Dr. Beenish Bashir

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Education:

- **Ph.D: Xinjiang Technical Institute of Physics & Chemistry, University of Chinese Academy of Sciences**

  Influence of Fluorine on Electronic Structures and Nonlinear Optical Effects of A Series of Borate Crystals 2014-2018

- **Masters: University of Sargodha, Pakistan**

  A Theoretical Study of Two-Dimensional Second-Order Non-Linear Optical Properties of Terpyridine Substituted Hexamolybdates 2010-2013

Professional Skills:

Expertise in Density Functional Theory (DFT)

VASP, CASTEP, GAUSSIAN-09w, DIAMOND, ChemDraw, ADF

Work Experience:

- **Current Job: Postdoc researcher** 06-15-2022-to date

  Department of Chemistry & Biochemistry, George Mason University (Fairfax Campus)

  Topic: Properties of Porphyrins using Computational Chemistry

- **Research Scholar** 2021-2022

  Materials Science and Engineering, Southern University of Science and Technology, Shenzhen, China

  Topic: Promoting Nitrogen Electroreduction to Ammonia by Non-Noble Metal Single-Atom Catalysts

- **Postdoc: Department of Chemistry, Tsinghua University, China** 2018-2020

  Topic: Computational Investigation on the Catalytic Mechanism and Bonding Analysis of Single Atom Catalyst

Research Interests:

- Electronic structure calculations for understanding the catalytic mechanism and kinetics of functional materials
- Electrochemical nitrogen reduction reaction (eNRR) performance of single atom catalysis (SACs)
- Exploring the structure-to-property correlation in transition metal SACs

- Surface properties of catalyst surface, including the structural, energetic, electronic properties, and chemical reactivity
- 2D Dye-sensitized solar cell materials
- Exploring structural properties and bandgap engineering of Nonlinear optical (NLO) materials and rare earth metal borates

Research Contributions:

- Exploring the stability, geometries, electronic structures, and catalytic mechanism of direct benzene oxidation to phenol over phosphomolybdic acid cluster-based metal single-atom catalyst (SAC)
- Modelling of functional, 2D polyoxometalate (POM) based terpyridine-substituted compounds
- Functionality of d^{10} cations (Zn, Cd) consolidated with fluorine (F^{-}) anions
- Explored the chemical nature of F^{-} and OH^{-} anions in borates under different metal cations

Publications:

1. **B. Bashir**, S. H. Talib, H. Xiao, and J. Li. A Comparative Theoretical Investigation on the Mechanism of Direct Benzene Oxidation to Phenol Over Fe-PMA Cluster. (To be submitted)
2. H. H. Yang, **B. Bashir**, and G. Luo. Metal Phthalocyanine Catalysts for Electrochemical Oxygen Reduction. (To be submitted)
3. **B. Bashir**, B. B. Zhang, S. L. Pan, and Z. H. Yang. Combination d^{10}-cations and fluorine anion as active participants to design novel borate/carbonate nonlinear optical materials. *J. Alloys Compd*. 2018, ***758***, 85–90.
4. **B. Bashir**, B. B. Zhang, M.-H. Lee, S. L. Pan, and Z. H. Yang. DFT-Based Comparative Study about the Influence of Fluorine and Hydroxyl Anions on Opto-Electric Properties of Borate Crystals: Choice for Better Anion. *Inorg. Chem*. 2017, ***56***, 5636–5645.
5. **B. Bashir**, B. B. Zhang, B.-H. Lei, Z. H. Yang, M.-H. Lee, and S. L. Pan. DFT Based Theoretical Study about the Contributions of Fluorine to Nonlinear Optical Properties in Borate Fluoride Crystals. *Cryst. Growth Des*. 2016, ***16***, 5067–5073.
6. S. H. Talib, Z. S. Lu, X. Yu, K. Ahmad, **B. Bashir**, Z. X. Yang, Jun Li. Theoretical Inspection of M_1-PMA Single-Atom Electrocatalyst: Ultra-High Performance for Water Splitting (HER/OER) and Oxygen Reduction Reactions (OER). *ACS Catal*. 2021, ***11***, 8929-8941.
7. S. H. Talib, Z. S. Lu, **B. Bashir**, S. Hussain, K. Ahmad, S. U. D. Khan, S. Haider, Z. Yang, K. Hermansson, J. Li. CO oxidation on MXene (Mo_2CS_2) supported single-atom catalyst: a termolecular Eley-Rideal mechanism, *Chin. Chem. Lett*. 2022, https://doi.org/10.1016/j.cclet.2022.04.010.
8. S. H. Talib, S. Baskaran, X. Yu, Q. Yu, **B. Bashir**, S. Muhammad, S. Hussain, X. Chen, J. Li. Non-noble metal single-atom catalyst of Co_1/MXene (Mo_2CS_2) for CO oxidation. *Sci. China Mater*. 2020, ***64***, 651-663.
9. N. Mushtaq, G. Chen, Q. Wang, **B. Bashir**, L. R. Sidra, X.-Z. Fang. Synthesis of polyamide-imides with different monomer sequence and its effect on transparency and thermal properties. *Polymer*, 2020, ***190***, 122218.
10. N. Gogoi, **B. Bashir**, P-C. Ma. Z. H. Yang. Supramolecular assembly of leaf-like fluorescent tetraphenylethylene through polymer-directd inter-locking. *Compos. Commun*. 2019, ***11***, 45–51.

11. T. Baiheti, S. J. Han, **B. Bashi**r, Z. H. Yang, H. H. Yu, S. L. Pan. Four new deep ultraviolet borates with isolated $B_{12}O_{24}$ groups: Synthesis, structure, and optical properties. *J. Solid State Chem*. 2019, ***273***, 112–116.
12. L. R. Sidra, G. Chen, N. Mushtaq, M. Kai, **B. Bashir**, X.-Z. Fang. Processable poly (benzoxazole imide)s derived from asymmetric benzoxazole diamines containing 4-phenoxy aniline: Synthesis, properties and isomeric effect. *Polym. Chem*. 2018, ***9***, 2785-2796.
13. S. Sambasivam, L. Liu, Y. Yang, G. Han, **B. Bashir**, Z. H. Yang, and S. L. Pan. Syntheses, crystal structures and characterization of three alkaline metal borates. *CrystEngComm*. 2017, ***19***, 2561–2569.
14. M. R. S. A. Janjua, M. Amin, M. Ali, **B. Bashir**, M. U. Khan, M. A. Iqbal, W. Guan, L. K. Yan, Z. M. Su. A DFT Study on the Two-Dimensional (2-D) Second-Order Nonlinear Optical (NLO) Response of Terpyridine-Substituted Hexamolybdates: Physical Insight of 2-D Inorganic-Organic Hybrid Functional Materials. *Eur. J. Inorg. Chem*. 2012, ***4***, 705–711.
15. M. R. S. A. Janjua, M. U. Khan, **B. Bashir**, M. A. Iqbal, Y. Song, S. A. R. Naqvi, Z. A. Khan. Effect of π-conjugation Spacer (-C≡C-) on the First Hyperpolarizabilities of Polymeric Chain Containing Polyoxometalate Cluster as a Side-Chain Pendant: A DFT Study. *Comput. Theoret. Chem*. 2012, ***994***, 34–40.

Key Conferences:

1. **B. Bashir**, Z. H. Yang, M.-H. Lee, and S. L. Pan. A DFT approach towards the role of luorine as NLO active participant in borate fluoride crystals. The **2016** National Symposium on Optical Materials. (***Poster***)
2. **B. Bashir**, M. R. S. A. Janjua, M. Amin, M. Ali, M. U. Khan, M. A. Iqbal, W. Guan, L. K. Yan, Z. M. Su, "A DFT Study on the Two-Dimensional (2-D) Second-Order Nonlinear Optical (NLO) Response of Terpyridine-Substituted Hexamolybdates: Physical Insight of 2-D Inorganic-Organic Hybrid Functional Materials. 10th International and 22nd National Chemistry Conference **2011**. (***Poster***)

References:

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