**PERSONAL INFORMATION**


**DR. HAFIZ HAMID RAZA**

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**CAREER OBJECTIVE**

To pursue my career as an outstanding professional in a challenging and dynamic environment where I can nurture and boost my skills to the utmost by complementing technical knowledge with practical experience.

## EDUCATION

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|---|---|
| **2024** | Ph.D Physics **(CGPA: 3.22/4.00)** |
| | Government College University, Lahore, Pakistan |
| | **Thesis Title:** Potential use of magnesium based hydrides in hydrogen storage: First principles study |
| **2018** | M.Phil Applied Physics **(CGPA: 3.43/4.00)** |
| | Government College University, Lahore, Pakistan |
| | **Thesis Title**: Optoelectronic and thermal properties of $LiXH_3$ (X=Ba, Sr and Cs) for hydrogen storage materials: A first principle study |
| | ▪ Density Functional Theory, Physics of Materials |
| **2016** | BS Computational Physics **(CGPA: 3.44/4.00)** |
| | University of the Punjab, Lahore, Pakistan |
| | **Thesis/Project Title**: A first principle calculations of Structural and Electronic Properties of ZnO by using Material Studio and Origin Pro Software |
| | ▪ Computational Physics, Quantum Mechanics, Classical Mechanics, Electro-Magnetic Theory, Solid State Physics |
| **2011** | Higher Secondary School Certificate **(838/1100)** |
| | Govt. Islamia College Civil Lines Lahore, Pakistan |
| **2009** | Secondary School Certificate **(894/1050)** |
| | The Learners Grammer Boys High School Shahdara Lahore, Pakistan |

## RESEARCH INTERESTS

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|---|---|
| • Density Functional Theory | • Computational Material Science |
| • Solid State Physics | • Hydrogen Storage materials |

**PUBLICATIONS**

1. **Hafiz Hamid Raza**, Maha Naeem, Hafiz Irfan Ali, Abdullah M. Al-Enizi, Amna Parveen, and Sadaf Jamal Gilani. “First-Principles Study of the Excitonic and Polaronic Effect of Hydride-Based Anti-perovskite $Cu_3HX$ (X = S, Se, Te).” Journal of Inorganic and Organometallic Polymers and Materials (2025).
2. **Hafiz Hamid Raza**, Maha Naeem, Hafiz Saad Ali, Amna Parveen, and Abdullah M. Al-Enizi. "First-Principles Investigation of $BX_3H_9$ (X= Ca, Sc, Ti) Hydrides: Structural, Electronic, Phonon, and Hydrogen Storage Properties." Journal of Physics and Chemistry of Solids (2025): 112800.
3. **Hafiz Hamid Raza**, G Murtaza, Maleeha Shafiq, and Saba Abdul Shakoor, First-principles calculations on structural, mechanical and thermodynamic properties of orthorhombic $Mg_2BeTMH_8$ (TM= Ni, Cu and Zn) for hydrogen storage applications. International Journal of Hydrogen Energy, 2024. 62: p. 637-651.
4. **Hafiz Hamid Raza**, Ghulam Murtaza, Zeesham Abbas, Samia Razzaq, Shahid M. Ramay and M. Irfan. “The structural, mechanical, phonon and pressure induced thermodynamic properties of $X_4Mg_4H_{12}$ (X=Rb and Cs) for hydrogen storage applications via PBE-GGA and TB-mBJ potentials”, Materials Science and Engineering: B 300, (2024): 117072.
5. Hafiz Irfan Ali, Nawaz Muhammad, G Murtaza, Maha Naeem, **Hafiz Hamid Raza**, Ahmad Usman, Saba Saleem, M Basit Shakir, Majed Y Almashnowi, and Muhammad Umair Ashraf, Exploration of physical aspects of $Li_2AgAsZ_6$ (Z= F, Cl, Br, I) double perovskites for energy harvesting perspectives. Inorganic Chemistry Communications, 2024: p. 113295.
6. Maha Naeem, Nawaz Muhammad, G. Muratza, **Hafiz Hamid Raza** and Hafiz Irfan Ali. "First principles investigations of chalcogenides perovskites for optoelectronic applications" Journal of Materials Research (2024).
7. Muhammad Umer, G. Murtaza, Nazir Ahmad, Ahmad Ayyaz, **Hafiz Hamid Raza**, Ahmad Usman, Ayesha Liaqat, Salim Manoharadas, First principles investigation of structural, mechanical, thermodynamic, and electronic properties of Al-based perovskites $XAlH_3$ (X=K, Rb, Cs) for hydrogen storage. International Journal of Hydrogen Energy, 2024. 61: p. 820-830.
8. Zeesham Abbas, Zeeshan Zafar, **Hafiz Hamid Raza**, Amna Parveen, and Shoyebmohamad F Shaikh, Density-functional quantum analysis of optoelectronic, elastic, thermodynamic and hydrogen storage properties of $AMgH_3$ (A= Be, Ca) perovskite-type hydrides: Prospects for clean energy hydrogen-storage fuel and optoelectronic applications. International Journal of Hydrogen Energy, 2024. 60: p. 212-228.

9. Saqib Ali, H Saad Ali, Khawar Ismail, Ali Raza Iftikhar, Hassan Ali, and **Hafiz Hamid Raza**, Theoretical investigation of double perovskite $A_2NbTbO_6$ (A= Ca, Sr, Ba) for optoelectronic applications under DFT approach. Optical and Quantum Electronics, 56(7), (2024) 1-15.

10. Zeesham Abbas, Kisa Fatima, Shafaat Hussain Mirza, **Hafiz Hamid Raza**, Shoyebmohamad F Shaikh, and Amna Parveen, A systematic first-principles investigation of the structural, electronic, optical, thermodynamic and transport properties of lead free pyrochlore oxides $Q_2Sb_2O_7$ (Q= Be, Ca, Sr) for low-Cost energy applications. Journal of Physics and Chemistry of Solids, 2024: p. 111950.
11. Saba Abdul Shakoor, G Murtaza, **Hafiz Hamid Raza**, Nazir Ahmad, Muryam Iftikhar, Abdul Hakim Shah, and Ahmad Ayyaz, Structural, electronic, thermoelectric, thermodynamic, and elastic properties of $XPH_2$ (X= Li, Na, K) for hydrogen storage application: A first principle study. Computational and Theoretical Chemistry, 2024: p. 114528.
12. Hafeez Ur Rehman, Nawaz Muhammad, G Murtaza, **Hafiz Hamid Raza**, Shahid M Ramay, M Irfan, and M Awais Rehman, The investigation of structural, electronic, thermal, and elastic properties of $X_2ZnH_4$ (X= K, Rb and Cs) for hydrogen storage applications: DFT study. Optical and Quantum Electronics, 2024. 56(4): p. 636.
13. **Hafiz Hamid Raza**, G. Murtaza, Samia Razzaq, and Abida Azam. "Improving thermodynamic properties and desorption temperature in $MgH_2$ by doping Be: DFT study", Molecular Simulation 49(5), (2023): 497-508.
14. **Hafiz Hamid Raza**, G. Murtaza, and Maleeha Shafiq. "Structural, phonon, thermodynamic, and electronic properties of $MgFeH_3$ at different pressures: DFT study." Computational and Theoretical Chemistry (2023): 114030.

15. M Irfan, G Murtaza, Nawaz Muhammad, Shaista Tahir, **Hafiz Hamid Raza**, B Sabir, Muryam Iftikhar, and S Sharif, Experimental and theoretical studies of structural, electronic and magnetic properties of $RE_2NiCrO_6$ (RE= Ce, Pr and Nd) double perovskites. Physica E: Low-dimensional Systems and Nanostructures, 2023. 148: p. 115635.
16. Ahmad Ayyaz, G. Murtaza, M. Umer, Ahmad Usman, and **Hafiz Hamid Raza**. "Structural, elastic, optoelectronic, and transport properties of Na-based halide double perovskites $Na_2CuMX_6$ (M= Sb, Bi, and X= Cl, Br) as renewable energy materials: A DFT insight" Journal of Materials Research (2023): 1-16.
17. Maleeha Shafiq, M Qasim Shah, G Murtaza, **Hafiz Hamid Raza**, S M Ramay, M Irfan, Pressure induced variations in the band structure, optical and mechanical properties of lead free double halides perovskites $K_2CuAsX_6$ (X = Cl, Br): A first-principles calculations, Inorganic Chemistry Communications, 156, (2023) 111262.

18. Maleeha Shafiq, G. Murtaza, M. Qasim Shah, **Hafiz Hamid Raza**, and Ahmad Ayyaz. "Structural, elastic, electronic, optical and thermoelectric properties of metal based ternary chalcopyrite semiconductor for photovoltaic application: First-principles studies." Optik (2023): 171502.
19. Khawar Ismail, G. Murtaza, Nessrin A. Kattan, **Hafiz Hamid Raza**, A. I. Aljameel, and Q. Mahmood. "Study of optical, thermoelectric and mechanical properties of cerium based perovskites $CePO_3$ (P= Be, Ca, Mg)." Physica B: Condensed Matter (2023): 415208.
20. Muryam Iftikhar, G. Murtaza, **Hafiz Hamid Raza**, Nawaz Muhammad, Shahid M. Ramay, and Ghulam Farid. "Computational determination of structural, electronic, magnetic and elastic properties of CsXB (X= Mg and Sr) $d^o$ half-Heusler alloys as potential spintronic materials." Indian Journal of Physics (2023): 1-8.
21. Syed Farhan Ali Shah, G. Murtaza, Khawar Ismail, **Hafiz Hamid Raza**, and Imran Javed Khan. "First principles investigation of transition metal hydrides $LiXH_3$ (X= Ti, Mn, and Cu) for hydrogen storage." Journal of Computational Electronics (2023): 1-9.
22. Zeesham Abbas, Kisa Fatima, Izabela Gorczyca, Syed Hassan Abbas Jaffery, Asif Ali, Muhammad Irfan, **Hafiz Hamid Raza** et al. "First-principles calculations to investigate electronic, optical, and thermoelectric properties of $Na_2GeX_3$ (X= S, Se, Te) for energy applications." Materials Science in Semiconductor Processing 154 (2023): 107206.
23. Abida Azam, Ramesh Sharma, Debidatta Behera, **Hafiz Hamid Raza**, H. Saad Ali, Shaimaa AM Abdelmohsen, Ashraf MM Abdelbacki, and Sanat Kumar Mukherjee. "Insight into the structural, optoelectronic, and thermoelectric properties of $Fe_2HfSi$ Heusler by DFT investigation." RSC advances 13, no. 23 (2023): 15437-15447.
24. Shoaib Muhammad, G Murtaza, Abida Azam, **Hafiz Hamid Raza**, RM Arif Khalil, Muhammad Iqbal Hussain, and 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, 2023: p. 2450358.
25. Samia Razzaq, Khawar Ismail, G. Murtaza, and **Hafiz Hamid Raza**. "Theoretical Study of Half-Heusler CsXAs (X= Ca, Sr, and Ba) from First Principle Calculations." Journal of Superconductivity and Novel Magnetism 35, no. 11 (2022): 3291-3299.
26. Zeesham Abbas, Kisa Fatima, Izabela Gorczyca, Muhammad Irfan, Najla Alotaibi, Thamraa Alshahrani, **Hafiz Hamid Raza**, and Shabbir Muhammad. "Proposition of new stable rare-earth ternary semiconductor sulfides of type $LaTlS_2$ (La= Er, Eu, Tb): Ab-initio study and prospects for optoelectronic, spintronic and thermoelectric applications." Materials Science in Semiconductor Processing 146 (2022): 106662.

27. Zeesham Abbas, Kisa Fatima, Syed Hassan Abbas Jaffery, Asif Ali, **Hafiz Hamid Raza**, Shabbir Muhammad, H. Algarni, Sajjad Hussain, and Jongwan Jung. "Ab-initio study of Nb-based complex materials: A new class of materials for optoelectronic applications." Journal of Computational Science 63 (2022): 101791.
28. Muhammad Abubakr, Kisa Fatima, Zeesham Abbas, Ahmad Hussain, Nawishta Jabeen, **Hafiz Hamid Raza**, Youness Chaib, Shabbir Muhammad, Saifeldin M. Siddeeg, and Izabela Gorczyca. "Effect of S, Se and Te replacement on structural, optoelectronic and transport properties of $SrXO_4$ (X= S, Se, Te) for energy applications: A first principles study." Journal of Solid State Chemistry 305 (2022): 122689.
29. Samia Razzaq, G. Murtaza, Rana Muhammad Arif Khalil, Nazir Ahmad, and **Hafiz Hamid Raza**. "Ab-initio calculation of electronic, mechanical, optical and phonon properties of $ZrXH_3$ (X= Co, Ni and Cu): A key towards potential hydrogen storage materials." International Journal of Modern Physics B 36, no. 17 (2022): 2250090.
30. Ikram Un Nabi Lone, M Mohamed Sheik Sirajuddeen, Nazir Ahmad Teli, **Hafiz Hamid Raza**, Saubia Khalid, and Raheel Hammad, DFT calculations on the ternary MScP, quaternary $MSc_2P$ (M= Cu, Zn), and Cu and Zn doped in semiconducting scandium phosphide by GGA and GGA+ U approach. Vacuum, 2021. 191: p. 110328.
31. Ikram Un Nabi Lone, M Mohamed Sheik Sirajuddeen, Saubia Khalid, and **Hafiz Hamid Raza**, First-principles study on electronic, magnetic, optical, mechanical, and thermodynamic properties of semiconducting gadolinium phosphide in GGA, GGA+ U, mBJ, GGA+ SOC and GGA+ SOC+ U approaches. Journal of Superconductivity and Novel Magnetism, 2021. 34: p. 1523-1538.
32. Zeesham Abbas, Nawishta Jabeen, Ahmad Hussain, Faisal Kabir, Thamraa Alshahrani, **Hafiz Hamid Raza**, Shabbir Muhammad, Sikander Azam, and Izabela Gorczyca. "Effect of Nb, Ta and V replacements on electronic, optical and elastic properties of $NbCu_3Se_4$: A GGA+ U study." Journal of Solid State Chemistry 301 (2021): 122338
33. Aditya Dey, Ramesh Sharma, Sajad Ahmed Dar, and **Hafiz Hamid Raza**. "A computational investigation on structural, mechanical, electronic, magnetic, thermoelectric, and optical properties of CrXPb (X= Sc, Ti) half-Heusler alloys." Journal of Superconductivity and Novel Magnetism 34 (2021): 781-796.
34. **Hafiz Hamid Raza**, G. Murtaza, Nawaz Muhammad, and Shahid M. Ramay. "First-principle investigation of $XSrH_3$ (X= K and Rb) perovskite-type hydrides for hydrogen storage." International Journal of Quantum Chemistry 120, no. 24 (2020): e26419.

35. Umm-e-Hani, G. Murtaza and **Hafiz Hamid Raza**. "Optoelectronic and thermal properties of cubic $SiMO_3$ (M= Sn, Pb) oxides for device application: a first principle study." Optical and Quantum Electronics 52 (2020): 1-21.
36. **Hafiz Hamid Raza**, G. Murtaza, and Rana M. Arif Khalil. "Optoelectronic and thermal properties of $LiXH_3$ (X= Ba, Sr and Cs) for hydrogen storage materials: a first principle study." Solid State Communications 299 (2019): 113659.

## CONFERENES

Guest Speaker in "International Conference on Emerging Trends & Innovation in Nanotechnology"

Organized by Department of Physics, Riphah International University Lahore, Pakistan

## PERSONAL SKILLS

| **Language (s)** | English | Urdu | Punjabi |
|---|---|---|---|
| **Computer Skills** | WIEN2k | CASTEP | BASH Scripting |
| | Python (3/5) | Dev C++ | Quantum ESPRESSO |

## TEACHING (Visiting)

2024 Quantum Mechanics, University of Central Punjab (UCP), Lahore, Pakistan
2024 Optics Lab, University of Central Punjab (UCP), Lahore, Pakistan
2024 General Physics Lab, University of Central Punjab (UCP), Lahore, Pakistan
2025 Fundamental Applications of Physics, University of Education, Lower Mall Lahore, Pakistan

## RESEARCH IMPACT & PROFILES

- **World's Top 2% Scientist** (Stanford University ranking, https://doi.org/10.17632/btchxktzyw.8)
- **Google Scholar Profile** https://scholar.google.com/citations?user=BvQVad4AAAAJ&hl=en

## REFERENCES

**References will be furnished on demand**.

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