SYED AWAIS ROUF

Address: House No. 12, Street No. 2,
Sirajpura Shalimar Town Baghbanpura
54000-Lahore, Pakistan.

CAREER OBJECTIVES

To professionalise myself in one of the world's best subjects, physics. My goal is to understand myself and my surroundings with facts and figures, cause and outcome, as well as to implement my knowledge and skills in useful practical work, to gain a respectable position in the society and serve humanity.

PERSONAL INFORMATION

FATHER'S NAME:	Abdul Rouf Shah (late)
DATE OF BIRTH:	18/10/1989
DOMICILE:	Lahore
NATIONALITY:	Pakistani
LANGUAGES:	Punjabi and Urdu (native speaker), English (professional), Finnish (elementary)
CONTACT:	+92 321 1685 161
EMAIL:	awais.physicist@gmail.com, syedawais.rouf@ue.edu.pk

QUALIFICATIONS

2013 – 2017

Marie Curie Early Stage Research Fellow (PhD obtained on 7th Nov 2017): Physics
University of Oulu (Oulu, Finland), secondments at Technical University of Berlin (Berlin, Germany), Bruker BioSpin GmBh, (Rheinstetten, Germany) and Slovak Academy of Sciences (Bratislava, Slovakia)
Research Topic: Paramagnetic Nuclear Magnetic Resonance Chemical Shift Theory: A Combined Ab-Initio/Density-Functional Theory Method
Supervisor: Prof. Dr. Juha Vaara

2012 – 2013

Bachelor of Education (B. Ed.): Professional Degree
University of the Punjab, Lahore, Pakistan.
Purpose of Degree: Teaching, Teacher Education

2010 – 2012

Master of Philosophy (M. Phil.): Physics
Department of Physics
University of the Punjab
Lahore, Pakistan.
Thesis Title: Magnetic Properties of Mn-Doped ZnO: A First-Principles Study

2006 – 2010

Bachelor of Science Honors (B. Sc. (Hons.)): Physics
Department of Physics
University of the Punjab
Lahore, Pakistan.
Specialisation: Solid-State Physics

ADDITIONAL SKILLS

- **Operating System**: Windows, Linux
- **Scientific Writing**: Word, LaTex
- **MS Office Tools**: Power point, Excel, Outlook
- **Programming**: R, Matlab, C, C++, Python (SciPy, NumPy, MatPlotlib)
- **Analysis and Visualization Tools**: Mathematica, Xmgrace, Originlab
- **Modelling Softwares**: Gimp, Molden, JMol, VMD, Avogadro, GabEdit, MaterialStudio
- **Computational Physics and/or Chemistry Codes**: SIESTA, ORCA, GAUSSIAN, TURBOMOLE, ReSpect, DALTON, CFOUR, Wien2k, CASTEP

SCHOLARSHIPS & AWARDS

- **HEC Approved Supervisor for MS/MPhil/PhD**. (2020-2023)
- **Marie Curie Early Stage Research (PhD) Fellowship**. (2013-2016).
- **Student Grant**, EUROMAR Conference (2015).
- **Award of Research Assistantship** during M. Phil. (2011).
- **Laptop Award** on Merit during M.Phil. from Govt. of Punjab, Lahore, Pakistan (2010).
- **Merit Scholarship** during B.Sc. (Hons) (2007).

EXPERIENCE

- **Assistant Professor of Physics** at the Department of Physics, University of Education, Lahore, Multan Campus, Multan, Pakistan from **23-10-2018 to present**.
- **Coordinator** at the Department of Physics, University of Education, Lahore, Multan Campus, Multan, Pakistan from **23-10-2018 to present**.
- **Doctoral Student Employed** in a Academy of Finland Project at NMR Research Unit, **University of Oulu, Oulu, Finland** from **Nov-2016** to **Dec-2017**.
- **Marie Curie Early Stage Researcher** from **Nov-2013** to **Nov-2016** at NMR Research Unit, **University of Oulu, Oulu, Finland**.
- **Visiting Researcher** (3^{rd} secondment for 3 months during year 2016) at **Slovak Academy of Sciences, Bratislava, Slovakia**.
- **Visiting Researcher** (2^{nd} secondment for 3 months during year 2015) at **Bruker BioSpin, GmBh, Rheinstetten, Germany**.
- **Visiting Researcher** (1^{st} secondment for 3 months during year 2014) at **Technical University of Berlin, Berlin, Germany**.
- **Science Educator** (from Oct-2012 to Oct-2013) at **Govt. High School Attoke Awan Lahore, Pakistan**.
- **Research Assistant** (part-time) from Jan-2012 to May-2012 at **Department of Physics, Lahore University of Management Sciences (LUMS), Lahore, Pakistan**.

LIST OF PUBLICATIONS

PUBLISHED ARTICLES <u>(IF = 119.568)</u>

1. T. M. Al-Daraghmeh, G. Nazir, O. Zayed, N. A. Kattan, **S. A. Rouf***, H. Albalawi, A. I. Aljameel, and I. Boukhris, "Tuning of optical, thermodynamic, and thermoelectric properties of Cs2CuBiX6 (X = Cl, Br, I) halide perovskites for solar cells and energy harvesting applications", Physica Scripta, (2024). **IF = 2.600**
2. N. A. Kattan, **Syed Awais Rouf***, H. D. Alkhaldi, M. Hassan, S. Al-Qaisi, A. I. Aljameel, H. Albalawi, I. Boukhris, Q. Mahmood, U. Mumtaz, "Study of Half metallic Ferromagnetism and Thermoelectric Properties of the Spinels $MgCo_2(S/Se)_4$ for Spintronic and Energy Harvesting", J. Inorganic and Organometallic Polymers and Materials, (2024). **IF = 3.900**
3. A. I. Aljameel, **Syed Awais Rouf***, B. O. Alsobhi, A. O. Alrashdi, J. Hakami, A. K. Alqorashi, H. Albalawi, I. kebaili, Q. Mahmood, "Half Metallic Ferromagnetism, Mechanical, Thermodynamic, and Thermoelectric Properties of Vacancy Ordered Double Perovskites $Rb_2(V/Cr)Cl_6$ for Spintronics", J. Inorganic and Organometallic Polymers and Materials, (2024). **IF = 3.900**

4. U. Mumtaz, **Syed Awais Rouf*,** H. T. Masood, A. A. Abd El-Moula, M. I. Hussain, N. Abbas, A. S. Alshomrany, N. Sfna, "Study of Structural, Mechanical, Thermodynamic, and Optical Properties of Rare-earth Based Perovskite Oxides $AcXO_3$ (X = Al, Ga, In)", Optical & Quantum Electronics, (2023). **IF = 3.000**
5. Q. Mahmood, Noura Dawas Alkhaldi, Sheikha lardhi, Ayman S. Alofi, **Syed Awais Rouf***, Tariq M. Al-Daraghmeh, Omar Zayed, Murefah mana AL-Anazy, El Sayed Yousef, "Stable Lead Free Double Perovskites $Cs_2XAu(Br/I)_6$ (X = Y, Sc) as an Emerging Aspirant for Solar Cells and Thermoelectric Applications", Materials Chemistry and Physics, (2024). **IF = 4.600**
6. M. Hassan, **Syed Awais Rouf***, "Impact of Terbium (Tb) on Ferromagnetism and Thermoelectric Behaviour of Spinels MgTb2(S/Se)4 for Spintronic", Materials Science & Engineering B, (2023). **IF = 3.600**
7. H. Albalawi**, **S. A. Rouf***, T. Zelai, N. A. Kattan, S. Bouzgarrou, Q. Mahmood, Samah Al-Qaisi, El Sayed Yousef, "The Study Optical, Thermoelectric, and Thermodynamic Properties of Double Perovskites K_2CuBiX_6 (X = Cl, Br, I) for Energy Harvesting", Materials Science & Engineering B, (2023). **IF = 3.600**
8. A. Mera, AK Almeshal, **S. A. Rouf***, T. Zelai, A.I. Aljameel, Othman Hakami, Q. Mahmood, "Modification of Band gaps by Changing Anions to Optimize the Double Perovskites K_2NaTlX_6 (X = Cl, Br, I) for Solar Cells and Transport Applications", Chem. Phys. Lett., (2023). **IF = 2.800**
9. **S. A. Rouf***, H. Albalawi, T. Zelai, O. Hakami, N. A. Kattan, Samah Al-Qaisi, S. Bouzgarrou, M. Younas, Khaild I. Hussein, Q. Mahmood, "Half Metallic Ferromagnetism and Thermoelectric Effect in Spinel Chalcogenides SrX_2S_4 (X = Mn, Fe, Co) for Spintronic and Energy Harvesting", J. Phys. Chem. Solids., (2023). **IF = 4.000**
10. A. Mera, **S. A. Rouf***, Taharh Zelai, N. A. Kattan, Q. Mahmood, "Study of Inorganic Double Perovskites Cs_2RbZI_6 (Z = Ga, In) as Energy Harvesting Aspirant: A DFT Approach", Opt Quant Electron., (2023). **IF = 3.000**
11. A. Mera, T. Zelai, **S. A. Rouf***, N. A. Kattan, Q. Mahmood, "First-principles Calculations to Investigate Mechanical, Thermoelectric and Optical Performance of Inorganic Double Perovskites Rb_2AgAlZ_6 (Z = Br, I) for Energy Harvesting", J. Mater. Research Tech., (2023). **IF = 6.267**
12. N. A. Kattan, **S. A. Rouf***, Q. Mahmood, M. mana AL-Anazy, M. A. Amin, H. H. Hegazy, M. Morsi, N. H. Alotaibi, H. H. Somaily, "Study of Optoelectronic and Thermoelectric Properties of Double Perovskites X_2HfI_6 (X = Ga, In, Tl) for Renewable Energy", Phys. Scr., (2023). **IF = 3.081**
13. M. Hasnain, Zaka Ullah, N. I. Sonil, W. Ahmad, A. Khalil, S. M. Ali, G. M. Mustafa, M. F. Nazar, **S. A. Rouf**, N. Shamain, K. Khan, "Ultrasensitive Strain Sensor based on Graphite Coated Fibrous Frameworks for Security Applications", Mater. Today Commun., (2023). **IF = 3.800**
14. R. Moussa, Y. Djalab, M. Maache, R. Khenata, Saad bin Omran, **S. A. Rouf**, M. W. Iqbal, A. Abdiche, W. Ahmed, M. Manzour, "An Investigation Using DFT Methods on the Electronic and Optical Properties, and Mechanical Behavior of the Wurtzite $ZnO_{1-x}Te_x$ Ternary Alloy", Current Applied Physics, (2023). **IF = 2.400**
15. Y. Djalab, R. Moussa, M. Maache, **S. A. Rouf**, A. Abdiche, R. Khenata, F. Soyalp, "Theoretical Investigations of Structural, Electronic, Optical and Elastic Properties of Wurtzite $ZnO_{1-x}Se_x$ Ternary Alloys using First Principle Method", J. Materials Research, (2022). **IF = 2.909**
16. N. A. Kattan, **S. A. Rouf***, N. Sfina, M. mana Al-Anazy, H. Ullah, A. Hakamy, A. Mera, Q. Mahmood, M. A. Amin, "Tuning of Band Gap by Anion Variation of Double Perovskites K_2AgInX_6 (X = Cl, Br) for Solar Cells and Thermoelectric Applications", J. Solid State Chemistry, (2022). **IF = 3.656**
17. **S. A. Rouf***, N. Akhtar, N. A. Kattan, J. Alzahrani, Q. Mahmood, Samah Al-Qaisi, M. Morsi, H. Albalawi, S. Alharthi, M. Amin, "Study of Ferromagnetism and Thermoelectric Behaviour of Thiospinels $MgFe_2(S/Se)_4$ for Spintronics and Energy Harvesting", Phys. Scr., (2022). **IF = 3.081**
18. T. I. Al-Muhimeed, J. Alzahrani, **S. A. Rouf***, S. Al-Qaisi, R. Anbarasan, Q. Mahmood, H. Albalawi, S. Alharthi, Mohammed A. Amin, H. H. Somaily, M. Morsi,

"Tuning of Band Gap by Anion Variation of Ga_2TiX_6 (X = Cl, Br, I) for Solar Cells and Renewable Energy", Phys. Scr., (2022). **IF = 3.081**

19. A. Mera, Q. Mahmood, **S. A. Rouf***, "Quantum Ferromagnetism in Transition Metals doped II-VI Semiconductors for Spintronic Applications: A Merging Technology", Solid State Communications, (2022). **IF = 1.934**
20. S. A. Rouf*, M. I. Hussain, U. Mumtaz, H. T. Masood, H. Albalawi, A. M. Majeed, R. M. A. Khalil, Q. Mahmood, "An Ab-Initio Study of Electronic and Optical Properties of $RhXO_3$ (X = Ga, Ag) Perovskites", Phys. Scr., (2022). **IF = 2.487**
21. T. Zelai, **S. A. Rouf***, Q. Mahmood, S. Bouzgarrou, Mohammed A. Amin, A. I. Aljameel, T. Ghrib, H. H. Hegazy, A. Mera, "First-Principles Study of Lead-Free Double Perovskites Ga_2PdX_6 (X = Cl, Br, and I) for Solar Cells and Renewable Energy", J. Mater. Research Tech., (2021). **IF = 5.039**
22. T. H. Flemban, H. Althib, S. Bouzgarrou, **S. A. Rouf***, M. H. Alhossainy, A. I. Aljameel, A. Mera, M. G. B. Ashiq, Q. Mahmood**, "First Principle Analysis of Lead-free Variant Perovskites Iodides for Optical and Thermoelectric Applications", J. Mater. Research Tech., (2021). **IF = 5.039**
23. H. Althib, T. H. Flemban, A. I. Aljameel, A. Mera, M. G. B. Ashiq, Q. Mahmood, B. Ul Haq, **S. A. Rouf**, "First Principle Study of $Zn/CdSc_2Se_4$ Electronic, Optical and Transport Properties for Energy Renewable Applications", Bulletin of Materials Science, (2021). **IF = 1.783**
24. M. I. Khan*, M. Touheed, M. S. Hasan, M. Siddique, **S. A. Rouf**, T. Ahmad, M. Iqbal, M. M. Almoneef,* and N. Alwadai, "Hydrothermal Synthesis, Characterization and Photocatalytic Activity of Mg doped MoS_2", Zeitschrift für Physikalische Chemie, International Journal of Research in Physical Chemistry and Chemical Physics, (2021). **IF = 2.408**
25. H. T. Masood, S. Anwar, **S. A. Rouf**, A. Nawaz, T. Javaid, T. Munir, W. DeJiang, "Synthesis of WO3 Nanosheet and its Application in CdTe Thin Film Solar Cells", J. Alloys and Compounds, (2021). **IF = 5.316**
26. A. A. AlObaid, **S. A. Rouf**, T. I. Al-Muhimeed, A. I. Aljameel, M. Morsi, H. H. Hegazy, T. Alshahrani**, G. Nazir, O. A. Alamri, Q. Mahmood*, "New Lead-Free Double Perovskites Rb2Ge(Cl/Br)6; A Promising Materials for Renewable Energy Applications", Mater. Chem. Phys., (2021). **IF = 4.094**
27. **S. A. Rouf***, M. I. Hussain, U. Mumtaz, A. M. Majeed, and H. T. Masood, "Structural, Electronic and Optical Properties of XGaO3 (X = V, Nb) Perovskites for Optoelectronic Applications: A DFT Study", J. Comp. Electronics, (2021). **IF = 1.532**
28. A. Maryam, M. N. Rasheed, M. Asghar, K. Fatima, M. Afzal, F. Iqbal, **S. A. Rouf**, M. Syvajarvi, and B. Zhu, "Preparation and Application of LiSiC-oxide for Low Temperature Solid Oxide Fuel Cells", Dig. J. Nanomater. Bios. 16, 2 (2021). **IF = 0.785**
29. Q. Mahmood, **S. A. Rouf**, E. Algrafy, G. Murtaza, S. M. Ramay, and A. Mahmood, "First Principle Analysis of Electronic, Optical and Thermoelectric Characteristics of XBiO3 (X = Al, Ga, In) Perovskites", Opto-Electronics Review, 28, 8 (2020). **IF = 1.438**
30. Q. Mahmood, **S. A. Rouf**, M. Rashid, M. Jamil, M. Sajjad and A. Laref, "Tailoring of Bandgap to Tune the Optical Properties of Ga1−xAlxY (Y = As, Sb) for Solar Cell Applications by Density Functional Theory Approach", Z. Naturforsch. 74(12)a: 1131 (2019). **IF = 1.414**
31. **S. A. Rouf**, V. B. Jakobsen, J. Mareš, N. D. Jensen, C. McKenzie, J. Vaara and U. G. Nielsen, "Assignment of Solid-State 13C and 1H NMR Spectra of Paramagnetic Ni(II) Acetylacetonate Complexes Aided by First-Principles Computations", Solid State NMR, 87, 29 (2017). **IF = 2.044**
32. **S. A. Rouf**, J. Mareš and Juha Vaara, "Relativistic Approximations to Paramagnetic NMR Chemical Shift and Shielding Anisotropy in Transition Metal Systems", J. Chem. Theory Comput. 13(8), 3731 (2017). **IF = 5.245**
33. Peter J. Cherry, **S. A. Rouf** and J. Vaara, "Paramagnetic Enhancement of Nuclear Spin-Spin Coupling", J. Chem. Theory Comput. 13(3), 1275 (2017). **IF = 5.245**

34. **S. A. Rouf**, J. Mareš and J. Vaara, "1H Chemical Shifts in Paramagnetic Co(II) Pyrazolylborate Complexes: A First-Principles Study", J. Chem. Theory Comput. 11(4), 1683 (2015). **IF = 5.245**
35. J. Vaara, **S. A. Rouf** and J. Mareš, "Magnetic Couplings in the Chemical Shift of Paramagnetic NMR", J. Chem. Theory Comput. 11(10), 4840 (2015). **IF = 5.245**

BOOK CHAPTER

1. **S. A. Rouf***, Z. Usman, H. T. Masood, A. M. Majeed, M. Sarwar and W. Abbas, "Synthesis and Purification of Carbon Nanotubes", accepted for publication in "Carbon Nanotubes - Redefining the World of Electronics" edited by Dr. Prasanta Ghosh, IntechOpen (2021).

RESEARCH FUNDING

1. NRPU (2021) Research Project by the HEC, Islamabad having total cost of Rs. 2866500/-.

RESEARCH SUPERVISION

MS Theses

1. M. Numair, "Investigation of Optoelectronic and Thermoelectric Properties of $ZnMgS_2$ Using Density Functional Theory", 2023.
2. Arooj Khalid, "DFT Study of Optoelectronic Properties of $CaZrO_3$ Under Pressure for Optoelectronic Applications", 2023.
3. Asim Junaid, "First-Principles Calculation of the Elastic Constant, Electrical and Optical Properties of Rare Earth Metals Doped Lanthanum Zinc Oxide", 2023.
4. Muhammad Adnan, "Structural, Mechanical and Optoelectronic Properties of Lanthanum Doped Tellurium Oxide Using Density Functional Theory", 2023.
5. Muhammad Nazim, "Computational Studies on the Solvent Effect of Silylamide Dissociation", 2023.
6. Mehr un Nissa, "Adsorptive Removal of Antibiotic Gatifloxacin from Aqueous Solution by Iron Oxide Nanoparticles", 2023.
7. Muqaddas Umar, "The Structural and Optical Properties of Chromium Arsenic Oxide $CrAsO_3$: A DFT Study", 2022.

BS Theses

8. Farman Hussain, "DFT Study of Ruddlesden–Popper (RP) Phased Ba_2SnO_4 Perovskite Oxide", 2023.
9. Muhammad Shafi, "Ab-initio Investigation of Optoelectronic Properties of $K_2ScTlCl_6$", 2023.
10. Sagheer Ahmad, "DFT Study of Electronic and Optical Response of Lead-free Halide Perovskite $CsGeBr_3$", 2023.
11. Sumiya Shaheen, "Structural, Electronic and Optical Properties of AcSnO3: A DFT Study", 2023.
12. Hamza Liaqat, "An Ab-Initio Study of Electronic Band Structures and Optical Response of Silver Tungstates $AgWO_4$", 2022.
13. Muhammad Faseeh ul Zaman Shah, "DFT Study of Structural, Electronic and Optical Properties of $AcGaO_3$", 2022.
14. Nasir Abbas, "DFT Study of Structural, Electronic and Optical Properties of $AcAlO_3$", 2022.
15. Muhammad Naoman, "Life Cycle of a Star and Estimation of Mass of Cygnus X-1", 2022.
16. M. Hamza, "Measurement of Balmer Decrement of Galaxies through 3D Data", 2021.
17. M. Zaid, "Globular Cluster: Measurement of Milky Way Center", 2021.
18. Umair Mumtaz, "Ab initio Investigation of Structural, Electronic and Optical Properties of $VGaO_3$", 2020.
19. M. Shoaib, "Structural Study of Planets within and Beyond Our Solar System", 2020.

ORGANIZATION

1. Seminar on "Differentiation of Normal and Tumorous Microvasculature Using Optical Coherence Tomography", UE Multan Campus, August 4th 2022.

2. An online Seminar on "Medical Imaging of Microrobots Towards in-vivo Applications", UE Multan Campus, Pakistan, July 21st 2022.
3. An online Seminar on "Introduction to Particle Accelerators: Evolution of Accelerators and Modern-Day Applications", UE Multan Campus, Pakistan, July 18th 2022.
4. An online Seminar on "Bandgap Tuning of Metal-oxides for Improved RS Characteristics of RRAM Devices: Using DFT Study", UE Multan Campus, Pakistan, June 4th 2022.
5. An online Seminar on "Advancements in Physics and Future Directions", UE Multan Campus, Pakistan, April 5th 2021.
6. An online Seminar on "Two-Phase Flow Simulations for Wettability Alteration of Reservoir Rocks using Nano-fluids for Application in Enhanced Oil Recovery", UE Multan Campus, Pakistan, April 1st 2021.
7. Seminar on "Fabrication of High Efficient Thin Film Solar Cells", UE, Multan Campus, Pakistan, Jan 21st 2020.

PARTICIPATION

1. Local mini pNMR symposium organised at TUB, Berlin, Germany on June, 25th 2014 with title "Paramagnetic chemical shifts in Co(II) pyrazolylborate complexes by first principle computation".
2. The pNMR Scientific Conference, 16th-18th of September 2014, Cambridge, UK.
3. FSRUO Autumn School 2014 Photon based research at roadmap infrastructures & IYCr 2014: Crystallography in Finland, Oct 20th-22th 2014, University of Oulu, Oulu, Finland.
4. Swedish Theoretical Chemistry Meeting 2014-New Horizons, Oct 27th-29th 2014, Uppsala University, Uppsala, Sweden.
5. NMR Research Group Seminar University of Oulu, Finland on 13th of Feb 2015 with title "Proton Chemical Shifts in Paramagnetic Co(II) Pyrazolylborate Complexes".
6. The Molecular Computational Science (CMS-2015), 15th-18th of March 2015, University of Warwick, Coventry, UK.
7. The 37th Finnish NMR Symposium and the 17th Kuopio Bio-NMR Workshop, 15th - 17th of April 2015, University of Eastern Finland, Kuopio, Finland.
8. EUROMAR Satellite Workshop "pNMR - From Rags to Riches: Challenges and Potentials of NMR on Paramagnetic Molecules", 4th-5th of July 2015, Prague, Czech Republic with title "NMR Chemical Shifts in Paramagnetic Molecules Using First-Principles Approach".
9. European Magnetic Resonance Conference (EUROMAR-2015), 5th -10th of July 2015, Prague Congress Centre, Prague, Czech Republic.
10. PNMR Secondment at Bruker GmBh-2015 Research Work Seminar, Rheinstetten, Germany on 10th of Aug 2015 with title "An Overview of Nuclear Magnetic Resonance (NMR) and Results of Calculations/Simulations".
11. The European Summer School in Quantum Chemistry (ESQC-2015), 6th -19th of Sep 2015, Hotel Torre Normanna, near Palermo, Sicily, Italy.
12. The International Chemical Congress of Pacific Basin Societies (PECIFICHEM-2015), 15th - 20th of Dec 2015, Honolulu, Hawaii, USA.
13. NMR Research Group Seminar, University of Oulu, Finland, on 18th of Mar 2016 with title "Relativistic Effects in the NMR Chemical Shifts of Paramagnetic Molecules Using First-Principles Approach".
14. Physics days 2016, 29th -31st of March 2016, Faculty of science, University of Oulu, Oulu, Finland.
15. "Theory and Applications of Computational Chemistry" - TACC 2016, conference at the University of Washington, Seattle, WA, USA on August 28th to September 2nd, 2016.
16. Final pNMR Workshop "Europe meets Italy with paramagnetic NMR" Venice, Italy on 27th-30th of Sep 2016 with title "NMR Chemical Shifts in Paramagnetic Molecules: A First-Principles Study".

17. NMR Research Group Seminar University of Oulu, Finland on 12th of May 2017 with title "NMR Chemical Shifts in Paramagnetic Molecules: Combined Ab Initio/DFT Study".
18. PIPS, Dialogue with Teachers on Promoting Social Harmony, December 14th-15th 2018, Lahore, Pakistan.
19. PHEC, Capacity Building Program, 29th February to 25th July 2020, Lahore, Pakistan.
20. One day Online Faculty Development Program on Challenges in Building Collaborations in Research and Innovation, Dr. M.G.R. Educational and Research Institute, India, May 9th 2020.
21. Virtual Session on Mindfulness with Dr. Ranjini Manian, Dr. M.G.R. Educational and Research Institute, India, June 23rd 2020.
22. ProQuest Ebook Central Advanced Training, HEC, Islamabad, Pakistan, Sep 16th 2020.
23. Online Course ACS Reviewer Lab, Oct 7th 2020.
24. 20th International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods, ICTP, Italy, February 23rd-25th 2021.
25. Workshop: 2D Materials for Spin-Orbitronics, ICTP, Italy, May 3rd-5th 2021.
26. Workshop on Physics and Chemistry of Solid/Liquid Interfaces for Energy Conversion and Storage, ICTP, Italy, May 24th-28th 2021.
27. Symposium on Atomistic Modelling and Simulation, Nyro Research India, June 7th-11th 2021.
28. Workshop on "Empowering knowledge on ethical publishing: Mastering the art of identifying predatory, fake and cloned journals" on June 8th 2022.
29. "Resume for Research and Innovation (R4RI), a Narrative CV Approach: The What, Why, and How Organisations can engage with it" on Monday 21st March 2022.

INTERESTED FIELDS & RESEARCH

- Computational Chemistry
- Computational Materials Science
- Computational Condensed Matter Physics
- Chemical Physics
- Optoelectronics
- Spintronics
- Spectroscopy and Molecular Properties
- Computational Materials Modelling

LIST OF REFERENCES

- Dr. Juha Vaara (PhD Supervisor)
  Professor
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  University of Oulu,
  Oulu, Finland FIN-90014
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- Dr. Qasim Mahmood (Post-PhD Collaborator)
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- Dr. Fakhar ul Inam (Co-supervised M. Phil Thesis)
  Professor

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