

# DR. GHULAM MURTAZA

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<https://scholar.google.co.uk/citations?user=WYPAqTQAAAAJ&hl=en>

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## Education and Training

2012

**Ph.D. (Physics)** University of the Punjab, Lahore, Pakistan.

-Department of Physics,

-Thesis: Ferromagnetism recognition approaches based on GaN and ZnO doped with  
Rare earth metals for Spintronics Applications

2007

**MPhil (Physics)** Bahauddin Zakariya University, Multan, Pakistan.

-Department of Physics

-Thesis: Structural & Magnetic Characterization of Cd-Sr Substituted W-type Barium  
Hexa-ferrites Synthesized through wet and dry methods

## Teaching and Research Experience

2020-till

**Associate Professor**

Centre for Advanced Studies in Physics,  
Government College University, Lahore

2012-2020

**Assistant Professor**

Centre for Advanced Studies in Physics,  
Government College University, Lahore

- Incharge of Accelerator Lab &

-Materials Synthesis and Simulation Laboratory

- Plan research regarding material sciences
- Teaching MPhil, PhD and BS students

**2008-2009**

**Visiting lecturer,**  
Department of Physics, University of the Punjab, Lahore  
-BS Courses taught: Basic Electronics, Semiconductor and Solid State Devices

## Awards, Scholarships and Honours

- |      |  |
|------|--|
| 2012 | <b>HEC</b> Approved Supervisor   |
| 2010 | <b>Qualify GRE general (2007) and GRE GAT (Subject) test</b> conducted by NTS  |
| 2009 | <b>Awarded IRSIP Scholarship for Ph.D., (six month experimental work) in the University of the York, UK</b> by Higher Education Commission, Islamabad, Pakistan. |
| 2007 | <b>2nd Position</b> in M.Phil. Physics Department, B.Z.U, Multan.  |
| 2007 | <b>Awarded Indigenous Scholarship</b> for Ph.D. study by Higher Education Commission, Islamabad, Pakistan.   |

## Academic and Research Interests

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|-------------------|---|
| Courses           | Advanced Quantum Mechanics<br>Basic Electronics<br>Semiconductor and Solid State Devices<br>Advanced Magnetic Materials and Devices<br>Nanotechnology and Renewable Energy Resources<br>Physics of Materials<br>Soft Condensed Matter Physics<br>Condensed Matter Physics and Complex Systems<br>ABC of DFT<br>Spintronics<br>Quantum Optic |
| Research Interest | Nanostructured Materials<br>Thin Films<br>Solar Materials<br>Magnetic Materials, Hard and Soft Ferrites<br>Semiconductor Device Physics<br>Spintronics (Half-Metallic, DMS)<br>Energy storage Materials<br>First Principle studies under the framework of DFT   |

## PhD Theses supervised

2022-2025	Tunable ferroelectric and ferromagnetic properties of monochalcogenides multiferroics for Non-Volatile Memory Devices, Mr. Irfan Aslam, in progress
2022-2025	Heterostructure alloys for spintronics, Ms. Abeera Ijaz Saeed, in progress
<b>2020-2023</b>	<b>Synthesis and Characterization of Thermoelectric Materials for Efficient Energy Harvesting, Mr. Akhlaq Ahmed, Completed</b>
2019-2022	Impact of Ni addition in the High Strength Carbide Austempered Ductile Iron, Mr. Farhan Ali, in progress
2019-2022	Structural, optoelectronic and magnetic properties of double perovskite compounds: First principles study, Mr. Hafiz Saad Ali, in progress
<b>2017-2020</b>	<b>Investigation of stable organic and inorganic perovskites for the applications of optoelectronic devices, Ms. Saba Maqsood, Completed</b>
<b>2019-2022</b>	<b>Potential use of magnesium based hydrides in hydrogen storage: First Principles study, Mr. Hafiz Hamid Raza, Completed</b>
<b>2017-2020</b>	<b>Tunability of microwave bandwidth and absorption loss in hexaferrite composites, Mr. Mohsin Ishfaq Piracha, Completed</b>
<b>2015-2018</b>	<b>Synthesis and electromagnetic properties of metal substituted Ba-based hexaferrites, Ms. Sidra Younus, Completed</b>
<b>2015-2018</b>	<b>First principle investigation of physical properties of perovskite oxides compounds through modified Becke-Johnson potential, Ms. Bushra Sabir, completed</b>
<b>2015-2018</b>	<b>Bandgap engineering of ternary chalcopyrite structures for photovoltaic applications: First principle study, Mr. Muhammad Shahzad Yaseen, completed</b>
<b>2015-2018</b>	<b>Tailoring physical properties of polymeric materials by ion implantation, Mr. Athar Naeem Akhtar, completed</b>
<b>2014-2017</b>	<b>Ion implantation and doping of rare earth metals to tailor the multiferroic properties of BiFeO<sub>3</sub>, Ms. Sadia Sharif, completed</b>

## MS/M.Phil Theses supervised

2023-2025

2023-2025

2023-2025

2022-2024 Exploration of the photovoltaic properties of oxide-based double perovskite: An experimental and theoretical approach by **Hummaira Khan**

2022-2024 Electronic, Magnetic, Elastic and Thermodynamic properties of Half-Heusler alloys for spintronic applications by **Maryam Touqir**

2022-2024 Synthesis of high-performance Ni-rich cathode materials for Li-ion batteries by **Urwa Tul Aysha**

2022-2024 Structural and Optoelectronic Properties of Lead-free Double Perovskite for Photovoltaic: An Experimental and Theoretical investigations by **M. Basit Shakir**

2021-2023 Synthesis and characterization of lead-free double perovskite for photovoltaic applications by **Ahmad Ayyaz**

2021-2023 Fabrication of Ni-rich layered oxide cathode material for high-performance Li-ion batteries by **Ahmad Usman**

2021-2023 Silicon Sensors Qualification for the phase-II upgrade of the CMS outer tracker by **Majid Hussain**

2020-2022 Experimental and theoretical investigation of Structural, electronic, optical and magnetic properties of double perovskite for spintronic applications by **Muhammad Irfan**

2020-2022 First principles investigation of transition metal hydride compound design for hydrogen storage performance by **SYED FARHAN ALI SHAH**

2020-2022 Structural, elastic, electronic, optical and thermoelectric properties of metal based chalcopyrite semiconductor for photovoltaic application: First principles studies by **Maleeha Shafiq**

2020-2022 Investigation of structural and electrochemical performance of sodium based layered transition metal oxide by **Shaista Tahir**

2019-2021 First principles study of the structural, electronic and optoelectronic properties of  $A_2BX_6$  double perovskite compounds by **M Ali Khalid**

2019-2021	Synthesis and Characterizations of $\text{SnO}_2/\text{TiO}_2/\text{MXene}$ composites for electron transport layer in dye sensitized solar cell by <b>M Bilal Jafer</b>
2019-2021	Synthesis and characterization of double perovskite oxide $\text{La}_2\text{B}/\text{SiO}_6$ (B= Co, Ni and Fe) compounds using solid state route by <b>Faizan Ul Hassan</b>
2019-2021	Synthesis and characterization of Na and Fe co-doped Lithium Cobalt Oxide Cathode for Li-ion batteries by <b>Ali Hamza</b>
2019-2021	First Principles Investigations of layered cathode material for Lithium-ion Batteries by <b>M Noukhaiz</b>
2018-2020	Characterization of La-doped $\text{BaZrO}_3$ compounds by solid-state reaction method for optoelectronic applications by <b>Khurram Shehzad</b>
2018-2020	A facile hydrothermal synthesis and characterization of double perovskite oxide $\text{A}_2\text{FeMnO}_6$ (A= Ba, La, Sr, and Ce) nanoparticles for optoelectronic applications by <b>Saqlain Dar</b>
2018-2020	Structural, electronic, optical and thermal properties of $\text{CsPb}_{1-x}\text{Ge}_x\text{I}_3$ compounds for solar cell applications: A first principle study by <b>Abdul Ghafar</b>
2018-2020	A first principle study of structural, electronic, thermoelectric and magnetic properties of Ti doped $\text{XTe}$ (where X= Ca, Sr and Ba) for spintronics applications, by <b>Khawar Ismail</b>
2017-2019	Synthesis and characterization of antiperovskite Oxide $\text{Ba}_3\text{SnO}$ for spintronic devices by <b>Naveed Jafer</b>
2017-2019	Synthesis and characterization of spinel ferrites adsorbents magnetic nanoparticles for water treatment, <b>Abdullah</b>
2017-2019	Structural, electronic, thermal, optical and magnetic properties of $(\text{AMnTe}_2, \text{A}=\text{Li, Na, K})$ for spintronics applications: A first principle study, by <b>Najma Yaqoob</b>
2016-2018	Optoelectronic and thermal properties of $\text{LiXH}_3$ (X=Ba, Sr and Cs) for hydrogen storage materials: A first principle study, by <b>Hafiz Hamid Raza</b>
2016-2018	Synthesis of Praseodymium doped Nano crystalline $\text{LiCo}_{1-x}\text{Pr}_x\text{O}_2$ cathode material by Sol-Gel method for Li-ion battery by <b>Kanza altaf</b>
2016-2018	Dosimetry analysis of cervical cancer patient using rapid arc treatment planning by <b>Farrukh Huma</b>
2016-2018	Influence of diamagnetic tin substitution on cobaltite $\text{LaCoO}_3$ emerging materials for spintronic devices by <b>Usman Meraj</b>

2016-2018	Synthesis and characterization of Ni doped Zinc Telluride semiconductors by solid state method by <b>Hafiz Muhammad Tahir Iqbal</b>
2016-2018	First principle study of electronic, optical and thermal properties of $ASnO_3$ ( $A = Ba, Sr, \text{ and } Cs$ ) for optoelectronics application by <b>Um-e-Hani</b>
2015-2017	On the properties of transition metal doped perovskite manganites: an experimental and theoretical investigation by <b>Ammara Sajawal</b>
2015-2017	Effect of Fe-Gd co-doped on perovskite manganites for the application of magnetic storage devices by <b>Iram Habib</b>
2014-2016	Synthesis and Characterization of Nano-Crystalline $LiCo_{1-x}La_xO_2$ (with $x=0.0, 0.04, 0.08, 0.12, 0.16$ and $0.2$ ) cathode material prepared by Sol-Gel process for Li-ion battery by Ch. <b>Ghulam Fareed</b>
2014-2016	Optical and structural properties of Cadmium Sulfide nano particles for solar cell applications by <b>Syed Muhammad Osama Ali</b>
2014-2016	Synthesis and characterization of Sn doped $BiFeO_3$ multiferroic nanoparticles by <b>Muhammad Umair</b>
2013-2015	Structural, morphological and optical properties of Lanthanum doped nanocrystalline $SnO_2$ , by <b>Hafiz Shahab Arif</b>
2013-2015	Investigation of structural, morphological, electronic and optical properties of Au irradiated ZnNiO thin films prepared by pulsed laser deposition, by <b>Hajira Hanif</b>
2013-2015	Synthesis and characterization of Li doped ZnS nanoparticles by <b>Hafiz Aftab Iqbal</b>
2013-2015	Synthesis and Characterization of Vanadium (V) doped Zinc Oxide ( $ZnO$ ) Nanoparticles Using Chemical Route by <b>Hafiz Saad Ali</b>
2013-2015	Synthesis and characterization of Cd-Mn doped $BiFeO_3$ multiferroic nanoparticles by <b>Bilal Ishaq</b>
2012-2014	Effects of carbon ions implantation on mechanical properties and corrosion resistance of magnesium alloys, by <b>Muhammad Kashif Mumtaz</b>
2012-2014	Synthesis and characterization of Nd-Mn substituted Y-type hexaferrites Using chemical method by <b>Muhammad Ehsan-ul-haq</b>

## PhD/MS/BS Theses Co-Supervised

2021-2023	Structural, thermoelectric, elastic, and electronic properties of metal hydride for hydrogen storage application: A first principle study by <b>Saba Abdul Shakoor</b> (MPhil Chemistry)
2018-2020	Hydrogen storage materials for fuel cells: A first principle calculation of physical properties by <b>Samia Razzaq</b> (MPhil Chemistry)
2019-2023	COMPUTATIONAL STUDY OF PEROVSKITE TYPE HYDRIDES $\text{EuXH}_3$ (Pd, Pt) FOR HYDROGEN STORAGE APPLICATIONS by <b>Muhammad Umer</b> (B.Sc. Hons. Chemistry)

## Workshops, Conferences and Seminars/Talks

2024	Invited Speaker, 6th International Workshop on Ion Beam Applications Technical Program 04-06 Dec. 2024 at National Centre for Physics, Islamabad
2024	Invited Speaker, International Conference on Emerging Trends in Physics 2024 (ICETP24), October, 8-9 at Department of Physics, University of Lahore
2024	Invited Speaker, 1 <sup>st</sup> International Conference on Applied Sciences and Technology (ICAST-2024) at Department of Physics, Baba Guru Nanak University Nankana Sahib, 24-25 October
2024	Invited Speaker, 5th Annual International Conference on Advances in Materials Science (AIMS) at Department of Physics, Education University Lahore, on November 27-28
2024	4th ii Science International Conference, Recent Advances in Photonics and Physical Sciences, organized at Lahore College Women University (LCWU) on March 4-6, 2024, Department of Physics
2024	Invited Speaker, International Conference on 3D Printed and Energy Conversion materials, January, 25-26, 2024, Department of Physics, University of the Punjab, Lahore.
2024	National training workshop, Capacity Building of the project directors/managers of PSDP projects on PMES, 9-11 January, 2024, organized by M/O PD&SI in collaboration with P&DD, Govt. of the Punjab, Lahore

- 2023      **AIMS-2023, the 4<sup>th</sup> Annual International Conference, organized by Department of Physics, Division of Science and Technology, University of Education, Lahore, November 29-30, 2023.**
- 2023      **Invited Speaker, 5<sup>th</sup> International Workshop on Ion Beam Applications, 11 - 13 September, NCP, Islamabad**
- 2023      **Invited Speaker, 2<sup>nd</sup> International Conference on emerging trends and Innovations in Nanotechnology, 17 and 18 June 2023, Department of Physics, Riphah International University, Lahore Campus**
- 2023      **Participate, International Biophysics Workshop Nanoscale Materials and Biological Physics March 20-21, 2023 LUMS, Lahore**
- 2023      **Invited Speaker, 2<sup>nd</sup> International Conference on “Emerging Trends in Physics” 20<sup>th</sup> – 22<sup>nd</sup> March 2023, LCUW, Lahore**
- 2023      **Invited Speaker, 1<sup>st</sup> International Conference on Physics Horizons and Multidisciplinary Science, 27-28 February 2023, COMSATS University, Islamabad- Lahore Campus**
- 2022      **Invited Speaker, 4<sup>th</sup> International Workshop on Ion Beam Applications, 03 - 05 October, NCP, Islamabad**
- 2022      **Invited Speaker, Recent Trends in Theoretical Physics, One day Research Symposium, June, 01, University of Sahiwal, Sahiwal**
- 2022      **International School on Physics & Allied Disciplines (ISPAD-2022) Nanosciences and Technology Activity, 14-18 March, 2022, NCP, Islamabad**
- 2022      **Organiser and Speaker, 17<sup>TH</sup> NATIONAL SYMPOSIUM ON FRONTIERS IN PHYSICS, Government College University, Lahore, December 01-03, 2022**
- 2020      **Invited Speaker, 1<sup>st</sup> International Conference on Advances in Materials Science (AIMS 23-24 July 2020) University of Education, Lahore**
- 2019      **Invited Speaker at, International Conference on Solid State Physics December 08, 2019, ICSSP-19, University of the Punjab**
- 2019      **PU International Symposium on Advanced Energy Storage Materials, on 4-6 November, University of the Punjab, Lahore**
- 2019      **International CASTEP training workshop 2019, 19<sup>th</sup> - 23<sup>rd</sup> August Oxford University, UK**



2019	<b>Invited Speaker, 16<sup>th</sup> International Symposium on Advanced Materials, 21-25 October, Islamabad, Pakistan</b>
2019	<b>Invited Speaker, 16<sup>th</sup> National Symposium Frontier in Physics, 29-31 Jan. 2019 GCU, Lahore</b>
2018	<b>Invited Speaker, International Symposium on applications of radioisotopes, November, Department of Physics, GC University, Lahore</b>
2018	<b>Invited Speaker, International Workshop on Ion Beam Applications, National Centre for Physics, Islamabad, 09-11 July</b>
2017	International Conference on Solid State Physics – 10-14 December, University of the Punjab, Lahore
2017	<b>Invited Speaker 15<sup>th</sup> National Symposium Frontier in Physics, 29-31 Jan. 2017 GCU, Lahore</b>
2016	<b>Invited Speaker on 14<sup>th</sup> National Symposium Frontier in Physics, 23-25 Nov. 2016 GCU, Lahore</b>
2016	National Workshop on Ion Beam Applications, National Centre for Physics, Islamabad, 2-3 June
2015	Invited speaker on one-day workshop, “Physics and Technology of Accelerators” National Centre for Physics, Islamabad, 23, November 2015
2014	International Conference on Physics and Contemporary Needs (ICPCN- 2014) CAPS-Physics, GC University, Lahore
2007	Conference on X-Ray diffraction study by <b>Khwarzmic Science Society</b> Center of Solid State Physics, Lahore, Pakistan.
2007	<b>7th International Symposium on Advanced Materials, Islamabad, Pakistan.</b>

## **Computer, Technical Skills and Research Projects**

Simulation Code WIEN2K, CASTEP

Math Packages Mathematica, **FORTRAN Programming, LabVIEW**

OS Windows, Mac OS X, Linux, DOS.

Computer Language Python

Instrument handling  
 X-Ray Diffractometer, Structure analysis  
 Vibrating Sample Magnetometer (VSM)  
 Thin Film Growth and Characterization  
 Scanning Electron Microscopy (SEM), Energy Dispersive Spectroscopy (EDS)  
 Atomic Force Microscopy (AFM)  
 Pelletron Accelerator  
 Magneto-optic Kerr effect (MOKE)  
 Molecular Beam Epitaxy (MBE)  
 Hydraulic press  
 Digital Furnace  
 Dielectric Measurements  
 I-V Characteristics measurements by 4-probe system (Hall effect)  
 Fourier Transform Infrared Spectroscopy (FTIR)  
 Solar Simulator

## Research Projects

**2019-2020** Magnetic Composites Materials, Emerging Designer Adsorbents for Aqueous Pollutants Removal and Water Treatments, Faculty research project, ORIC GC University, Lahore, Total Award Amount: Rs. 300,000/-

**2012-2013** Synthesis, characterization, and first principles study of vanadium doped half-metallic ferromagnetic II-VI (ZnS, ZnSe, and ZnTe) systems, **Higher Education Commission, Pakistan**, Total Award Amount: Rs. 50,0000/- Approved.

2012-2013 Synthesize and characterization of impurity doped Fe<sub>3</sub>O<sub>4</sub> nanoparticles by chemical route, **GC University, Lahore**, Completed. CASP Rs. 100000/-

## List of Journal Publications

Year 2026

1. Urwa tu Ayesha, [G. Murtaza](#), Synthesis, characterization, and DFT simulation to analyze electrochemical performance of ternary transition metal oxides LiNi<sub>0.80</sub>X<sub>0.10</sub>Nb<sub>0.10</sub>O<sub>2</sub>(X=Cu, Zn, Y) for lithium-ion batteries, Journal of Physics and Chemistry of Solids 208 (2026) 113074

Year 2025

2. Sundus Ajmal, [G. Murtaza](#), Fizza Aftab, Wajid Ali, Ahmad Ayyaz, Ali Akremi,

- and Imed Boukhris, A Computational Investigation of Structural, Electronic, Thermoelectric, and Electrochemical Properties of Binary Transition Metal  $\text{NaTM}_{1/3}\text{Fe}_{2/3}\text{O}_{2-\delta}$  (TM = Ag, Nb, W) as Na-ion Battery Cathode Materials, *Journal of The Electrochemical Society* 172 (2025) 080527
3. M. Awais Ahmed, Shoaib Ullah, Khalil Ur Rehman, [G. Murtaza](#), Ahmad Ayyaz, M. Irfan, Imen Kebaili, Ali El-Rayyes, A First-Principles Study of the Structural, Optoelectronic and Thermoelectric Properties of  $\text{Ba}_2\text{XIO}_6$  (X = Li, K and Rb) for Energy Harvesting, *Brazilian Journal of Physics* (2025) 55:221
  4. Fizza Aftab, [G. Murtaza](#), Sundas Ajmal, Ahmad Ayyaz, Ali Akremi, Samah Al-Qaisi, Hind Albalawi, Mohd Taukeer Khan, First-principles investigation of transition metal-substituted layered oxides  $\text{KMn}_{2/3}\text{TM}_{1/3}\text{O}_2$  (TM = Cr, Nb, Ag) as promising cathode materials for potassium-ion batteries, *Journal of Physics and Chemistry of Solids*, 207 (2025) 112962
  5. Sayada Ayesha Zia Bukhari, Ayesha Parveen, Muhammad Sajid, Hassan Ali, Gamil A. A. M. Al-Hazmi, Khawar Ismail, [Ghulam Murtaza](#), Yazen. M. Alawaideh, Muhammad Jamil, First-principles study of structural, electronic, optical, and thermoelectric properties of  $\text{BaTMSe}_2$  (TM = Fe, Co, and Ni) for optoelectronic devices, *Journal of Sol-Gel Science and Technology* (2025) 1-15
  6. Ahmad Ayyaz, [G Murtaza](#), Exploring hydrogen storage potential, thermodynamic, and optoelectronic characteristics of novel double perovskite hydrides  $\text{Na}_2\text{LiXH}_6$  (X = Al, Sc, and Ga): DFT analysis, *Journal of Energy Storage* 122 (2025) 116650
  7. Samah Al-Qaisi, Nazia Iram, N. Sfina, Abderrazak Boutramine, Hamad Rahman Jappor, Amani H. Alfaifi, Hind Saeed Alzahrani, Habib Rached, Malak Azmat Ali, [G. Murtaza](#), Comprehensive DFT Study of  $\text{K}_2\text{TiZiI}_6$  (Z = Al, In) Double Perovskites: Structural Stability and Potential for Optoelectronic and Thermoelectric Energy Harvesting, *Physica B: Condensed Matter* (2025)
  8. Mudassir Ishfaq, Ali Raza Iftikhar, Hassan Ali, Khawar Ismail, [Ghulam Murtaza](#), Gamil A. A. M. Al-Hazmi, Muhammad Jamil, Theoretical analysis of double perovskite  $\text{A}_2\text{HfNiO}_6$  (where A = Ba, Ca, and Sr) for structural, elastic optical, electronic, thermoelectric and magnetic properties for spintronics applications, *Materials Science and Engineering B* 317 (2025) 118198
  9. Ahmad Usman, [G. Murtaza](#), Ahmad Ayyaz, Imed Boukhris, Hafiz Irfan Ali, M. Basit Shakir, Hanof Dawas Alkhalidi, Maryam Touqir, Thamraa Alshahrani, Muhammad Umair Ashraf, First-principles exploration of redox, electronic, thermoelectric, and thermodynamic properties of binary transition metal  $\text{NaX}_{1/3}\text{Mn}_{2/3}\text{O}_2$  (X = Ag, W, Zr) for enhanced performance of Na-ion batteries, *Inorganic Chemistry Communications*, 175 (2025) 114157
  10. Maryam Touqir, [G. Murtaza](#), Ahmad Ayyaz, Ahmad Usman, M. Basit Shakir, Saba Saleem, Hummaira khan, Muhammad Umair Ashraf, Khalid M. Elhindi, First-principles calculations to investigate Electronic, half-metallicity, thermodynamics, thermoelectric and mechanical properties of new Half-Heusler alloys  $\text{FeCoZ}$  (Z = Si, Ge, and Pb) *Computational and Theoretical Chemistry*, (2025)
  11. Sidra Younus, [G. Murtaza](#), Haya Alhummiyany, M Hassan, Murefah Mana Al-Anazy, Q Mahmood, El Sayed Yousef and Ali S Alshomrany, Investigation of structural, magnetic, and dielectric properties of  $\text{BaFe}_{12}\text{O}_{19}/\text{Pr}_{1-x}\text{Sr}_x\text{Co}_y\text{Mn}_{1-y}\text{O}_3$  composites; an emerging aspirant for high frequency applications, *Physica Scripta*, 100 (2025) 015925
  12. Maryam Masood, [Ghulam Murtaza](#), Nadia Ahmad, Maryam Touqir, Iram Hafiz, Ahmad Usman, Ahmad Ayyaz, Nazir Ahmad, An ab-initio study of the physical

- properties of Ge-based perovskites ( $X\text{GeH}_3$ :  $X=\text{Mg}$ ,  $\text{Ca}$ , and  $\text{Sr}$ ) for potential hydrogen storage application, *International Journal of Hydrogen Energy* 97 (2025)981-993
13. Ahmad Usman, [G. Murtaza](#), Muhammad Younas, Ali Akremi, Ahmad Ayyaz , Haya Alhummiyany, Syed Kashif Ali, Kanza Altaf, Hisham S.M. Abd-Rabboh, Sadia Sharif, Q. Mahmood, Study of Pr doped nanocrystalline  $\text{LiCoO}_2$  cathode material for spintronic, *Materials Chemistry and Physics* 329 (2025) 130133  
and energy storage applications: A theoretical and experimental analysis
  14. Ahmad Ayyaz, [G. Murtaza](#), Synthesis, Characterization, and Photocatalytic Performance of Gold Ions Implanted  $\text{TiO}_2/\text{Graphene}$  Nanocomposites for Efficient Dye Photodegradation, *Ceramics International* (2025)
  15. Ahmad Ayyaz, Imed Boukhris, Ahmad Fraz, Afaf Khadr Alqorashi, Q. Mahmood, Lamiaa Galal Amin, [G. Murtaza](#), M. Basit Shakir, Exploring Energy Harvesting Potential of Lithium-Based Halide Perovskites  $\text{Li}_2\text{CuSbZ}_6$  ( $Z=\text{Cl}$ ,  $\text{Br}$ ): First Principles Approach, *Materials Science in Semiconductor Processing*, 185 (2025) 108968
  16. Zoha Afzal, Sajid Butt, Muhammad Rizwan, Sajid Ur Rehman, Saeeda Sajjad, Zahid Usman, [G. Murtaza](#), Density Functional Theory (DFT) Perspectives of Thermoelectric Transportation in Sr-doped  $\text{LaCoO}_3$ , *Next Materials* 7(2025)100383
  17. Mudassir Ishfaq, Muniba Urooj, Muhammad Sajid, Khawar Ismail, Rimsha Baqeel, Ejaz Ahmad Khera, Rajwali Khan, Sattam Al Otaibi, Khaled Althubeiti, Hassan Ali, [Ghulam Murtaza](#), Muhammad Jamil, First principles investigation of structural, electronic, optical, transport properties of double perovskites  $\text{X}_2\text{TaTbO}_6$  ( $X= \text{Ca}$ ,  $\text{Sr}$ ,  $\text{Ba}$ ) for optoelectronic and energy harvesting applications, *Journal of Physics and Chemistry of Solids* 197 (2025) 112432
  18. Hummaira Khan, [G. Murtaza](#), Ahmad Ayyaz, M. Basit Shakir, Maryam Touqir, Khubaib Iqbal, Ahmad Usman, Sohail Mumtaz, Ihab Mohamed Moussa, Structural stability, optoelectronic, thermoelectric, and elastic characteristics of  $\text{X}_2\text{ScBiO}_6$  ( $X= \text{Mg}$ ,  $\text{Ca}$ , and  $\text{Ba}$ ) double perovskites for energy harvesting: First-principles analysis, *Materials Science in Semiconductor Processing*, 185 (2025) 108911

## Year 2024

19. Ahmad Ayyaz, G. Murtaza, Huda Alkhalidi, Haya Alhummiyany, Akhlaq Ahmed, Hisham S.M. Abd-Rabboh, Q. Mahmood, M. S. Al-Buriah, H. Elhosiny Ali, Investigation of Structure, Morphology, Dielectric, and Optoelectronic Properties of La-Doped  $\text{BaZrO}_3$ : Experimental and DFT Analysis, *Journal of Materials Science: Materials in Electronics* 35 (2024)2110
20. Hafiz Irfan Ali, Nawaz Muhammad, G. Murtaza, Maha Naeem, Hafiz Hamid Raza, Ahmad Usman, Saba Saleem, M. Basit Shakir, Majed Y. Almashnowi, Muhammad Umair Ashraf, Amel Ayari-Akkari, *Exploration of physical aspects of  $\text{Li}_2\text{AgAsZ}_6$  ( $Z = \text{F}$ ,  $\text{Cl}$ ,  $\text{Br}$ ,  $\text{I}$ ) double perovskites for energy harvesting perspectives*, *Inorganic Chemistry Communications*, 170 (2024) 113295

21. Saba Saleem, Nawaz Muhammad, **G. Murtaza**, DFT Study of Structural, Electronic, Magnetic, Elastic, and Thermoelectric Properties of Ta-based Half-Heusler Alloys CsTaX (X=C, Si, and Ge) for Spintronics and Thermoelectric Technologies, Computational and Theoretical Chemistry (2025)
22. M. Basit Shakir, **G. Murtaza**, Ahmad Ayyaz, Maryam Touqir, Hummaira Khan, Ali Akremi, Hafiz Irfan Ali, Ahmad Usman, Abeer S. Altowyan, Khubaib Iqbal, Computational insight on  $K_2AuBiX_6$  (X = F, Cl, Br, I) double perovskites to comprehensively investigate mechanical, optoelectronic, and thermoelectric features for green energy applications, Materials Science and Engineering: B, 310, ( 2024) 117667
23. Maha Naeem, Nawaz Muhammad, **G. Murtaza** , Hafz Hamid Raza , Hafz Irfan Ali, First principles investigations of chalcogenides perovskites for optoelectronic applications, Journal of Material Research (2024)
24. Maryam Touqir, **G. Murtaza**, Ab initio analysis of structural, electronic, magnetic, thermodynamics, and elastic properties of the Half-metallic Half Heusler alloy  $ZMnAs$  (Z= Be, Mg) for spintronics application, Materials Semiconductor and processing 184(2024)108807
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