

DR. GHULAM MURTAZA

Centre for Advanced Studies in Physics,
Government College University,
Lahore-54000, Pakistan.

Cell #+92-3214263536

Email: gmrai@gcu.edu.pk, murtazarai@hotmail.com,

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

Academic and Research Interests

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

PhD Theses supervised

2022-2025 Tunable ferrelcetric and ferrmagnetic properties of monochalcogenides multiferroics for Non-Volatile Memory Devices, Mr. Irfan Aslam, in progress

2022-2025 Huesllor alloys for spintronics, Ms. Abeera Ijaz Saeed, in progress

2020-2023 **Synthesis and Characterization of Thermoelectric Materials for Efficient Energy Harvesting, Mr. Akhlaq Ahmed, Completed**

2019-2022 Impact of Ni addition in the High Strength Carbidic 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

2017-2020 **Investigation of stable organic and inorganic perovskites for the applications of optoelectronic devices, Ms. Saba Maqsood, Completed**

2019-2022 **Potential use of magnesium based hydrides in hydrogen storage: First Principles study, Mr. Hafiz Hamid Raza, Completed**

2017-2020 **Tunability of microwave bandwidth and absorption loss in hexaferrite composites, Mr. Mohsin Ishfaq Piracha, Completed**

2015-2018 **Synthesis and electromagnetic properties of metal substituted Ba-based hexaferrites, Ms. Sidra Younus, Completed**

2015-2018 **First principle investigation of physical properties of perovskite oxides compounds through modified Becke-Johnson potential, Ms. Bushra Sabir, completed**

2015-2018 **Bandgap engineering of ternary chalcopyrite structures for photovoltaic applications: First principle study, Mr. Muhammad Shahzad Yaseen, completed**

2015-2018 **Tailoring physical properties of polymeric materials by ion implantation, Mr. Athar Naeem Akhtar, completed**

2014-2017 **Ion implantation and doping of rare earth metals to tailor the multiferroic properties of BiFeO₃, Ms. Sadia Sharif, completed**

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 M Bilal Jafer
2019-2021	Synthesis and characterization of double perovskite oxide $\text{La}_2\text{B}/\text{SiO}_6$ ($\text{B}=\text{Co, Ni and Fe}$) compounds using solid state route by Faizan Ul Hassan
2019-2021	Synthesis and characterization of Na and Fe co-doped Lithium Cobalt Oxide Cathode for Li-ion batteries by Ali Hamza
2019-2021	First Principles Investigations of layered cathode material for Lithium-ion Batteries by M Noukhaiz
2018-2020	Characterization of La-doped BaZrO_3 compounds by solid-state reaction method for optoelectronic applications by Khurram Shehzad
2018-2020	A facile hydrothermal synthesis and characterization of double perovskite oxide A_2FeMnO_6 ($\text{A}=\text{Ba, La, Sr, and Ce}$) nanoparticles for optoelectronic applications by Saqlain Dar
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 Abdul Ghafar
2018-2020	A first principle study of structural, electronic, thermoelectric and magnetic properties of Ti doped XTe (where $\text{X}=\text{Ca, Sr and Ba}$) for spintronics applications, by Khawar Ismail
2017-2019	Synthesis and characterization of antiperovskite Oxide Ba_3SnO for spintronic devices by Naveed Jafer
2017-2019	Synthesis and characterization of spinel ferrites adsorbents magnetic nanoparticles for water treatment, Abdullah
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 Najma Yaqoob
2016-2018	Optoelectronic and thermal properties of LiXH_3 ($\text{X}=\text{Ba, Sr and Cs}$) for hydrogen storage materials: A first principle study, by Hafiz Hamid Raza
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 Kanza altaf
2016-2018	Dosimetry analysis of cervical cancer patient using rapid arc treatment planning by Farrukh Huma
2016-2018	Influence of diamagnetic tin substitution on cobaltite LaCoO_3 emerging materials for spintronic devices by Usman Meraj

2016-2018 Synthesis and characterization of Ni doped Zinc Telluride semiconductors by solid state method by **Hafiz Muhammad Tahir Iqbal**

2016-2018 First principle study of electronic, optical and thermal properties of $ASnO_3$ ($A = Ba, Sr, \text{ and } Cs$) for optoelectronics application by **Um-e-Hani**

2015-2017 On the properties of transition metal doped perovskite manganites: an experimental and theoretical investigation by **Ammara Sajjawal**

2015-2017 Effect of Fe-Gd co-doped on perovskite manganites for the application of magnetic storage devices by **Iram Habib**

2014-2016 Synthesis and Characterization of Nano-Crystalline $LiCo_{1-x}La_xO_2$ (with $x=0.0, 0.04, 0.08, 0.12, 0.16 \text{ and } 0.2$) cathode material prepared by Sol-Gel process for Li-ion battery by Ch. **Ghulam Fareed**

2014-2016 Optical and structural properties of Cadmium Sulfide nano particles for solar cell applications by **Syed Muhammad Osama Ali**

2014-2016 Synthesis and characterization of Sn doped $BiFeO_3$ multiferroic nanoparticles by **Muhammad Umair**

2013-2015 Structural, morphological and optical properties of Lanthanum doped nanocrystalline SnO_2 , by **Hafiz Shahab Arif**

2013-2015 Investigation of structural, morphological, electronic and optical properties of Au irradiated $ZnNiO$ thin films prepared by pulsed laser deposition, by **Hajira Hanif**

2013-2015 Synthesis and characterization of Li doped ZnS nanoparticles by **Hafiz Aftab Iqbal**

2013-2015 Synthesis and Characterization of Vanadium (V) doped Zinc Oxide (ZnO) Nanoparticles Using Chemical Route by **Hafiz Saad Ali**

2013-2015 Synthesis and characterization of Cd-Mn doped $BiFeO_3$ multiferroic nanoparticles by **Bilal Ishaq**

2012-2014 Effects of carbon ions implantation on mechanical properties and corrosion resistance of magnesium alloys, by **Muhammad Kashif Mumtaz**

2012-2014 Synthesis and characterization of Nd-Mn substituted Y-type hexaferrites Using chemical method by **Muhammad Ehsan-ul-haq**

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 Saba Abdul Shakoor (MPhil Chemistry)
2018-2020	Hydrogen storage materials for fuel cells: A first principle calculation of physical properties by Samia Razzaq (MPhil Chemistry)
2019-2023	COMPUTATIONAL STUDY OF PEROVSKITE TYPE HYDRIDES EuXH ₃ (Pd, Pt) FOR HYDROGEN STORAGE APPLICATIONS by Muhammad Umer (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, 1st 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 4th Annual International Conference, organized by Department of Physics, Division of Science and Technology, University of Education, Lahore, November 29-30, 2023.**

2023 **Invited Speaker, 5th International Workshop on Ion Beam Applications, 11 - 13 September, NCP, Islamabad**

2023 **Invited Speaker, 2nd 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, 2nd International Conference on “Emerging Trends in Physics” 20th – 22nd March 2023, LCUW, Lahore**

2023 **Invited Speaker, 1st International Conference on Physics Horizons and Multidisciplinary Science, 27-28 February 2023, COMSATS University, Islamabad- Lahore Campus**

2022 **Invited Speaker, 4th 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, 17TH NATIONAL SYMPOSIUM ON FRONTIERS IN PHYSICS, Government College University, Lahore, December 01-03, 2022**

2020 **Invited Speaker, 1st 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, 19th - 23rd August Oxford University, UK**

2019 **Invited Speaker, 16th International Symposium on Advanced Materials, 21-25 October, Islamabad, Pakistan**

2019 **Invited Speaker, 16th National Symposium Frontier in Physics, 29-31 Jan. 2019 GCU, Lahore**

2018 **Invited Speaker, International Symposium on applications of radioisotopes, November, Department of Physics, GC University, Lahore**

2018 **Invited Speaker, International Workshop on Ion Beam Applications, National Centre for Physics, Islamabad, 09-11 July**

2017 International Conference on Solid State Physics – 10-14 December, University of the Punjab, Lahore

2017 **Invited Speaker 15th National Symposium Frontier in Physics, 29-31 Jan. 2017 GCU, Lahore**

2016 **Invited Speaker on 14th National Symposium Frontier in Physics, 23-25 Nov. 2016 GCU, Lahore**

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 **Khwarzimic Science Society** Center of Solid State Physics, Lahore, Pakistan.

2007 **7th International Symposium on Advanced Materials, Islamabad, Pakistan.**

Computer, Technical Skills and Research Projects

Simultion 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_3O_4 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 $LiNi0.80X0.10Nb0.10O2$ (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 NaTM₁/3Fe₂/3O₂– δ (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 Ba₂XIO₆ (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 KMn_{2/3}TM_{1/3}O₂ (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 BaTMS₂ (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 Na₂LiXH₆ (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 K₂TIZI₆ (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 A₂HfNiO₆ (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 Alkhaldi, Maryam Touqir, Thamraa Alshahrani, Muhammad Umair Ashraf, First-principles exploration of redox, electronic, thermoelectric, and thermodynamic properties of binary transition metal NaX_{1/3}Mn_{2/3}O₂ (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 FeCoZ (Z = Si, Ge, and Pb) Computational and Theoretical Chemistry, (2025)
11. Sidra Younus, **G. Murtaza**, Haya Alhummiany, M Hassan, Murefah Mana Al-Anazy, Q Mahmood, El Sayed Yousef and Ali S Alshomrany, Investigation of structural, magnetic, and dielectric properties of BaFe₁₂O₁₉/Pr_{1-x}S_xCoyMn_{1-y}O₃ 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=Mg, Ca, and 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 Alhummiany, Syed Kashif Ali, Kanza Altaf, Hisham S.M. Abd-Rabboh, Sadia Sharif, Q. Mahmood, Study of Pr doped nanocrystalline 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 TiO_2 /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=Cl, 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 LaCoO_3 , Next Materials 7(2025)100383
17. Mudassir Ishfaq, Muniba Urooj, Muhammad Sajid, Khawar Ismail, Rimsha Baeqel, 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 $X_2\text{TaTbO}_6$ (X= Ca, Sr, 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 $X_2\text{ScBiO}_6$ (X= Mg, Ca, and 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 Alkhaldi, Haya Alhummiany, Akhlaq Ahmed, Hisham S.M. Abd-Rabboh, Q. Mahmood, M. S. Al-Burahi, H. Elhosiny Ali, Investigation of Structure, Morphology, Dielectric, and Optoelectronic Properties of La-Doped 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 = F, Cl, Br, 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
25. Ahmad Ayyaz, Samah Saidi, Noura Dawas Alkhaldi, **G. Murtaza**, N. Sfina, Q. Mahmood, Lead-Free Double Perovskites Rb_2TlSbX_6 (X=Cl, Br, and I) As an Emerging Aspirant for Solar Cells and Green Energy Applications, Solar Energy 279 (2024) 112844
26. Ahmad Ayyaz, G. Murtaza, Akhlaq Ahmed, J. El Ghoul, Mayeen Uddin Khandaker, Revealing vibrational, elastic, electro-optic, and thermoelectric aspects of double perovskites Na_2ScCuX_6 (X=Cl, Br) for energy harvesting applications by implementing DFT approach, Materials Chemistry and Physics 325 (2024) 129808
27. Basit Shakir, **G. Murtaza**, Probing the Structural, Electronic, Thermodynamic, Optical, and Thermoelectric Features of Lead-Free Double Perovskites Na_2ScAgZ_6 (Z=Br, I) for Green Energy Harvesting, Inorganic Chemistry Communications (2024)
28. Ahmad Usman, **G Murtaza**, Synthesis, characterization, and evaluation of improved electrochemical performance of vanadium and zinc co-doped Ni-rich oxide cathode materials: Experimental and first-principles study, Ionics (2024)
29. **G. Murtaza**, M. Usman Meraj, M. Hassan, Muhammad Younas, Nuriyah Mohammed Aloufi; Haya Alhummiany, Murefah mana Al-Anazy, Abdulaziz A Alshihri; Syed Tahir Abbas Shah; Q. Mahmood, Study of structural and magnetic properties of Sn doped cobaltite perovskite $LaCoO_3$: Experimental and DFT Approach, Journal of Materials Science: Materials in Electronics (2024)
30. Hafeez Ur Rehman, Muhammad Jameel, Ning Wang, **G. Murtaza**, Maleeha Shafiq, Muhammad Usman, Zahid Usman, Muhammad Zulfiqar, Moonis Ali Khan, A DFT Investigation on Halide Double Perovskites X_2ScTlI_6 (X= Rb, Cs) For Thermoelectric and optoelectronic applications, Materials Today Communications (2024)
31. Ahmad Ayyaz, **G. Murtaza**, Investigation of Promising Lead-Free Double Perovskites Rb_2TlBiZ_6 (Z=Cl, Br, and I) as Sustainable Alternatives for Photovoltaic and Wasted Heat Conversion Applications: First Principles Analysis, Journal of Inorganic and Organometallic Polymers and Materials (2024)
32. Ahmad Ayyaz, **G. Murtaza**, Norah Algethami, Ahmad Usman, M. Basit Shakir, Q. Mahmood, Influence of alkali metal cation modifications on physical characteristics

of double perovskites $\text{Rb}_2\text{XTlBr}_6$ (X=Li, Na, K): First-principles study for solar energy and thermoelectric applications, *Physica B: Condensed Matter* 690(2024) 416245

33. Murefah Mana Al-Anazy, Ahmad Ayyaz, **G. Murtaza**, Abdulaziz A. Alshihri, Ahmad Usman, DFT insight on stability, optoelectronic, and thermoelectric features of Na_3XO (X = Cu, Ag) anti-perovskites: Promising materials for sustainable energy applications, *International Journal of Quantum Chemistry* (2024)

34. Urwa tul Ayesha, **G. Murtaza**, First Principles Calculations of Novel Binary Transition Metal Oxides $\text{NaCr}_{0.5}\text{X}_{0.5}\text{O}_2$ (X = Y, Tc, Rh) for Na-Ion Batteries, *Journal of the Electrochemical Society* (2024)

35. H. Saad Ali, **G. Murtaza**, Ahmad Ayyaz, Khawar Ismail, Maryam Touqir, Hafeez Ur Rehman, Yousef Mohammed Alanazi, First-principles predictions of structure, half-metallic antiferromagnetism, optoelectronic, and elastic properties of double perovskites A_2TaNiO_6 (A = Ca, Sr, and Ba) for energy harvesting, *Materials Science in Semiconductor Processing* 181 (2024) 108638

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References

Prof. Dr. M. Azhar Iqbal

Ex Chairman
Department of Physics,
University of the Punjab,
Lahore.

Tel: +92-42-99239238, 03334210963

E-mail: iqbalma@yahoo.com

Prof. Dr. Yongbing Xu

Chair in Nanotechnology
Head, Spintronics and Nanodevices Laboratory
Department of Electronic Engineering
Heslington, York YO10 5DD, UK

Tel: +44-1904-432349
Fax: +44-1904-432335
E-mail: yx2@ohm.york.ac.uk

Prof. Dr. Riaz Ahmad
Dean
Faculty of Mathematical and Physical Sciences
Director IOP
Chairman/Department of Physics,
Govt. College University, Lahore,
Pakistan
Tel:+92-42-99211589
E-mail: ahriaz@gcu.edu.pk

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