

# **YASIR ALTAF**

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## **INTRODUCTION**

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Self-motivated learner and a team player with a proven track record of honoring professionalism. Strong verbal and written communication skills for a range of audience. Passionate teacher and researcher with years of teaching experience initially in high school and college, and now at university level with experience of teaching a variety of basic and advanced courses. Steadily growing as a researcher and leading a research group consisting of BS and MS Chemistry students. History of involvement in administrative responsibilities along teaching and research with current additional role as Coordinator of the department of Chemistry (Campus Head of Department). Always eager to take lead in problem-solving and happy to learn from the seniors. Respectful toward cultural, religious and ethnic diversity. Habitual of staying updated and learning new skills with the purpose of gaining information and trying for novelty and innovation.

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## **EDUCATION**

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<b>2019</b>	<b>Ph.D., Chemistry, Victoria University of Wellington, New Zealand</b>
	Concentrations: Theoretical and Computational Chemistry, Basics of Organometallic Synthesis
	Thesis: <i>Computational Chemistry of Compounds with Donor-Acceptor Interactions</i>
	Supervisor: Matthias Lein, Ph.D. (Computational Chemistry)
	Co-Supervisor: Prof. Martyn Coles (Organometallic Synthesis)
<b>2014</b>	<b>M.S. Chemistry, COMSATS University Islamabad, Abbottabad Campus, Pakistan</b>
	Concentrations: Organic Synthesis
	Thesis: <i>Synthesis, Characterization and DFT Studies of New Benzanthrone Derivatives</i>
	Thesis Advisor: Farhan Ahmad Khan, Ph.D.
<b>2011</b>	<b>M.Sc., Chemistry, The University of Azad Jammu and Kashmir, Muzaffarabad, AJK, Pakistan</b>
	Concentrations: Organic, Inorganic, Physical, Biochemistry
<b>2008</b>	<b>B.Sc., The University of Azad Jammu and Kashmir, Muzaffarabad, AJK, Pakistan</b>
	Concentrations: Botany, Chemistry, Zoology
<b>2006</b>	<b>HSSC, AJK Board of Intermediate and Secondary Education, Mirpur, AJK, Pakistan</b>
	Concentrations: Pre-medical
<b>2003</b>	<b>SSC, AJK Board of Intermediate and Secondary Education, Mirpur, AJK, Pakistan</b>
	Elective Subjects: Biology, Chemistry, Physics

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## EXPERIENCE

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<b>Sep 2020 to date</b>	<b>Assistant Professor of Chemistry</b> University of Education, Lahore, Pakistan, Jauharabad Campus <b>Courses Taught:</b> Quantum Chemistry and Gas Phase Equilibrium, Fundamentals of Physical Chemistry, Introduction to Biochemistry, Environmental Chemistry, Advanced Physical Chemistry, Electroanalytical Techniques, Medicinal Chemistry, Advanced Photochemistry, Organic Polymer Chemistry, Atomic Spectrophotometry, Fundamentals of Inorganic Chemistry, Fundamentals of Organic Chemistry, Analytical Chemistry <b>Supervision of Research Projects:</b> 11 BS students (all graduated) and 28 MS students <b>Additional Charge:</b> Coordinator, Department of Chemistry w.e.f September 2025, Member visiting faculty hiring committee, Member chemicals inspection committee
<b>2019 (T2), 2017 (T1 and T2)</b>	<b>Sessional Assistant, School of Chemical and Physical Sciences</b> Victoria University of Wellington, New Zealand <b>Courses:</b> Concepts of Chemistry, Principles of Chemistry, Chemical Synthesis – Laboratory Course, Chemical Materials and Methods
<b>Jan 2015-Dec 2015</b>	<b>Head of Sciences, Punjab College Kotli, AJK, Pakistan</b> <b>Roles:</b> Meetings with the science staff to devise strategy for improvement in teaching, meetings with the parents to listen to their grievances regarding the problems of their children in science subjects and providing them with the feedback on the progress of their children, meetings with the principal to discuss progress and further improvements needed
<b>Aug 2014-Jun 2016</b>	<b>Lecturer, Punjab College Kotli, AJK, Pakistan</b> <b>Courses:</b> General Chemistry, Physical Chemistry, Organic Chemistry, Inorganic Chemistry
<b>2011-12 and 2008-09</b>	<b>Science Teacher, Greenland Public Secondary School and Girls Inter College, Chowki Kalah, Kotli, AJK, Pakistan</b> Subjects: Biology, Chemistry, Physics

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## DIGITAL SKILLS AND COMPUTING

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Experience of working on different operating systems and programs such as

Windows and Linux (Advanced user)

Latex (Advanced user)

MS Office (Advanced user)

ChemBioOffice (Advanced user)

Programming in *Python* (beginner)

Experience of Computational Software such as

Gaussian, Multiwfn, and GUIs such as GaussView (Excellent user)

ORCA, Quantum ESPRESSO (Intermediate user)

ADF, GAMESS (Basic user)

Experience of high-performance cluster-computing on *Heisenberg*, *Raapoi* and *NESI* clusters, New Zealand

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## REPRESENTATIVE PUBLICATIONS

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M. K. Shehzad, **Y. Altaf**, M. Z. Mehdi, F. Ahmed, & F. Abbas (2025). Computational insight into Thieno [3, 2-b] thiophene based nonfused-ring electron acceptors as organic solar cells precursors. *Journal of Molecular Liquids*, 128878.

A. Khurshid, **Y. Altaf**, N. Zafar *et al.* (2025) Palladium (II) Pyridylidene Sulfonamide (PYSA) Catalysts Featuring Ortho-Substitution Allow for Improved Electrocatalytic CO<sub>2</sub> Reduction. *Inorganic Chemistry Communications*, 73: 113838.

Z. Umar, **Y. Altaf**, F. Ahmed, N. U. Hassan *et al.* (2024) Band structure engineering to improve the optical and thermoelectric properties of Rb<sub>2</sub>AgXBr<sub>6</sub> (X= Al, In, Ga) for energy applications within DFT framework. *Materials Science and Engineering: B*, 310: 117728 (from the thesis of my MS student Zunash Umar).

A. Zafar, **Y. Altaf**, A. Zafar, *et al.* (2024). Unveiling the effects of thallium and bismuth p-n doping on germanium-based clusters (n<sub>5</sub> to n<sub>12</sub>) for applications in semiconductor materials. *Materials Science in Semiconductor Processing*, 184: 108818 (from the thesis of my MS student Ayesha Zafar)

R. Hasan, **Y. Altaf**, N. Jabeen, N. U. Hassan *et al.* (2024). ZnS@Fe<sub>2</sub>O<sub>3</sub> core-shell nanorod arrays for supercapattery applications: theoretical evaluation of faradic and non-faradic behavior using Dunn's model. *Journal of Electroanalytical Chemistry*, 966: 118411 (from thesis of my MS student Rabbia Hasan).

A. R. Raza, S. L. Rubab, M. Ashfaq, **Y. Altaf**, M. N. Tahir, *et al.* (2023). Evaluation of antimicrobial, anticholinesterase potential of indole derivatives and unexpectedly synthesized novel benzodiazine: Characterization, DFT and Hirshfeld charge analysis. *Molecules*, 28(13): 5024-5043.

S. L. Rubab, A. R. Raza, B. Nisar, M. Ashfaq, **Y. Altaf** *et al.* (2023). Synthesis, crystal structure, DFT calculations, Hirshfeld surface analysis and in silico drug-target profiling of (R)-2-(2-(1, 3-dioxoisoindolin-2-yl) propanamido) benzoic acid methyl ester. *Molecules*, 28(11): 4375-4392.

M. Naseem, S. Asghar, U. Farooq, A. Lakhani, **Y. Altaf**, M. Hashmi (2023). Determination of the absolute configuration of Ballonigrin Lactone A using DFT calculations. *ACS Omega*: 8(2): 1923-1928. (from the thesis of my MS student Misbah Naseem)

**Y. Altaf**, S Ullah., F. A. Khan, A. Maalik, S. L. Rubab, M. A. Hashmi (2021). Finding new precursors for light harvesting materials: A computational study of the fluorescence potential of benzanthrone dyes. *ACS Omega*, 6(47): 32334-32341.

**Y. Altaf**, M. Yar, M. A. Hashmi (2020). Main-group metal cyclophane complexes with high coordination numbers. *RSC Advances* 10(51): 30796-30805.

M. Anker, **Y. Altaf**, M. Lein, M. Coles (2019). Reaction of In-Zn bonds with organic azides: products that result from hetero- and homobimetallic behavior. *Dalton Transactions*. 48(44): 16588-16594.

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## CONFERENCES AND WORKSHOPS

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### Role as Organizer:

International Conference on Recent Trends in Natural Sciences – Hybrid

2024: Conference Secretary

2023: Conference Organizing Team

2022: Conference Organizing Team

### Participation:

2019: 6TH Computational Molecular Science Conference, University of Warwick, UK

2014: Workshop on Modern Techniques in Structural Chemistry and Structural Biology, COMSATS University Islamabad (Abbottabad Campus), Pakistan

2013: 12th International and 24th National Chemistry Conference", Bahauddin Zakariya University (BZU), Multan

2010: 9th "Youth in Governance" Workshop held at Mirpur University of Science and Technology

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## GRANTS AND SCHOLARSHIPS

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2016: Dalian Institute of Chemical Physics Doctoral Scholarship (Not availed, started PhD at VUW, NZ)

2016: Victoria Doctoral Scholarship, Victoria University of Wellington, New Zealand

2003: Postgraduate College Kotli Excellence Scholarship

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## REFERENCES

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Available on request

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## KEY RESEARCH PROJECTS SUPERVISED

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### MS Chemistry

2025	<b>Muhammad Farhan Waris</b> DFT Analysis of Alkaline Earth Metal Chlorohydrides as Energy-Harvesting Materials
2025	<b>Hafiza Nimra Zafar</b> Tailoring of DAD Type Benzothiadiazole-based Molecules to Design Organic Solar Cell Precursors
2025	<b>Kaneez Fatima</b> Computational Exploration of Indacenodithiophene-6-Cyanide Derivatives as Organic Solar Cell Precursors
2025	<b>Sadia Malik</b> Synergistic Effect of Reduced Graphene Oxide-based Composite in Hybrid Electrodes for Supercapacitor Applications
2025	<b>Sana Qaisar</b> Computational Insight into Optical and Thermoelectric Properties of Silver-based on Half-heuslers
2025	<b>Maaz Ur Rehman</b> DFT Study of Benzothiadiazole-based Non-Fullerene Acceptors for Photovoltaic Applications
2025	<b>Muhammad Zain Mehdi</b> Effect of Annealing on Electrochemical Properties of Neodymium Sulfide ( $Nd_2S_3$ )
2025	<b>Muhammad Hasnain</b> Bioaccumulation and Health-Risk Assessment of Heavy Metals in Selected Fruits and Vegetables at District Khushab
2025	<b>Romaisha Zahid</b> Computational Study of A-D-A-D-A Type Y21 Acceptor-based Organic Solar Cell Precursors
2025	<b>Ishna Saghir</b>
2025	<b>Muqaddas Ijaz</b> Computational Study of Structure and Electronic Properties of Aluminum-Doped Selenium Clusters
2025	<b>Sajida Bibi</b> Impact of Changing Hydrostatic Pressure on Thermodynamic and Thermoelectric Properties of Cerium Oxide: A DFT Study
2024	<b>Aiman Zafar</b> Computational Investigation of Gallium Decorated Boron-Nitrogen Sheets as the Single Atom Catalysts for Nitrous Oxide Reduction
2024	<b>Ayesha Zafar</b>

	Computational Study of Thermochemical Properties of p-n Doped Germanium Clusters
<b>2024</b>	<b>Muhammad Kamran Shehzad</b>
	Tailored Small Organic Molecules Designed by End-Capped Acceptors for Enhanced Photovoltaic Properties
<b>2024</b>	<b>Rabbia Hasan</b>
	Synthesis and Electrochemical Properties of ZnS-Fe <sub>2</sub> O <sub>3</sub> Nanostructures for Supercapacitor Applications
<b>2024</b>	<b>Rabia Masood</b>
	Graphene Blended TiO <sub>2</sub> Material as Anode Precursor for Lithium-Ion Batteries
<b>2024</b>	<b>Zunash Umar</b>
	Computational Study of Optical and Thermoelectric Properties of Rubidium Bromide Based Double Perovskites
<b>2024</b>	<b>Asia Chaudary</b>
	In Silico Investigation of Interaction of Hyaluronan with Bovine Serum Albumin
<b>2023</b>	<b>Sana Batool</b>
	Absolute Configuration of Neo-Clarodanes Obtained from Sand Olive ( <i>Dodonaea angustifolia</i> ): A Computational Study
<b>2023</b>	<b>Misbah Naseem</b>
	Stereochemical Investigation of Diterpenoids Extracted from Ostostegia ( <i>Ballota limbata</i> ) by Density Functional Theory Calculations
<b>2023</b>	<b>Hafiz Fazal Ur Rehman</b>
	A DFT Study of Cyclooctatetraene Stabilization Using Push-Pull and Clamping Substituents
<b>BS Chemistry</b>	
<b>2022</b>	<b>Javaria Khalid</b>
	Computational Study of Vertical Excited States of Flavonoids Having Fluorescence Potential
<b>2022</b>	<b>Marriam Batool</b>
	Computational Investigation of the Structural and Thermodynamic Properties of Silver Imidazolium-Based Cyclophane Complexes
<b>2022</b>	<b>Muhammad Kamran Shehzad</b>
	Structural and Thermodynamic Features of Indium-Zinc Heterobimetallic Complexes
<b>2022</b>	<b>Ayesha Zafar</b>
	Searching New Precursors for Defluoridation: A Computational Insight into the Interaction of Fluoride ion with Different Clusters
<b>2022</b>	<b>Zarish Nayyab Gul</b>
	Study of the Interaction energy of Carbon monoxide with Clusters