IACS Building, Stony Brook University, NY 11794.
+1 (631) 632 2340
arshad.mehmood@stonybrook.edu
arshadmehmood118.github.io

Arshad Mehmood, Ph.D.

Highlights

• Outstanding Ph.D. Dissertation Award • Three years of university-level teaching experience • Mentored 9 undergrad, 3 Master's, 5 REU and 4 Ph.D. students • Secured 150K GPU hours on NREL HPC systems • Extensive experience with HPC clusters • h-index: 10

Current Position

May. 2024 **Senior Research Scientist**, *Stony Brook University*, DoIT and Institute for Advanced Computational Science (IACS), Stony Brook, NY.

I conduct independent and collaborative research, support faculty and students with HPC applications, and contribute to grants and publications. I provide scientific user support, develop training materials, and lead workshops. My independent research includes mentoring undergraduates in simulating electronically excited molecules and quantum dots, studying non-adiabatic dynamics, developing and efficient implementation of electronic structure visualization tools on high-performance computer hardware.

Education

Dec. 2020 **Ph.D. Chemistry**, *Texas Christian University*, Department of Chemistry, Fort Worth, TX.

Thesis: A Computational Toolkit to Understand Orbital Overlap and Chemical Reactivity

Advisor: Prof. Benjamin G. Janesko

Dec. 2011 **M.Phil. Physical Chemistry**, *Islamia University Bahawalpur*, Pakistan.

Thesis: Development of Ion Selective Electrode Based on Lambda Cyfluthrin

Sep. 2009 **M.Sc. Physical Chemistry**, *Islamia University Bahawalpur*, Pakistan.

Aug. 2007 **B.Sc. Chemistry, Mathematics, Physics**, *Islamia University Bahawalpur*, Pakistan.

Research Experience

2021–2024 **Postdoctoral Associate**, *Stony Brook University*, IACS, Stony Brook, NY.

Advisor: Prof. Benjamin G. Levine

First-principles Simulations of Ultrafast Spectroscopy Observables

I applied *ab-initio* non-adiabatic molecular dynamics simulations and GPU-accelerated Time-dependent Complete Active Space Configuration Interaction methods to simulate the excited state dynamics and time-resolved ultrafast spectrum of prototypical organic molecules.

Partner with the NSF Center for Adapting Flaws into Features (CAFF)

I employ electronic structure methods to investigate the role of defects in materials and advance collaborative scientific approaches to harness the unique properties of these defects. The projects include modeling defect-driven photochemistry in carbon dots, quantifying hot-electron transfer efficiency in AuNR@TiO_2 core-shell heterostructures, and analyzing electronic coupling interactions between organic dyes and quantum dots interfaces.

2015–2020 **Doctoral Researcher**, *Texas Christian University*, Fort Worth, TX.

A Computational Toolkit to Understand Orbital Overlap and Chemical Reactivity

The major Ph.D. project involved the development, implementation, and applications of the Orbital Overlap Range Function, EDR($\mathbf{r}$;d), and derived descriptors Orbital Overlap Distance, D($\mathbf{r}$), and Atomic-averaged Overlap Distance, D_A. Implemented these tools to Multiwfn package and developed a FORTRAN based open-source program to compute these descriptors. Applied these tools to quantify the reactivities of molecular surfaces, nanoclusters, solvent softness-hardness, protein-ligand interactions, drug-development and bond stretching.

Quantum Crystallography and Theoretical Modeling of Crystal Structures

This work focuses on the modeling of crystal structures and the integration of theoretical and experimental high-resolution charge density analysis for small molecules, drug structures, organometallics, and cocrystals utilizing single crystal X-ray diffraction. The investigation primarily entails identifying the topological characteristics of charge density, as well as quantifying electrostatic interaction energies and non-covalent interactions through the application of diverse theoretical methodologies.

2009–2011 **M.Phil. Researcher**, *Islamia University Bahawalpur*, Pakistan.

Development of Ion Selective Electrode Based on Lambda Cyfluthrin

The M.Phil. research project was focused on the development, characterization, and applications of novel ion-selective electrodes based on Cyfluthrins for the determination of chloride ions concentrations in aqueous pharmaceutical samples.

2008–2009 **M.Sc. Researcher**, *Islamia University Bahawalpur*, Pakistan.

Development of All-solid-state H^+ Ion-selective Electrodes

Worked on the synthesis of Polyaniline and its applications for the development of a pH electrode to determine H^+ ions concentrations in aqueous solutions.

Teaching Experience

2015–2016 **Teaching Assistant**, *Texas Christian University*, Department of Chemistry, Fort Worth.

TA for GenChem (30 students), PChem-I (12 students) and PChem-II (7 students).

2012–2015 **Lecturer of Chemistry**, *GC University Lahore*, Pakistan.

Taught undergraduate courses in PChem-I, PChem-II, Solid State Chemistry, Rotational and Vibrational Spectroscopy for classes of more than 50 students and a master's level course on Advanced Chemical Kinetics for a class of 24 students.

2009–2010 **Lecturer of Chemistry (visiting)**, *Islamia University Bahawalpur*, Pakistan.

Taught PChem-I and PChem-II courses for classes of more than 50 students.

Awards and Honors

Aug. 2023 **NVIDIA GPU Award for Best GPU Poster (Finalist)**, *ACS COMP Division*, ACS Fall 2023 Meeting, San Francisco, CA.

Dec. 2020 **Outstanding Ph.D. Dissertation Award**, *College of Science & Engineering*, Texas Christian University, Fort Worth, TX.

July 2018 **TCU GSRF Travel Award**, *Computational Chemistry Gordon Research Conference*, July 22-27, 2018, Mount Snow, West Dover, VT.

Apr. 2018 **Best Oral Presentation Award**, *51st Annual Meeting-in-Miniature of American Chemical Society Dallas-Fort Worth Section*, April 21, 2018, Dallas, TX.

Mar. 2018 **Wiley Best Poster Award**, *27th Austin Symposium on Molecular Structure and Dynamics at Dallas*, March 3-5, 2018, Dallas, TX.

July 2016 **American Crystallographic Association Travel Award**, *66th Annual Meeting of American Crystallographic Association (ACA)*, July 22–26, 2016, Denver, CO.

Dec. 2014 **Best Teacher Award 2014**, *Department of Chemistry, GC University Lahore*, Pakistan.

Leadership & Outreach

Apr. 2017 **Organizer**, *50th Annual Meeting-in-Miniature of American Chemical Society Dallas-Fort Worth Section*, April 29, 2017, Fort Worth, TX, USA.

Oct. 2016 **Volunteer**, *Chemistry Connections 2016*, October 14, 2016, Fort Worth Museum of Science and History, Fort Worth, TX.

July 2016 **Invited Chair of the General Interest II Session**, *66th Annual Meeting of American Crystallographic Association (ACA)*, July 22–26, 2016, Denver, CO.

Apr. 2014 **Organizer**, *1st International Conference on Forensic Science and Justice*, October 21–24, 2014, GC University Lahore, Pakistan.

Selected Publications

Google Scholar Total citations: 307 Citations since 2022: 262 h-index: 10

* *indicates corresponding author*

[34] Bian, Z.; Gomez, E.; Gruebele, M.; Levine, B. G.; Link, S.; Mehmood, A.; Nie, S. Bottom-up carbon dots: purification, single-particle dynamics, and electronic structure. *Chem. Sci.* **2025**, *Advance Article*, DOI: 10.1039/D4SC05843G.

[33] Mehmood*, A.; Janesko, B. G., An orbital-overlap complement to σ-hole electrostatic potentials. *PCCP*. **2025**, *27* (2), 861-867.

[32] Stamm, J.; Priyadarsini, S. S.; Sandhu, S.; Chakraborty, A.; Shen, J.; Kwon, S.; Sandhu, J.; Wicka, C.; Mehmood, A.; Levine, B. G.; et al. Factors governing H_3^+ formation from methyl halogens and pseudohalogens. *Nat. Commun.*. **2025**, *16* (1), 410.

[31] Ibele, L. M.; Mehmood, A.; Levine, B. G.; Avagliano, D. Ab Initio Multiple Spawning Nonadiabatic Dynamics with Different CASPT2 Flavors: A Fully Open-Source PySpawn/OpenMolcas Interface.. *J. Chem. Theory Comput.* **2024**, *20*(18), 8140-8151.

[30] Mehmood, A.; Silfies, M. C.; Durden, A.; Allison, T. K.; Levine, B. G. Simulating ultrafast transient absorption spectra from first principles using a time-dependent configuration interaction probe. *J. Chem. Phys.* **2024**, *161*, 044107.

[29] Ostovar, B.; Lee, S. A.; Mehmood, A.; Farrell, K.; Searles, E. K.; Bourgeois, B.; Chiang, W.; Misiura, A.; Niklas Gross, N.; Al-Zubeidi A.; Dione, J. A.; Landes, C. F.; Zanni, M.; Levine, B. G.; Link, S. The role of the plasmon in interfacial charge transfer. *Science Advances* **2024**, *10* (27), eadp3353.

[28] Kulikov, O. A.; Mehmood, A.; Vodzinsky, S. Supramolecular blends of C-alkylpyrogallol[4]arenes and polytetrahydrofurans. *Results in Chemistry* **2024**, *11*, 101804.

[27] Hernández, H. M.; Ohtsuka, S.; Mehmood, A.; Bordenca, J.; Wen, W.; Levine, B. G.; Johnson, C. J. Resonance Effects from Substituents on L-Type Ligands Mediate Synthetic Control of Gold Nanocluster Frontier Orbital Energies. *J. Phys. Chem. Lett* **2024**, *15* (40), 10244-10251.

[26] Sowa, J. K.; Cadena, D. M.; Mehmood, A.; Levine, B. G.; Roberts, S. T.; Rossky, P. J. IR Spectroscopy of Carboxylate-Passivated Semiconducting Nanocrystals: Simulation and Experiment. *J. Phys. Chem. C* **2024**, *128* (21), 8724-8731.

[25] Bian, Z.; Wallum, A.; Mehmood, A.; Gomez, E.; Wang, Z.; Pandit, S.; Nie, S.; Link, S.; Levine, B. G.; Gruebele, M. Properties of carbon dots versus small molecules from 'bottom-up' synthesis. *ACS Nano* **2023**, *17* (22), 22788-22799.

[24] Silfies, M. C.; Mehmood, A.; Kowzan, G.; Hohenstein, E. G.; Levine, B. G.; Allison, T. K. Ultrafast internal conversion and photochromism in gas-phase salicylideneaniline. *J. Chem. Phys.* **2023**, *159*, 104304.

[23] Khanam, H.; Mehmood*, A.; Ahmed, A.; Noureen, S.; In the pursuit of a 'disappearing solvatomorph' of antipyrine-dipicolinic acid (ANT-DPA) co-crystal: explained through relative stability and charge density analyses. *CrystEngComm* **2023**, *25*, 6478-6488.

[22] Iqbal, I.; Mehmood, A.; Noureen, S.; Lecomte , C.; Ahmed, A.; Crystal engineering, electron density analysis, and in situ variable temperature studies on co-crystal between nicotinic acid and gallic acid sesquihydrate. *CrystEngComm* **2023**, *25*, 770-784.

[21] Bilal, A.; Mehmood, A.; Noureen, S.; Lecomte , C.; Ahmed, A.; Crystal engineering of a co-crystal of antipyrine and 2-chlorobenzoic acid: relative energetic contributions based on multipolar refinement. *CrystEngComm* **2022**, *24*, 7758-7770.

[20] Kulikov, O. V.; Mehmood, A.; Sevryugina, Y. V., Polymerizable Channel-like Stacks Derived from Cyclic Tetrameric Diacetylenes. *Results in Materials* **2022**, *13*, 100262.

[19] Akram, S.; Mehmood, A.; Noureen, S.; Lecomte , C.; Ahmed, A.; Thermal-induced Transformation of Glutamic Acid to Pyroglutamic Acid and Self-cocrystallization: A Charge–Density Analysis. *Acta. Cryst. C.* **2022**, *78*, 72-80.

[18] Iqbal, A.; Mehmood, A.; Noureen, S.; Ahmed, A.; Crystal Engineering of Co-crystal of Nicotinic Acid and Pyrogallol: An Experimental and Theoretical Electron Density Analysis. *Acta. Cryst. B.* **2021**, *77*, 1035-1047.

[17] Enciso, A. E.; Lorandi, F.; Mehmood, A.; Fantin, M.; Szczepaniak, G.; Janesko, B. J.; Matyjaszewski, K.; p-Substituted Tris(2-pyridylmethyl)amines as Ligands for Highly Active ATRP Catalysts: Facile Synthesis and Characterization. *Angew. Chem. Int. Ed.* **2020**, *59*,14910-14920.

[16] Mehmood*, A.; Janesko, B. G., Extending the Marcus μ-Scale of Solvent Softness Using Conceptual Density Functional Theory and the Orbital Overlap Distance: Method and Application to Ionic Liquids. *J. Solution Chem* **2020**, *49*, 614–628.

[15] Mehmood, A.; Fahim, A.; Ahmed, M.; Noureen, S., Regioselectivity of Reduction of Nitro Groups in 3, 5-dinitrosalicylic Acid Monohydrate Explored by Experimental and Theoretical Charge Density Analysis. *J. Mol. Struct* **2020**, *1216* (4), 128483.

[14] Hasil, A.; Mehmood, A.; Noureen, S.; Ahmed, M., Experimental and Theoretical Charge Density Analysis of Skin Whitening Agent Kojic Acid. *J. Mol. Struct* **2020**, *1216* (4), 128295.

[13] Sharma, V.; Mehmood, A.; Janesko, B. G.; Simanek, E. E., Efficient Syntheses of Macrocycles Ranging from 22–28 Atoms Through Spontaneous Dimerization to Yield bis-hydrazones. *RSC Adv.* **2020**, *10* (6), 3217-3220.

[12] Faroque, M. U.; Mehmood, A.; Noureen, S.; Ahmed, M., Crystal Engineering and Electrostatic Properties of Co-crystals of Pyrimethamine with Benzoic Acid and Gallic Acid. *J. Mol. Struct.* **2020**, 128183.

[11] Sharma, V.; Mehmood, A.; Janesko, B. G.; Simanek, E. E., A Hydrogen Bond and Strong Electron Withdrawing Group Lead to the Formation of Surprisingly Stable, Cyclic Hemiaminals. *Tetrahedron Lett.* **2019**, 151334.

[10] Hasil, A.; Mehmood, A.; Ahmed, M., Experimental and Theoretical Charge-Density Analysis of Hippuric Acid: Insight Into its Binding with Human Serum Albumin. *Acta Cryst. B* **2019**, *75* (4), 750-762.

[9] Yepremyan, A.; Mehmood, A.; Asgari, P.; Janesko, B. G.; Simanek, E. E., Synthesis of Macrocycles Derived from Substituted Triazines. *ChemBioChem* **2019**, *20* (2), 241-246.

[8] Mehmood, A.; Jones, S. I.; Tao, P.; Janesko, B. G., An Orbital-Overlap Complement to Ligand and Binding Site Electrostatic Potential Maps. *J. Chem. Inf. Model.* **2018**, *58* (9), 1836-1846.

[7] Mehmood*, A.; Janesko, B. G., Predicting Ion Mobility Collision Cross Sections Directly from Standard Quantum Chemistry Software. *J. Mass Spectrom.* **2018**, *53* (5), 432-434.

[6] Yepremyan, A.; Mehmood, A.; Brewer, S. M.; Barnett, M. M.; Janesko, B. G.; Akkaraju, G.; Simanek, E. E.; Green, K. N., A New Triazine Bearing a Pyrazolone Group Capable of Copper, Nickel, and Zinc Chelation. *RSC Adv.* **2018**, *8* (6), 3024-3035.

[5] Mehmood, A.; Janesko, B. G., An Orbital-Overlap Complement to Atomic Partial Charge. *Angew. Chem. Int. Ed.* **2017**, *56* (24), 6878-6881.

[4] Kulikov, O. V.; Sevryugina, Y. V.; Mehmood, A.; Saraogi, I., Characterization of Aggregated Morphologies Derived from Mono- and Bis-arylbenzamides – Potential Alpha-helix Mimetics. *New J. Chem.* **2017**, *41* (15), 7417-7423.

[3] Mehmood*, A.; Janesko, B. G., The Electron Delocalization Range in Stretched Bonds. *Int. J. Quantum Chem* **2016**, *116* (23), 1783-1795.

[2] Mehmood*, A.; Bano, S.; Fahim, A.; Parveen, R.; Khurshid, S., Efficient Removal of Crystal Violet and Eosin B from Aqueous Solution Using Syzygium Cumini Leaves: A Comparative Study of Acidic and Basic Dyes on a Single Adsorbent. *Korean J. Chem. Eng.* **2015**, *32* (5), 882-895.

[1] Khurshid, S.; Kausar, S.; Afzal, S.; Adnan, A.; Mehmood, A.; Arshad, M.; Bukhari, Z. A., Adsorption Study of Nymphaea Alba for the Removal of Manganese from Industrial Waste Water. *Int. J. Phys. Sci.* **2013**, *8* (45), 2057-2062.

Oral Presentations

[7] Mehmood, A., Deciphering the Hidden Dance of Excited State Processes: How the Simulated Ultrafast Signals Complement the Experiment. ACS Spring Meeting, March 17-21, **2024**, New Orleans, LA.

[6] Mehmood, A., Painting with Light: A Journey of Interpretation. SBU Postdoc Spotlight, November 16th, **2023**, Stony Brook, NY.

[5] Mehmood, A., Deciphering the Hidden Dance of Excited State Processes: How Simulated Ultrafast Signals Complement the Experiment. SBU-BNL Photochemistry Symposium, November 1st, **2023**, Stony Brook, NY.

[4] Mehmood, A.; Levine, B. G., First-principles Simulations of Transient Absorption Spectrum to Probe the Ultrafast Proton Transfer Dynamics. ACS Spring Meeting, March 20-24, **2022**, San Diego, CA.

[3] Mehmood, A.; Janesko, B. G., An Orbital-Overlap Complement to Atomic Partial Charge. 51st Annual Meeting-in-Miniature of American Chemical Society Dallas-Fort Worth Section, April 21, **2018**, Dallas, TX.

[2] Mehmood, A.; Janesko, B. G.; Sevryugina, Y., Experimental and Theoretical Charge Density Analysis of 1-(2,3-Dichlorophenyl)piperazinium chloride, 66th Annual Meeting of American Crystallographic Association (ACA), July 22–26, **2016**, Denver, CO.

[1] Mehmood, A.; Janesko, B. G., Quantifying Electron Delocalization in Stretched Bonds. American Chemical Society 71st South Western/67th South Eastern Regional Meeting, November 4-7, **2015**, Memphis, TN.

Poster Presentations

[7] Mehmood, A.; Levine, B. G., Simulations of Ultrafast Spectroscopy Observables Using the GPU-accelerated Time-dependent Complete Active Space Configuration Interaction Method. ACS Fall Meeting, August 13-17, **2023**, San Francisco, CA. (Finalist for NVIDIA GPU Award)

[6] Mehmood, A.; Levine, B. G., First-principles Simulations of Transient Absorption Spectrum. American Conference on Theoretical Chemistry, July 25-28, **2022**, Tahoe City, CA.

[5] Mehmood, A.; Janesko, B. G., An Orbital-overlap Scale for Solvent Hardness and Softness. The Michael and Sally McCracken Annual Student Research Symposium, April 12, **2019**, Fort Worth, TX.

[4] Mehmood, A.; Janesko, B. G., An Orbital-Overlap Complement to Atomic Partial Charge. Computational Chemistry Gordon Research Conference, July 22-27, **2018**, Mount Snow, West Dover, VT.

[3] Mehmood, A.; Janesko, B. G., An Orbital-Overlap Complement to Atomic Partial Charge. The Michael and Sally McCracken Annual Student Research Symposium, April 20, **2018**, Fort Worth, TX.

[2] Mehmood, A.; Janesko, B. G., An Orbital-Overlap Complement to Atomic Partial Charge. 27th Austin Symposium on Molecular Structure and Dynamics at Dallas, March 3-5, **2018**, Dallas, TX.

[1] Mehmood, A.; Janesko, B. G., Quantifying Electron Delocalization in Stretched Bonds. 26th Austin Symposium on Molecular Structure and Dynamics at Dallas, March 5-7, **2016**, Dallas, TX.

Research Mentoring Experience

NSF REU Students

2021-Present *Stony Brook University*: Kevin Torres (Ph.D. student, NYU), Trevor D. Lata (Researcher U. Arizona), Michael J. Rivera (U. Puerto Rico), Peter Scully (Tufts U.) and Ubaidullah S. Hassan (The Cooper Union).

Undergraduate Students

2021-Present *Stony Brook University*: Pen Chang (Ph.D. student, Yale), Zain Zaidi (Stony Brook U.) and Nikita Basok (Stony Brook U.).

2018-2019 *Texas Christian University*: Alexandra Blitch (Advantis Global)

2013-2015 *GC University Lahore*: Sheher Bano (Teacher), Fatima Akbar (Teacher), Jamal Afzal (Postdoc Shandong U.), Mamoona Anwar (Teacher) and Saima Amin

M.S. Students

2023-Present *Stony Brook University*: Satoshi Ohtsuka

2013-2015 *GC University Lahore*: Abbas Ali and Shahid Majeed (Assis. Professor)

Ph.D. Students

2022-Present *Stony Brook University*: Eric Marants, Ari Pereira, Andrew Nicoll and Ying You.

Professional Society Memberships

2016–Present American Chemical Society (ACS)

2019–Present American Physical Society (APS)

2016–Present American Crystallographic Association (ACA)

Grants

Jan. 2025 **Allocation Proposal NREL Kestrel**, *Theoretical Insights into Fluorescence and Non-Radiative Mechanisms in Carbon Dots*, Approved with 150,000 GPU hours allocation.

Aug. 2023 **Allocation Proposal NSF ACCESS**, *Simulation of excited-state dynamics and ultrafast transient absorption spectrum of 2,2'-dihydroxy azobenzene*, Approved with 50,000 GPU hours allocation.

Mar. 2021 **Allocation Proposal NSF XSEDE**, *Simulation of ultrafast spectroscopy observables and excited state intramolecular proton transfer (ESIPT) dynamics of 1-Hydroxy-2-acetonaphthone*, Approved with 2,500 GPU hours allocation.

Computational Expertise

Languages Proficient in: PYTHON, FORTRAN, BASH, Intermediate in: C++ , Wolfram Mathematica

Modeling Gaussian, CP2K, QUANTUM ESPRESSO, CRYSTAL, MOLPRO, OPENMOLCAS, TeraChem

Certifications

Sept. 2023 **SciPhD Business of Science**, Stony Brook University.

June 2023 **Applied Machine Learning in Python**, University of Michigan.

May 2023 **College Teaching Seminars**, Stony Brook University.

Peer-review Services

[5] Journal of Chemical Physics

[4] RSC Advances
[3] Crystal Growth & Design
[2] International Journal of Environmental Science and Technology
[1] Spectroscopy Letters

References

Prof. Benjamin G. Levine
IACS Endowed Professor of Chemistry
Institute for Advanced Computational Science and Department of Chemistry
Stony Brook University, Stony Brook, NY, 11794
Telephone: +1 (631) 632 2381
Email: ben.levine@stonybrook.edu

Prof. Benjamin G. Janesko
Professor & Chemistry Department Chair
Department of Chemistry & Biochemistry
Texas Christian University, Fort Worth, TX, 76129
Telephone: +1 (817) 257 6202
Email: b.janesko@tcu.edu

Prof. Martin Gruebele
Professor of Physics
Professor of Beckman Institute for Advanced Science and Technology
Professor of Center for Biophysics and Quantitative Biology
Professor of Center for Advanced Study
Professor of Carle Illinois College of Medicine
Department of Chemistry
University of Illinois at Urbana-Champaign, Urbana, IL 61801
Telephone: +1 (217) 333 1624
Email: myerscou@illinois.edu