Dr. Muhammad Rouf Alvi

Assistant Professor (TTS)

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Other Information: Pakistani, Married

Currently, I am serving as an Assistant Professor (TTS) of Chemistry at University of Education Lahore, Multan Campus, since Nov. 29, 2021. After PhD, I have teaching and research experience of almost 13 Years (completed two postdocs from Xiamen University, China, and worked as an Assistant Professor at University of the Punjab, Lahore, Pakistan). I have published 19 research articles (12 as a first/corresponding author) with more than 65 impact factor in international journals. I have supervised several BS/MSc and more than 11 MS/MPhil research students.

Research & Teaching Interests:

- Activation and functionalization of the small molecules by frustrated Lewis pairs, exciting for the industrial applications.
- Machine learning approach to predict properties and applications in chemical materials
- Prediction and elucidation of the reaction mechanisms, aromaticity, and stability of organic and organometallic compounds.
- Synthesis of organic, organosilicon and organometallic compounds interesting for molecular electronics
- Teaching organic chemistry, organometallic chemistry, and techniques of organic syntheses.

Academic Qualification / Education:

• **PhD Chemistry**	Oct 2007 – Apr 2012	Department of Chemistry–BMC, Uppsala University, Sweden
• **MSc Chemistry**	Oct 2001 – Sep 2003	Institute of Chemistry, University of the Punjab, Lahore, Pakistan
• **BSc**	Sep 1998 – Aug 2001	Govt. College Bahawalnagar, Islamia University Bahawalpur, Pakistan
• **FSc (HSSC)**	Sep 1996 – Aug 1998	Government College (University) Lahore, Pakistan
• **Matric (SSC)**	Sep 1994 – Aug 1996	Government Higher Secondary School, Qabula (Pakpattan), Pakistan

Post-PhD Teaching & Research Experience:

• **Assistant Professor**	Nov 2021 – Present	Department of Chemistry, Division of Science and Technology, University of Education, Lahore, Multan Campus, Pakistan.
• **Postdoc Researcher**	Jan 2016 – May 2021	Department of Chemistry, College of Chemistry and Chemical Engineering, Xiamen University, China
• **Assistant Professor**	Sep 2012 – Dec. 2015	Institute of Chemistry, University of the Punjab, Lahore, Pakistan

Pre-PhD Experience:

• **School Teaching**	Jan 2006 – Oct 2007	Alhamd Institute of Sciences, Township, Lahore
• **R & D Chemist**	Aug 2004 – May 2005	Shafi Reso-Chem, 3-KM Bulhar Road off 22-KM Ferozepur Road, Lahore
• **Environmental Chemist**	Sep 2003 – Apr 2004	Dada Enterprises Kasure, 2-KM Ferozepur Road, Kasure
• **R & D Chemist**	Jun 2003 – Jul 2003	Qarshi Industries, Lahore

Professional Skills:

• **Instrument & Techniques**	Modern synthetic and structure analysis tools, such as NMR, GC-MS, IR, UV-Vis, Glove Box, Schlenk techniques etc.
• **Computational Chemistry Software/Program**	Gaussian, Amsterdam Density Functional (ADF) Modeling Suite, Multi Wavefunction (Multiwfn) program, Spartan (Chemistry) Software, Molcas (ab initio Quantum Chemistry) Software, Natural Bond Orbital (NBO) Program, EDDB and AIMAll (Atoms in Molecules) Software

Research Summary (Research Projects):

❖ **Since 2016**

Theoretical investigation of the main group and organometallic compounds.

- Designing unprecedented approaches to activate small molecules; such as N_2, CO_2, CO, NO and H_2, for industrially value-added products.
- Prediction and elucidation of the reaction mechanisms, aromaticity, and stability of organic and organometallic compounds.
- Probing general rules and discerning the origin of thermodynamic stabilities of main-group aliphatic

and aromatic polyenes.

- Tuning aromaticity and antiaromaticity of the main-group compounds and organometallics in the singlet and triplet electronic states.
- Understanding mechanistic details of the challenging reactions.

❖ **2012–2015 (As an Assistant Professor)**

- Theoretical investigation of silenes and silaaromatics.

❖ **2007–2012 (As a PhD student)**

- Synthesis of low-coordinated organosilicon and organogermanium compounds, such as, silenes, silenolates and germenolates.
- Experimental development of a new acid catalyzed protocol for the hypersilyl protection of a wide range of functionalized alcohols, thiols and carboxylic acids.
- Theoretical study of silenes and silaaromatics (with switching properties for molecular electronics).

Publications:

Articles (with ISI Web of Science Impact Factor)

Total IF = 65.2

1st/Corr. = 41.7

1 **Alvi Muhammad Rouf**,* Alvi Muhammad Rouf,* Muhammad Aamir, Faiza Sharif, Nafeesa Akbar, Seerat Zahra, “Potential Formation of Antiaromatic Silolosiloles (Disilapentalenes) from Their Saturated Diketosilolosilole Precursors via a [1,3]-Si → O Sigmatropic Shift,” *Organometallics* **2025**, *44*, 2410. IF = 2.9.

2 Khadijah Mohammedsaleh Katubi, **Alvi Muhammad Rouf**,* Bilal Siddique, Muhammad Faizan Nazar,* Ghulam Jillani Ansari, Z.A. Alrowaili, M.S. Al-Buriahi, “Machine learning-assisted chemical space generation of small molecule organic semiconductors for efficient photodetectors,” *Computational Materials Science* **2024**, *241*, 113037. IF = 3.3.

3 Ali Raza, Zaka Ullah,* Adnan Khalil, Rashida Batool, Sajjad Haider, Kamran Alam, Nazmina Imrose Sonil, **Alvi Muhammad Rouf**, Muhammad Faizan Nazar,* “Facile fabrication of a graphene-based chemical sensor with ultrasensitivity for nitrobenzene,” *RSC Advances* **2024**, *14*, 9799-9804. IF = 4.6.

4 Fatimah Mohammed A. Alzahrani, **Alvi Muhammad Rouf**,* Jawayria Najeeb, Sumaira Naeem, Bilal Siddique, Muhammad Faizan Nazar, Z.A. Alrowaili, Imed Boukhris, M.S. Al-Buriahi, "Computational design of new polymers having low exciton binding energy for organic solar cells fabrication: Chemical generation and visualization," *Journal of Photochemistry & Photobiology, A: Chemistry* **2024**, *450*, 115457(1-13). IF = 4.7.

5 **Alvi Muhammad Rouf**,* Jun Zhu* “An unprecedented route to achieve persistent 1*H*-azirine,” *Physical Chemistry Chemical Physics* **2023**,*25*, 18, 12602–12606. IF = 2.9.

6 Feiying You, Jie Zeng, **Alvi Muhammad Rouf**, Shisheng Dong, Jun Zhu* Theoretical Study on Reaction Mechanisms of Dinitrogen Activation and Coupling by Carbene-Stabilized Borylenes in Comparison with Intramolecular C–H Bond Activation, *Chemistry – An Asian Journal* **2022**, *17*, 22, e202200232. IF = 3.3.

7 **Alvi Muhammad Rouf**, Yuanyuan Huang, Shicheng Dong, Jun Zhu* "Systematic Design of Frustrated Lewis Pair Containing Methyleneborane and Carbene for Dinitrogen Activation," *Inorganic Chemistry* **2021**, *60*, 5598-5606. IF = 4.7.

8 **Alvi Muhammad Rouf**, Chenshu Dai, Shicheng Dong, Jun Zhu* "Screening Borane Species for Dinitrogen Activation," *Inorganic Chemistry* **2020**, *59*, 11770–11781. IF = 4.7.

9 Jiashun Wu, **Alvi Muhammad Rouf**, Yuanyuan Huang, Danling Zhuang, Jun Zhu* "Theoretical Study on the Stability and Aromaticity in Silapentafulvenes towards Triplet Ground State Species," *Physical Chemistry Chemical Physics* **2020**, *22*, 4668**–**4676. IF = 3.3.

10 **Alvi Muhammad Rouf**, Chenshu Dai, Fangzhou Xu, Jun Zhu* "Dinitrogen Activation by Tricoordinated Boron Species: A Systematic Design," *Advanced Theory and Simulations* **2020**, *3*, 1900205(1–7). IF = 2.9.

11 **Alvi Muhammad Rouf**,* Sajid Iqbal, Anam Ejaz "Chalcogenborines and Derivatives: Probing the Origin of Relative Thermodynamic Stabilities," *ChemistrySelect* **2020**, *5*, 83**–**90. IF = 2.0.

12 Lu Lin, Qin Zhu, **Alvi Muhammad Rouf**, Jun Zhu* "Probing the Aromaticity and Stability of Metallatricycles by DFT Calculations: Towards Clar Structure in Organometallic Chemistry," *Organometallics* **2020**, *39*, 80**–**86. IF = 2.9.

13 Danling Zhuang, **Alvi Muhammad Rouf**, Yuanyuan Li, Chenshu Dai, Jun Zhu* "Aromaticity-promoted CO_2 Capture by P/N-Based Frustrated Lewis Pairs: A Theoretical Study," *Chemistry – An Asian Journal* **2020**, *15*, 266**–**272. IF = 3.3.

14 Qin Zhu, Lu Lin, **Alvi Muhammad Rouf**, Jun Zhu* "Reaction Mechanisms on Unusual 1,2-Migrations of *N*-Heterocyclic Carbene-Ligated Transition Metal Complexes," *Chemistry – An Asian Journal* **2019**, *14*, 3313**–**3319. IF = 3.3.

15 **Alvi Muhammad Rouf**, Jingjing Wu, Jun Zhu* "Probing a General Rule Towards Thermodynamic Stabilities of Mono BN-doped Lower Polyenes", *Chemistry – An Asian Journal* **2017**, *12*, 605–614. IF = 4.1.

16 **Alvi Muhammad Rouf*** Muhammad Imran Abdullah, Munawar Ali Munawar, Sajid Iqbal, Azeem Intisar, "Structure, stability and aromaticity of 2,4,6,1,3,5-trisilatriphosphabenzene versus 2,4,6-trisilatriazine: A quantum chemical approach", *Computational and Theoretical Chemistry* **2015**, *1065*, 18–26. IF = 2.8.

17 Henrik Löfås, Andreas Orthaber, Burkhard O. Jahn, **Alvi M. Rouf**, Anton Grigoriev* Sasha Ott, Rajeeve Ahuja, Henrik Ottosson* "A New Class of Molecular Conductance Switches Based on the [1,3]-Silyl Migration from Silanes to Silenes", *Journal of Physical Chemisry C* **2013**, *117*, 10909–

10918. IF = 3.2.

18 **Alvi Muhammad Rouf**, Burkhard O. Jahn, Henrik Ottosson* "Computational Investigation of Brook-type Silabenzenes and Their Possible Formation through [1,3]-Si→O Silyl Shifts", *Organometallics* **2013**, *32*, 16–28. IF = 2.9.

19 **Alvi Muhammad Rouf**, Henrik Ottosson* "Silaphenolates and Silaphenylthiolates: Two Unexplored Unsaturated Silicon Compound Classes Influenced by Aromaticity", *Molecules* **2012**, *17*, 369–389. IF = 4.6.

Book Chapter

H. Ottosson, **A. M. Rouf**, "4.4.2.5. Silenes (Update 1, 2011)" *Science of Synthesis, Knowledge Updates* **2011/3**, pp. 37–46. Georg Thieme Verlag KG, Stuttgart, Germany.

PhD Thesis

"Low-coordinate Organosilicon Chemistry: Fundamentals, Excursions Outside the Field, and Potential Applications", *Interfaculty Units, Acta Universitatis Upsaliensis,* **2012**. urn:nbn:se:uu:diva-169796.

References:

- **Professor Jun Zhu:** State Key Laboratory of physical chemistry of solid surfaces, Department of Chemistry, College of Chemistry and Chemical Engineering, Xiamen University, China. E-mail: jun.zhu@xmu.edu.cn

- **Associate Professor Henrik Ottosson:** Department of Chemistry – Ångström Laboratory, Uppsala University, Box 523, 75120 Uppsala, Sweden. E-mail: henrik.ottosson@kemi.uu.se