

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

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

• 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 Cu₃HX (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 BX₃H₉ (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 Mg₂BeTMH₈ (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 X₄Mg₄H₁₂ (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 Li₂AgAsZ₆ (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 XAlH₃ (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 AMgH₃ (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 CePO₃ (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° 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 LiXH₃ (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 Na₂GeX₃ (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 Fe₂HfSi 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 LaTlS₂ (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 SrXO₄ (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 ZrXH₃ (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 MSc₂P (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 NbCu₃Se₄: 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 XSrH₃ (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 ($\text{M} = \text{Sn, Pb}$) 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 ($\text{X} = \text{Ba, Sr and Cs}$) for hydrogen storage materials: a first principle study." *Solid State Communications* 299 (2019): 113659.

CONFERENCES

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.