# CURRICULUM VITAE

## A. PERSONAL DATA:


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|---|---|
| Name: | **Dr. Muhammad Iqbal Hussain** |
| Father's Name: | Muhammad Yar |
| Date of Birth: | April 1, 1981 |
| Domicile: | Muzaffar Garh (Punjab, Pakistan). |
| Identity Card No.: | 32303-0780751-1 |
| Marital Status: | Married |
| Religion: | Islam |
| Nationality: | Pakistani |
| Postal Address: | House # 272, B-Block, Citi Housing Phase-I, Multan. |
| Official Address: | Department of Physics, University of Education, Lahore Multan Campus, Bosan Road, Multan Pakistan. |
| Permanent Address: | Chah Baloch Wala, Mouza Khokhar, Tehsil Kot Addu District Kot Addu, Pakistan. |
| E-mail Address: | miqbal@ue.edu.pk |
| Phone No. (Mobile): | +92 345 4742132 |


## B. ACADEMIC QUALIFICATIONS:

| Certificate/Degree (Duration) | Name and Address of Institution | From - To | Division /Grade | Major Subjects Studied |
|---|---|---|---|---|
| Secondary School Certificate (S.S.C) | Govt. High School, Gourmani Pakistan | 1994-1996 | 1st / A | English, Mathematics, Physics, Chemistry etc. |
| Faculty of Science (F.Sc. Pre-engineering) | Govt. Degree College Muzaffar Garh Pakistan | 1996-1998 | 2nd / B | English, Physics, Mathematics, Chemistry etc. |
| Bachelor of Science (B. Sc.) | Govt. Degree College Muzaffar Garh Pakistan | 1998-2001 | 1st / A | English, Physics, Mathematics (A & B courses) |
| Master of Science ( (MSc Physics with Specialization Industrial Electronics) (Two years) | Bahauddin Zakariya University Multan, Pakistan | 2001-2003 | 1st / A | Physics |
| Master of Philosophy in Physics (M. Phil.) (Two years) | COMSATS Institute of Information Technology, Lahore, Pakistan. | 2009-2011 | 1st | Physics |
| PhD | Bahauddin Zakariya University Multan, Pakistan | 2017-2021 | 1st | Physics |

**M. PHIL DISSERTATION TITLE:**
"*Entangled Coherent States Based on Even-Odd Coherent States with Average Photon Number as Relative Phase*"

**PhD DISSERTATION TITLE:**
"*First Principles Study of the Physical Properties of Perovskite Materials for Optoelectronic Applications*" supervised by Dr. Rana M. Arif Khalil, Institute of Physics, Bahauddin Zakariya University, Multan, Pakistan.

## C. MEMBERSHIP OF ORGANIZATIONS: -

1. Member of the Departmental Board of Studies for the Department of Physics, University of Education, Lahore from 29.05.2018 to 21.08.2019, and then 20.11.2024 to date.

## D. TEACHING/NON-TEACHING EXPERIENCE:

| Institution / Organisation | Position Held | From-To | Responsibility |
|---|---|---|---|
| Department of Physics, University of Education, Lahore Multan Campus | Lecturer (BPS-18) | 31-10-2017 To date | Taught various courses to BS/MS level students and supervised BS/MS research work. |
| Registrar's Office, University of Education, Lahore, Pakistan. | Look after charge of the Registrar's Office | 16-09-2017 to 27-09-2017 | Looking after day to day matters of the Registrar's Office |
| Registrar's Office, University of Education, Lahore, Pakistan. | Deputy Director (Management) (BPS-18)/Re-assigned duties | 09-11-2016 To 30-10-2017 | - dealing appointments BPS-17 & above.<br>- preparing agendas, writing minutes, and conducting meetings of Syndicates, Academic Councils, Selection Boards, Board of Advanced Studies & Research (BASR), etc.<br>- Dealing with official routine matters |
| Registrar's Office, University of Education, Lahore, Pakistan. | Assistant Director (BPS-17) | 31-7-2013 T0 08-11-2016 | - dealing appointments BPS-17 & above.<br>- preparing agenda, writing minutes, and conducting meetings of Syndicate, Academic Councils, Selection Boards, Board of Advanced Studies & Research (BASR), etc.<br>- Dealing with official routine matters |

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|---|---|---|---|
| Registrar's Office, University of Education, Lahore, Pakistan. | Administrative Officer (BPS-16) | 29-5-2006 To 30-7-2013 | -Worked in Registrar's office and performed multiples routine assignments.<br>-dealt FDP program/Ph.D. (off campus) related matters |

## E. M.Phil/Ph.D. THESES / PROJECTS SUPERVISION:

**MS Thesis Co-supervision**

1. Ms. Mubashra Sheikh (research work in progress)
   Registration No. 25-UE-12028

2. Mr. Moeen Abbas (research work in progress)
   Registration No. 25-UE-12029

3. "***The computational study of the phase stability, optoelectronic, and mechanical properties of ternary perovskites for optoelectronic applications***", Rabia Rizwan (F22BPHYS3E).

4. ***"DFT aided prediction of the structural, optoelectronic, and elastic properties of perovskite oxides CoXO3 (X=Ir, Rh) for energy harvesting applications***", Esha Tul Razia (F22BPHYS3E).

**BS Thesis Supervision**

1. "***Ab-Initio* Investigation of Structural, Electronic and Optical Properties of $VGaO_3$**", Umair Mumtaz (bsf1602302).

2. "**Computational Studies of the Structural and Optoelectronic Properties of Halide Double Perovskite**" Muhammad Asif (bsf2205940)

## F. COURSES TAUGHT TO BS/MS LEVEL CLASSES

Optical Properties of Solids, Atomic and Molecular Physics, Circuit Analysis, Mathematical Method of Physics-I & II, Mechanics-I & II, Modern physics and electronics, Fundamentals of digital electronics, Applied physics, Computational Physics, Advanced Mathematical Methods of Physics, Computing Tools for Physics etc.

## G. ADMINISTRATIVE RESPONSIBILITIES:

1. Member of the Board of Studies for the Department of Physics, Division of Science & Technology, University of Education, Lahore from 29.05.2018 to 21.08.2019 and 20.11.2024 to date.
2. Coordinator sports at the University of Education, Lahore, Multan Campus from 27.09.2018 to 21.08.2019, and 02.02.2026 to date.
3. Coordinator Security at the University of Education, Lahore, Multan Campus from 01.08.2024 to 22.08.2025.

## H. DISTINCTIONS:

1. Declared and included in the prestigious Stanford University/Elsevier Top 2% Scientists list (2025) of the World.
2. Secured 2nd position in order of merit of M.Sc. (Physics) during session 2001-2003, Bahauddin Zakariya University, Multan.
3. Achieved First Class throughout the Academic Career except F.Sc.

## I. SPECIAL TRAINING/COURSES:

1. Certificate awarded on completion of 3-day orientation session on Peace Building organized by Centre for Policing and Security at University of Education, Multan Campus from 4-6th April 2019.
2. Achieved Certificate of participation by Pak Institute for Peace Studies (PIPS) on participation in 2-days dialogue on "Promoting Social Harmony and Critical Consciousness" from 14-15th December 2018.
3. Attended 3-days HEC's "Indigenous on Campus Training under modern University Governance program" from 15-17th December 2015 organized at Directorate of Research, University of Education, Lahore.
4. Attended training program on "Developing & Assessing Research Proposal" from 27-30th July 2015 organized by HEC Tertiary Education Support Program at the Centre for Executive Education (CEE), Institute of Business Administration, Karachi.
5. Attended 5 days HEC's "Indigenous on Campus Training under Modern University Governance program" from 2-7th February 2015 organized at the Directorate of Research, University of Education, Lahore.
6. On successful training of National Cadet Corps, received a "Certificate of Service in National Cadet Corps (NCC)" during F.Sc. in academic session 1996-1998.

## J. CONFERENCES/ WORKSHOPS/ MEETINGS ATTENDED:

1. Online talk of the article titled "Computational study of the structural and optoelectronic properties of $AGaO_3$ (A = Sc, Ti, Ag) using LDA+U Functional for optoelectronic applications" at AIMS-2022, held on December 15-16, 2022 by the Department of Physics, DSnT, University of Education, Lahore, Pakistan.
2. Oral presentation of the article titled "*Ab-initio* study of the Structural, Electronic, Mechanical, and Optical Properties of Tantalum-based perovskite oxides $ATaO_3$ (A = Rb, Fr) for Optoelectronic Applications" at AIMS-2021, held online on October 5-6, 2021 by the Department of Physics, DSnT, University of Education, Lahore, Pakistan.
3. Invited Speaker in iiScience International Conference entitled "Light Generation, Sensing and Energy Resources" held at the Department of Physics Women University Multan from 2-4th March 2020.
4. Arranged and attended the 2nd International Conference-2010 organized by the University of Education, Lahore from 20-21st September 2010.
5. Arranged and attended 1st International Conference-2006 organized by University of Education, Lahore.

## K. RESEARCH PUBLICATIONS

**International Publications in peer reviewed impact factor Journals (h-index=21)**

1. **Muhammad Iqbal Hussain,** R.M.A. Khalil, F. Hussain, M. Imran, A.M. Rana, S. Kim, "Investigations of Structural, Electronic and Optical properties of TM-$GaO_3$ (TM= Sc, Ti, Ag) Perovskite Oxides for Optoelectronic applications: A First Principles study", Materials Research Express, 7(1) (2020) 1-12. https://doi.org/10.1088/2053-1591/ab619c.

2. R.M.A. Khalil, F. Hussain, **Muhammad Iqbal Hussain,** A. Parveen, M. Imran, G. Murtaza, M.A. Sattar, A.M. Rana, S. Kim: "The Investigation of optoelectronic, magnetic and dynamical properties of Ce and Ti doped 2D blue phosphorene: A dispersion corrected DFT study", Journal of Alloys and Compounds 827 (2020) 1-10. https://doi.org/10.1016/j.jallcom.2020.154255.

3. **Muhammad Iqbal Hussain**, R.M.A. Khalil, S. Boota, F. Hussain, M. Imran, G. Murtaza, A.M. Rana, M.A. Sattar: "The structural, electronic and dynamical investigations of $NdMn_2O_5$ and $La_2CoMnO_6$ for optoelectronic applications: A first principles study", Optik - International Journal for Light and Electron Optics 204 (2020) 1-10. https://doi.org/10.1016/j.ijleo.2019.164165.

4. **Muhammad Iqbal Hussain**, R.M.A. Khalil, F. Hussain, M. Imran, A.M. Rana, S. Kim: "Investigation of structural, electronic and optical properties of $YInO_3$(Y=Rb, Cs, Fr) perovskite oxides using mBJ approximation for optoelectronic applications: A first principles study", Materials Science in Semiconductor processing 113 (2020) 1-9. https://doi.org/10.1016/j.mssp.2020.105064.

5. **Muhammad Iqbal Hussain**, R.M.A. Khalil, F. Hussain, A.M. Rana, M. Imran "*Ab-initio* prediction of the mechanical, magnetic and thermoelectric behaviour of perovskite oxides $XGaO_3$ (X = Sc, Ti, Ag) using LDA+U functional: For optoelectronic devices", Journal of Molecular Graphics and Modelling 99 (2020) 1-11. https://doi.org/10.1016/j.jmgm.2020.107621.

6. **Muhammad Iqbal Hussain**, R.M.A. Khalil, F. Hussain, A.M. Rana, G. Murtaza, M. Imran "Probing the structural, electronic, mechanical strength and optical properties of tantalum-based oxide perovskites $ATaO_3$ (A = Rb, Fr) for optoelectronic applications: First-principles investigations", Optik - International Journal for Light and Electron Optics 219 (2020) 1-10. https://doi.org/10.1016/j.ijleo.2020.165027.

7. R.M.A. Khalil, **Muhammad Iqbal Hussain**, F. Hussain, A.M. Rana, G. Murtaza, M. Shakeel, H. M. Asif Javed "Structural, Vibrational, Mechanical and Optoelectronic Properties of $LiBH_4$ for Hydrogen Storage and Optoelectronic Devices: First Principles Study", The International Journal of Quantum Chemistry 121(4) (2020) 1-14. http://dx.doi.org/10.1002/qua.26444.

8. **Muhammad Iqbal Hussain**, R.M.A. Khalil, F. Hussain, A.M. Rana "*Ab-initio* prediction of the structural, electronic and optical behavior of novel combinations of ternary perovskite oxides $ATiO_3$ (A = Rb, Cs, Fr) using Hubbard 'U' correction for optoelectronic devices", Journal of Computational Electronics 19(4) (2020) 1-11. https://doi.org/10.1007/s10825-020-01571-w.

9. **Muhammad Iqbal Hussain**, R.M.A. Khalil, F. Hussain, A.M. Rana "DFT based insight into the magnetic and thermoelectric characteristics of $XTaO_3$ (X = Rb, Fr) ternary perovskite oxides for optoelectronic applications", International Journal of Energy Research 45(2) (2020) 1-13. https://doi.org/10.1002/er.5968.

10. A. Ali, R. Raza, R.M.A. Khalil, **Muhammad Iqbal Hussain** "Electrochemical Analysis of Titanate based Anode for Direct Carbon Fuel Cell", ACS Applied Energy Materials 3(9) (2020) 9182-9189. https://doi.org/10.1021/acsaem.0c01532.

11. R.M.A. Khalil, **Muhammad Iqbal Hussain**, M. Imran, F. Hussain, N. Saeed, G. Murtaza, A.M. Rana, C. Mahata "First-Principles Simulation of Structural, Electronic and Optical Properties of Cerium Trisulfide ($Ce_2S_3$) Compound", Journal of Electronic Materials 50(4) (2020) 1637–1643 https://doi.org/10.1007/s11664-020-08478-z.

12. S. Hayat, R.M.A. Khalil, **Muhammad Iqbal Hussain**, A.M. Rana, F. Hussain "First-principles investigations of the structural, optoelectronic, magnetic and thermodynamic properties of hydride perovskites $XCuH_3$ (X= Co, Ni, Zn) for hydrogen storage applications", Optik - International Journal for Light and Electron Optics 228 (2021) 1-18. https://doi.org/10.1016/j.ijleo.2020.166187.

13. R.M.A. Khalil, **Muhammad Iqbal Hussain**, Nyla Saeed, A.M. Rana, F. Hussain "The prediction of structural, electronic, optical and vibrational behavior of $ThS_2$ for nuclear fuel applications: A DFT study", Optical and Quantum Electronics 53(11) (2021) 1-15. https://doi.org/10.1007/s11082-020-02698-7.

14. E.A. Khera, H. Ullah, M. Imran, N.A. Niaz, R.M.A. Khalil, U. Resheed, A.M. Rana, **Muhammad Iqbal Hussain**, C. Mahata, S. Kim "*ab-initio* study of oxygen vacancy effects on structural, electronic and thermoelectric behavior of $AZr_{1-x}M_xO_3$ (A = Ba, Ca, Sr; M= Al, Cu, x = 0.25) for application of memory devices", Journal of Molecular Graphics and Modelling 103 (2021) 1-13. https://doi.org/10.1016/j.jmgm.2020.107825.

15. R.M.A. Khalil, S. Hayat, **Muhammad Iqbal Hussain**, A.M. Rana, F. Hussain "DFT based First Principles Study of Novel Combinations of Perovskite-type Hydrides $XGaH_3$ (X= Rb, Cs, Fr) for Hydrogen Storage Applications", AIP Advances 11(2) (2021) 1-14. https://doi.org/10.1063/5.0037790.

16. **Muhammad Iqbal Hussain**, R.M.A. Khalil, F. Hussain "Computational Exploration of Structural, Electronic, and Optical Properties of Novel Combinations of Inorganic Ruddlesden–Popper Layered Perovskites $Bi_2XO_4$ (X = Be, Mg) using Tran and Blaha-Modified Becke–Johnson Approach for Optoelectronic Applications", Energy Technology 9 (5) (2021) 1-23. https://doi.org/10.1002/ente.202001026.

17. R. M. Arif Khalil, **Muhammad Iqbal Hussain,** A. Batool, Fayyaz Hussain, A. M. Rana, N. Luqman "Computational Study of $TbMn_2O_5$ and $Tb_2MnCoO_6$ to Probe the Structural, Vibrational and Optoelectronic Properties using PBE + U functional", Optik - International Journal for Light and Electron Optics, 241 (2021) 1-11. https://doi.org/10.1016/j.ijleo.2021.166835.

18. Syed Awais Rouf, **Muhammad Iqbal Hussain**, Umair Mumtaz, Abdul Mannan Majeed, Hafiz Tariq Masood, A density functional theory study of the structural,

electronic and optical properties of $XGaO_3$ (X = V, Nb) perovskites for optoelectronic applications, Journal of Computational Electronics 20(4) (2021) 1484-1495. https://doi.org/10.1007/s10825-021-01718-3.

**19.** R.M.Arif Khalil, **Muhammad Iqbal Hussain**, Rabail Fatima, Fayyaz Hussain, A.M. Rana, H.H. Hegazy, Abeer Mera, Effect of dopants on the structural, optoelectronic and magnetic properties of pristine AgGaO3 perovskite: A first principles study, Optik - International Journal for Light and Electron Optics, 244 (2021) 1-11. https://doi.org/10.1016/j.ijleo.2021.167555.

**20.** Shafqat Hayat, R.M.Arif Khalil, **Muhammad Iqbal Hussain**, A.M. Rana, Fayyaz Hussain, *Ab-initio* study of the structural, optoelectronic, magnetic, hydrogen storage properties and mechanical behaviour of novel combinations of hydride perovskites $LiXH_3$ (X = Cr, Fe, Co & Zn) for hydrogen storage applications, Journal of Computational Electronics 20(6) (2021) 2284–2299. https://doi.org/10.1007/s10825-021-01807-3.

**21.** Syed Awais Rouf, **Muhammad Iqbal Hussain**, Umair Mumtaz, Hafiz Tariq Masood, et al., An ab-initio study of electronic and optical properties of $RhXO_3$ (X = Ga, Ag) perovskites, Physica Scripta 97(2) (2022) 1-10. https://doi.org/10.1088/1402-4896/ac4b34.

**22.** Shafqat Hayat, R.M. Arif Khalil, **Muhammad Iqbal Hussain**, A.M. Rana, Fayyaz Hussain, A DFT study of perovskite type halides $KBeBr_3$, $RbBeBr_3$, and $CsBeBr_3$ in triclinic phase for advanced optoelectronic devices, Solid State Communications 344(1) (2022) 1-15. https://doi.org/10.1016/j.ssc.2022.114674.

**23.** R.M. Arif Khalil, **Muhammad Iqbal Hussain**, Nadia Luqman, Fayyaz Hussain, Anwar Manzoor Rana, Muhammad Saeed Akhtar, Rana Farhat Mehmood, DFT based study of the structural, optoelectronic, mechanical and magnetic properties of $Ti_3AC_2$ (A=P, As, Cd) for coating applications, RSC Advances 12(7) (2022) 4395-4407. https://doi.org/10.1039/D1RA07856A.

**24.** R. M. Arif Khalil, **Muhammad Iqbal Hussain**, A. M. Rana, Fayyaz Hussain, Neelam Inam, H. H. Somaily, Shafqat Hayat, First principles study of the structural, optoelectronic and mechanical properties of $XLaS_2$ (X=Cu, Zn) for optoelectronic applications, Optik - International Journal for Light and Electron Optics, 258 (2022) 1-10. https://doi.org/10.1016/j.ijleo.2022.168940.

**25.** R. M. Arif Khalil, **Muhammad Iqbal Hussain**, Saba Arshad, Fayyaz Hussain, Anwar Manzoor Rana, Hafiz M. Asif Javed, First-principles simulation: study of the structural, electronic, mechanical and optical properties of disulfide $XS_2$ (X=Ta, Ti) compounds for optoelectronic applications, Surface Review and Letters, 29(6), 2250083 (2022) 1-11. https://doi.org/10.1142/S0218625X22500834.

**26.** Amjad Ali, Sajid Munir, Mubushar Majeed, A. Khalil, **Muhammad Iqbal Hussain**, and Rizwan Raza, Effect of Manganese Catalysts on the Performance of Anodes in Direct Carbon Fuel Cells, ACS Applied Energy Materials, 5(6) (2022) 6878-6885. https://doi.org/10.1021/acsaem.2c00450.

**27.** **Muhammad Iqbal Hussain**, R.M. Arif Khalil, Density functional theory studies of the structural, optoelectronic, bond stiffness and lattice dynamical properties of double perovskite oxides $M_2YVO_6$ (M= Mg, Sr): promising candidates for

optoelectronic applications, Materials Science in Semiconductor processing 152 (2022) 1-11. https://doi.org/10.1016/j.mssp.2022.107050.

**28.** Ayesha Zia, G. Murtaza, Khawar Ismail, R.M. Arif Khalil, **Muhammad Iqbal Hussain**, *Ab-initio* calculations of the structural, electronic and optical response of $KXCl_3$ (X = Be, Ca and Sr) for optoelectronic applications, Computational Condensed Matter 33 (2022) 1-9. https://doi.org/10.1016/j.cocom.2022.e00737.

**29.** R.M. Arif Khalil, **Muhammad Iqbal Hussain**, Nyla Saeed, Fayyaz Hussain, Anwar Manzoor Rana, Exploration of the structural, optoelectronic and vibrational behavior of $Sb_2S_3$ through first principles approach for phenomenal applications in solar cells, Optical and Quantum Electronics 54(12) (2022) 1-14. https://doi.org/10.1007/s11082-022-04190-w.

**30.** Bisma Tariq, G. Murtaza, Hassan Ali, Samia Razzaq, R.M.A. Khalil, **Muhammad Iqbal Hussain**, Khawar Ismail, Ghazanfar Nazir, Nouf H. Alotaibi, First-principles study of the structural, half-metallic ferromagnetism, magnetic, and transport properties of $KXO_2$ (X = Pr, Nd, and Pm) hexagonal oxides, Solid State Communications 370 (2023) 1-8. https://doi.org/10.1016/j.ssc.2023.115229.

**31.** R. M. Arif Khalil, **Muhammad Iqbal Hussain**, Bushra Karim, Hind Albalawi, Khaild I. Hussein and Fayyaz Hussain, DFT-based systematic study on the structural, optoelectronic, thermodynamic, vibrational and mechanical behavior of Ruddlesden Popper perovskites $Sr_2XO_4$ (X = Zr, Hf) for optoelectronic applications, International Journal of Quantum Chemistry 123(22) (2023) 1-17. https://doi.org/10.1002/qua.27216.

**32.** Shoaib Muhammad, G. Murtaza, Abida Azam, H.H. Raza, R.M.A. Khalil, **Muhammad Iqbal Hussain**, M. Waqas Iqbal, Tailoring Magnesium based hydrides as potential and Reversible Materials for solid-state hydrogen storage: A First-principles study, International Journal of Modern Physics B 38(26) (2023) 1-20. https://doi.org/10.1142/S0217979224503582.

**33.** Muhammad Ali, R.M. Arif Khalil, **Muhammad Iqbal Hussain**, Fayyaz Hussain, Exploration of the structural, optoelectronic, magnetic, elastic, vibrational, and thermodynamic properties of molybdenum-based chalcogenides $A_2MoSe_4$ (A =Li, K) for photovoltaics and spintronics applications: A first-principles study, Journal of Molecular Modeling 29(11) (2023) 1-16. https://doi.org/10.1007/s00894-023-05751-w.

**34.** Rabail Fatima, R.M. Arif Khalil, **Muhammad Iqbal Hussain**, Fayyaz Hussain, Computational study of the structural, optoelectronic and thermoelectric properties of scandium based ternary chalcogenides $XScSe_2$ (X = Li, Rb) for applications in Photovoltaic cell, Journal of Computational Electronics 23(1) (2023) 82-93. https://doi.org/10.1007/s10825-023-02110-z.

**35.** Rabail Fatima, R.M. Arif Khalil, **Muhammad Iqbal Hussain**, Fayyaz Hussain, Ultraviolet active novel chalcogenides $BAlTe_2$ (B = Rb, Cs): the structural, optoelectronic, mechanical, and vibrational properties for energy harvesting applications through first principles approach**,** Optical Materials Express 14(3) (2024) 607-628. https://doi.org/10.1364/OME.506814.

**36.** R.M. Arif Khalil, **Muhammad Iqbal Hussain**, Mushahid Hussain Shah, Tahani I. Al Muhimeed, Ghazanfar Nazir, Fayyaz Hussain, Umair Mumtaz, The exploration of physical properties of 2D MXenes $M_3N_2$ (M= Ti, Hf, Zr, Mo) through the first principles approach: The energy harvesting materials**,** Computational Materials Science 238 (2024) 1-8. https://doi.org/10.1016/j.commatsci.2024.112947.

**37.** Mushahid Hussain Shah, R.M. Arif Khalil, Muhammad Usman, **Muhammad Iqbal Hussain**, Fayyaz Hussain, Munirah D. Albaqami, Saikh Mohammad, Jamal Abdul Nasir, First-Principles prediction of the structural stability, optoelectronic, magnetic properties and mechanical response of olivine type $LiMPO_4$ (M = Ni, Cu) phosphate materials for energy storage applications**,** Computational and Theoretical Chemistry 1235 (2024) 1-10. https://doi.org/10.1016/j.comptc.2024.114579.

**38.** R.M. Arif Khalil, Mushahid Hussain Shah, **Muhammad Iqbal Hussain**, Nouf H. Alotaibi, Saikh Mohammad, Fayyaz Hussain, Ghulam Meeladi, *Ab-initio* study about the structural, optoelectronic, magnetic, and elastic properties of novel combinations of 2D MXenes $M_3C_2$ (M= Zr, Mo) for energy harvesting applications**,** Physica B: Condensed Matter 685 (2024) 1-9. https://doi.org/10.1016/j.physb.2024.416016.

**39.** R.M. Arif Khalil, **Muhammad Iqbal Hussain**, Shumaila Zafar, Rabail Fatima, et al., Comprehensive analysis of the phase stability, optoelectronic, mechanical, thermodynamic and vibrational properties for prospective optoelectronic applications of novel combinations of chalcogenides $XScTe_2$ (X= Li, Rb) by employing density functional theory**,** Journal of Materials Science 59(19) (2024) 8374-8391. https://doi.org/10.1007/s10853-024-09677-3.

**40.** Umair Mumtaz, Syed Awais Rouf, Hafiz Tariq Masood, A. A. Abd El-Moula, **Muhammad Iqbal Hussain**, Nasir Abbas, *et al.*, Study of structural, mechanical, thermodynamic, and optical properties of rare-earth based perovskite oxides AcXO3 (X = Al, Ga, In)**,** Optical and Quantum Electronics 56(7) (2024) 1-10. https://doi.org/10.1007/s11082-024-06977-5.

**41.** R.M. Arif Khalil, **Muhammad Iqbal Hussain**, Ayesha Asma, Fayyaz Hussain, Rabail Fatima, Ammar Mohamed Tighezza, Mohamed Ouladsmane, Jamal Abdul Nasir, Ultraviolet active novel chalcogenides $AScSe_2$ (A= K, Cs): The structural, optoelectronic, mechanical, vibrational, and thermodynamical properties for energy harvesting applications**,** Materials Science in Semiconductor Processing 182 (2024) 1-13. https://doi.org/10.1016/j.mssp.2024.108735.

**42.** Rabail Fatima, R.M. Arif Khalil, **Muhammad Iqbal Hussain**, Fayyaz Hussain, DFT insight into the phase stability, optoelectronic, elastic, vibrational, and thermodynamic properties of metal chalcogenides RbKM (M = S, Se, Te) for energy harvesting technology**,** Materials Science in Semiconductor Processing 184 (2024) 1-12. https://doi.org/10.1016/j.mssp.2024.108854.

**43.** R. M. Arif Khalil, Muhammad Iqbal Hussain, Ali Raza, Rabail Fatima, Fayyaz Hussain, Manawwer Alam, Rizwan Wahab, Muhammad Ali & Jamal Abdul Nasir "Computational investigation of the phase stability, electronic, optical, phonon spectrum, and elastic behavior of layered perovskites $Ca_2XO_4$ (X = Zr, Hf) for optoelectronic applications, Journal of Molecular Modeling 31(4) 2025 1-13". https://doi.org/10.1007/s00894-025-06537-y.

**44.** Rabail Fatima, R. M. Arif Khalil, **Muhammad Iqbal Hussain**, First principles insight of $Cu_2CdMSe_4$ (M = Zr, Hf) quaternary chalcogenides as eco-friendly materials for optoelectronic and photovoltaic applications**,** Inorganic Chemistry Communications 174(1) (2025) 1-13. https://doi.org/10.1016/j.inoche.2025.114031.

**45.** Rabail Fatima, R. M. Arif Khalil, **Muhammad Iqbal Hussain**, Fayyaz Hussain**,** Insight into the physical characteristics of novel inorganic chalcogenides $MAg_3Se_4$ (M=V, Nb, Ta) with exceptional stability using WIEN2K for its applications in photovoltaics**,** Journal of the Indian Chemical Society 102 (6) (2025) 1-21. https://doi.org/10.1016/j.jics.2025.101705.

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## L. REVIEWED PUBLICATIONS:

- More than 60 various Elsevier and IOP articles are reviewed till date.

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