshawar.
5. Awarded certificate for the participation ***Solar cell characterization Technology*** **(**April 1-3 2016) GIK Institute of Engineering science and Technology Topi Pakistan**.**
6. Awarded certificate for the participation Two Days National Workshop **"*Plasma Physics*"** "April 26-27 2016" in National Center of Physics Quaid Azam University Islamabad.
7. Awarded certificate for the participation ***3rd International Conference Material Modelling and Simulation*** in University of Malakand KpK Pakistan 3-6 July 2013.
8. Awarded certificate for the participation online international symposium on "Impact of Covid-19 on Higher Education in South Asia" on 3rd January 2021in Bombay University of India.
9. Awarded certificate for the participation online international Conference on **"Nanotechnology- Smart Materials: Research : Commercialization"** in Maharaga Agrasen Institute of Technology India held on January 28, 2021.

TEACHING & ADMINISTRATIVE EXPERIENCE

1. Oct 04, 2018-till-date working as Lecturer Department of Physics Khushal Khan Khattak University Karak, KP, Pakistan.
2. Member Board of studies Department of Physics and Nano Technology Khushal Khan Khattak university Karak

3. Member of Program Team QEC Khushal Khan Khattak University Karak Sep 2019 till Date..
4. Member Admission Committee Department of Physics, Chemistry and Nano Technology Khushal Khan Kattak University Karak.
5. Chip Proctor department of Physics 20 March 2020 till date
6. BS Coordinator & Exam Coordinator department of Physics Spring 2021 till date
7. Undergraduate BS-Lab In charge department of Physics Spring 2021 till date

Thesis Supervision

BS Student

1. Study Structural, Mechanical, and Electrical properties of Ca Doped Mn Ferrite DFT and Experimental approach. (Luqman Amin & Rizwan Ullah 2018).
2. Density functional theory study of Graphite as an anode material for Lithium ion battery (Hazrat Amin 2019)
3. Investigation of Structural, Electrical and Thermo-electrical properties of single-crystal TiC using Density Functional Theory (Junaid Ahmad & Majid Khan 2021).
4. Density Functional theory study of Co doped Fe2O3 for optical Applications (Afnan Ahmad, Zohid Rehman, and Omer alam 2024)
5. First Principle study tri-doped Fe2O3 for opto-electronic Applications (Saqib Jamil, Alam zeb, Umar Javed 2024)
6. DFT study of cubic Halide Compounds for structural, electronic and optical properties: Review Study. (Muhammad Asim, Aftab Khan, Mehtab Khan (InProgress 2015)

MPhil Students

1. First Principle study of Silicon as an anode material for Lithium ion battery (Munazam Gul 2020)
2. MD Simulation study of Metal Silicide as an anode material for Lithium ion battery (Zai Ur Rahman 2022).
3. First-Principle Study of Cerium oxide (CeO2) and Fe doped Cerium oxide for opto-electronic Applications (Zeshan Ahmad 2024)
4. Atomistic modelling of Structural and Opto-Electronic Properties of I3OX (X= Rb and Ca) Anti-Perovskite compounds for Photovoltaic Application (Mr. Shaukat Mehmood 2025)

KNOWLEDGE (KNOW HOW

1. Best knowledge of PC usage and command on applications such as **MS office**, **Internet**.

2.Use of other office Equipment's and Machines such as Scanners, Photocopiers and Faxes.

3. Advance user of **Fortran, Material studio, WIEN2k, SIESTA, VASP, VESTA, VMD & ORIGIN PRO8 etc**

4. Proposal Writing.

PERSONAL INFORMATION:

Father Name:	**Rafi Ullah**
Domicile:	**Lower Dir**
Nationality:	**Pakistani**
Religion:	**Islam**
M-Status:	**Single**
Contact	**+92-343-9725776**
C.N.I.C #:	**15307-0266201-9**
Passport	**BB4142011**
Date of Birth:	**MAY-25-1991**
Permanent Address:	**Village & P.O Tindudog Tehsil Adenzai District Lower Dir.**
Home Address:	**Village & P.O Tindudog Tehsil Adenzai District Lower Dir**
Current Address:	**Hostel #9, Room 26, University of Peshawar, University Campus**

HOBBIES/EXTRACURRICULAR ACTIVATES

Worked for One years with a community base organization namely Falahi Tanzeem Nawjawana Tindudog based at Union Council Tazagram Dir (lower) Khyber Pakhtunkhawa

1. To raise awareness among the people
2. Protection of environment
3. *Self help*
4. Social Development
5. Women and Development
6. Bad effects of intoxing Drug

Reading books

Playing Cricket

A member of the village social welfare committee

REFERENCES

PUBLICATION (SCI)

[1] EFFECT OF STRAIN ON ELECTRONIC STRUCTURAL AND PHOTOCATALYTIC PROPERTIES OF MX2 (M=MO, W X=S). **(2024).** *Indian Journal of Pure & Applied Physics*. https://doi.org/10.56042/ijpap.v62i11.12747

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[3] Khalid, S., Ma, Y., Sun, X., Zhou, G., Wu, H., Lu, G., Yang, Z., Khan, J., Khenata, R., & Bouhemadou, A. **(2019).** Electronic and optical properties of Tl4GeX3 (X = S, Se and Te) compounds for optoelectronics applications: insights from DFT-computations. ***Journal of Materials Research and Technology,*** *9*(1), 413–420. https://doi.org/10.1016/j.jmrt.2019.10.070

[4] Khan, J., Al-Anazy, M. M., Yousef, E. S., D, D., Sharma, R., & Moayad, A. J. A. **(2023).** Comprehensive analysis of novel cubic HgCrO3 perovskite: a first principles, structural, thermodynamic, and magnetic properties study for spintronic applications. ***RSC Advances,*** *13*(48), 33603–33612. https://doi.org/10.1039/d3ra06392e

[5] Khan, J., Ali, G., Samreen, A., Ahmad, S., Ahmad, S., Egilmez, M., Amin, S., & Khan, N. **(2022).** Quantum-dot sensitized hierarchical NiO p–n heterojunction for effective photocatalytic performance. ***RSC Advances***, *12*(50), 32459–32470. https://doi.org/10.1039/d2ra05657g

[6] Khan, J., Dutta, A., Mundad, T., Boukhris, I., Al-Buriahi, M. S., & Adawi, H. **(2025).** First principles Studies on structural, elastic, electronic, optical properties of MGSRPB and MGSRSI Half Heusler alloys. ***Journal of Inorganic and Organometallic Polymers and Materials*.** https://doi.org/10.1007/s10904-024-03557-8

[7] Khan, J., Iqbal, Y., Rehman, F., Alam, J., Rahim, M., Hussain, S., Sharif, M. N., & Khan, M. A. (2024). Exploring Rare-Earth compound ErMn2Si2 for thermoelectric and photoelectrochemical applications using Density functional theory. ***Journal of Magnetism and Magnetic Materials***, *600*, 172156. https://doi.org/10.1016/j.jmmm.2024.172156

[8] Khan, J., Khalid, S., Uddin, W., Khenata, R., Khan, M., Rehman, S. U., Ahmad, M., Wang, S., Huang, W., Omran, S. B., & Fawad, M. **(2021).** A new approach to study combination mixture organic solvent ethylene carbonate with lithium-ion for alkali-ion battery: A density functional theory. ***Journal of Materials Research and Technology*,** *11*, 1672–1677. https://doi.org/10.1016/j.jmrt.2021.02.009

[9] Khan, J., Khan, M., Sharma, T., Boukhris, I., & Al-Buriahi, M. S. **(2024).** Advanced computational insights into CS2NASCX6 (X = CL, BR) 6 Double perovskites: structural stability, elastic properties, and optical characteristics for Next-Generation Photovoltaics. ***Journal of Computational Chemistry***, *46*(1). https://doi.org/10.1002/jcc.70010

[10] Khan, J., Khan, M., Uddin, W., Begum, P., Ahmad, F., Khan, B., Sharif, M. N., & Khan, M. A. (2024). Elucidating Li+-Ion Interactions with Ethylene Carbonate: Insights from Vibrational Infrared Spectroscopy, Electron Affinity Analysis, and Charge Dynamics to Enhance Lithium-Ion Battery Performance. ***Energy Technology*.** https://doi.org/10.1002/ente.202401235

[11] Khan, J., Khan, M., Uddin, W., Dutta, A., Ullah, S., & Alanazi, A. K. **(2024).** Comprehensive atomistic modulating of THCU2X2 (X = N, P, AS, SB, Bi) compounds for Opto-Electronic and Thermo-Electric applications. ***Journal of Electronic Materials*.** https://doi.org/10.1007/s11664-024-11671-z

[12] Khan, J., Khan, M., Uddin, W., Paghunda, N., Rehman, F., Shah, A. H., Rahman, A. U., & Ahmad, Z. (2024). Atomistic modulating of structural, elastic, and optoelectronic behavior of pure TiO2 and Fe/TiO2 for photoelectrochemical water splitting application. ***Results in Optics***, *16*, 100730. https://doi.org/10.1016/j.rio.2024.100730

[13] Khan, J., Khan, M., Uddin, W., Prodhan, R. K., Alanazi, A. K., Ullah, S., Rauf, A., Al-Awthan, Y. S., Bahattab, O. S., Hemeg, H. A., Aljazzar, S. O., & Al-Humaidi, J. Y. **(2024).** First-Principles study on the structural, optoelectronic, and elastic properties of halide perovskites XSNCL3 (X = RB, CS) for photoelectrode applications. ***Journal of Inorganic and Organometallic Polymers and Materials***. https://doi.org/10.1007/s10904-024-03518-1

[14] Khan, J., Lawati, D. R., Dutta, A., Almutairi, F. N., & Ayari-Akkari, A. **(2025).** Insight to structural, mechanical, electronic and optical properties of YSbPd and YSbPt half Heusles: an ab-initio investigation. ***Optical and Quantum Electronics***, *57*(2). https://doi.org/10.1007/s11082-024-08020-z

[15] Khan, J., Uddin, W., Dutta, A., Boukhris, I., & Albalawi, H. **(2024).** Mapping structural, electronic and optoelectronics features in Na2TlSbY6 (Y = Cl,Br): Implications for next-generation photovoltaics. *Polyhedron*, 117381. https://doi.org/10.1016/j.poly.2024.117381

[16] Lawati, D. R., Khan, J., Dutta, A., Akila, B., Algethami, N., & Al-Buriahi. **(2025).** Investigating structural and electronic features, band gap modulation, and optical absorption in ASNCL3 (A = NA, K) perovskites for optoelectronic applications. ***Solid State Communications***, 115850. https://doi.org/10.1016/j.ssc.2025.115850

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[18] Uddin, W., Nawabi, M. Y., Rehman, S. U., Hu, G., Khan, J., & Shen, X. **(2021).** Determination of P-Dimethylaminobenzaldehyde by using a Briggs–Rauscher electrochemical oscillator. ***Russian Journal of Electrochemistry***, *57*(12), 1213–1223. https://doi.org/10.1134/s1023193521110094

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[21] Khan, M. Y.; Jehangir, M. A.; Israr, N.; Hassan, A.; Younis, U.; Khan, J.; Khan, M.; Khan, A.; Souwaileh, A. A. First-Principles Study of CS3SBX6 (X = F, CL) for scintillation and optoelectronic applications. **Physica B Condensed Matter 2025**, 417150. https://doi.org/10.1016/j.physb.2025.417150.

[22] **Khan, J.**, Dutta, A., Al-Muhimeed, T. I., & Ahmad, S. H. A. (2025). Unveiling the multifunctional potential of K2YCuX6 (X=Cl,Br): Structural, mechanical and optical insights for renewable energy frontiers. ***International Journal of Modern Physics B***. https://doi.org/10.1142/s0217979225501747

[23] **Junaid Khan** Tanvi Sharma Norah Algethami and M. S. Al-Buriahi (2025). Structural, opto-electronic, and elastic responses of double perovskite K_2NaTiA_6 (A=Cl and Br) for photovoltaic application: A DFT study ***International Journal of Modern Physics B.*** *https://doi.org/10.1142/S0217979225501735*

[24] Uddin, W., Alanazi, A. K., Khan, J., & Khan, M. A. (2025). A novel approach to distinguish coumaric isomers using Briggs-Rauscher electrochemical oscillator. **Journal of Applied Electrochemistry.** https://doi.org/10.1007/s10800-025-02317-x

[25] Khan, J., Khan, M., Sharma, T., Parveen, A., & Gilani, S. J. (2025). Structural and optoelectronic investigations of AGeO3 (A=Mg,Cd) perovskites: A first-principles study. ***International Journal of Modern Physics B***. https://doi.org/10.1142/s0217979225501954