Hassan Nadeem

Education

Ph.D. Bioengineering **Jan 2023 — Present**
University of Illinois Urbana-Champaign
GPA: 4.00 | Member, Phi Kappa Phi Honor Society

M.S. Nuclear Engineering **Nov 2015 — Nov 2017**
Pakistan Institute of Engineering and Applied Sciences, Pakistan

B.S. Mathematics **Sept 2011 — Aug 2015**
National University of Sciences and Technology, Pakistan

Current Research Projects

Ph.D. Bioengineering – PI: Dr. Diwakar Shukla

- **Iterative generative modeling of protein structural ensembles.** Development of a framework for generating diverse and physically realistic protein conformational ensembles through iterative fusion of diffusion-based structure prediction models and inverse folding networks. This approach aims to couple sequence–structure consistency with conformational diversity to better capture thermodynamically relevant states beyond single-structure predictions.
- **Protein language model representations for fitness prediction of natural products.** Leveraging embeddings from large-scale protein language models to predict functional fitness, activity, and evolutionary compatibility of natural product biosynthetic enzymes (e.g. ProcM). The goal is to integrate sequence-derived representations with supervised and semi-supervised learning to guide discovery and optimization.
- **Predictive modeling of charge transport in oligopeptides.** Integration of large-scale molecular dynamics simulations, generative flow-based models, and scanning tunneling microscopy break-junction (STM-BJ) experiments to characterize structure–conductance relationships and develop predictive models of charge transport in short peptides.
- **Molecular design principles of proteomimetic brush polymers.** Use of molecular dynamics simulations to elucidate conformational behavior, solvent interactions, and emergent material properties of proteomimetic brush polymers, enabling rational design of sequence-defined polymer architectures.
- **Mechanistic origin of reflectivity in cephalopod reflectin proteins.** Combining molecular dynamics simulations with experimental reflectivity measurements to characterize the molecular and mesoscale origins of optical reflection in cephalopod reflectin proteins and to uncover design principles for bioinspired photonic materials.
- **Computational design of epitopes for molecularly imprinted polymers.** Development of computational pipelines for designing peptide epitopes that selectively bind molecularly imprinted polymers (MIPs), with applications in targeting and detecting cancer biomarkers.

Experience

Senior Scientist **Dec 2019 — Dec 2021**
Pakistan Atomic Energy Commission

- Developed and implemented novel core loading pattern optimization algorithms for Pressurized Light Water Reactors (PWRs), with the potential to increase effective full power days by approximately 15 days per operating cycle.
- Served as Quality Assurance (QA) Engineer, conducting internal audits, coordinating with cross-functional teams, and overseeing development and implementation of Corrective Action Plans in compliance with regulatory standards.
- Lead Instructor for Radiation Protection Training (RPT), training approximately 300 officers and technicians annually on radiation safety, nuclear safety culture, and reactor fundamentals.
- Organized and coordinated technical workshops, regulatory missions, and peer reviews involving national and international bodies, including PNRA, IAEA, and WANO.

Junior Scientist **Nov 2017 — Dec 2019**
Pakistan Atomic Energy Commission

- Delivered foundational mathematics and science courses to newly inducted engineers (20 per cohort) and technicians (50 per cohort), strengthening technical readiness for plant operations.
- Conducted Radiation Protection Training for nuclear power plant personnel, ensuring compliance with operational safety standards.
- Completed structured on-the-job training rotations in the Operations Division, Maintenance Division (Nuclear Island Systems), and Health Physics Department, gaining hands-on experience in reactor systems and radiological safety.

Certificates / Awards / Honors

University of Illinois Urbana-Champaign

- Graduate College Mentoring Certificate 2025 - Graduate College
- Mavis Future Faculty Fellowship 2024 - The Grainger College of Engineering

Pakistan Atomic Energy Commission

- Excellence in Performance Award (2019)

Pakistan Institute of Engineering and Applied Sciences, Pakistan

- Excellence in Research Award (2017)
- Pakistan Atomic Energy Commission Post-Graduate Fellowship (2015 – 2017)
  Covered tuition fee, stipend, lodging, transport for 2 years

National University of Sciences and Technology, Pakistan

- President's Gold Medal for highest GPA (2015)
- Merit Scholarship Award (8 consecutive semesters 2011-2015)

Publications & Preprints

- Samajdar, R.[†], **Nadeem, H.**[†], Moghe, N., Shukla, D., & Schroeder, C. M. (2026). Solvent environment influences molecular conformation and electron transport in peptides. *The Journal of Physical Chemistry Letters*, *17*(21), 6004–6013. doi:10.1021/acs.jpclett.6c01257
- **Nadeem, H.**, & Shukla, D. (2025). Ensemble adaptive sampling scheme: Identifying an optimal sampling strategy via policy ranking. *Journal of Chemical Theory and Computation*, *21*(9), 4626–4639. doi:10.1021/acs.jctc.4c01488
- Zhao, C., **Nadeem, H.**, & Shukla, D. (2025). Structural basis for negative regulation of ABA signaling by ROP11 GTPase. (accepted for publication), *Journal of Chemical Information and Modeling*. doi.org/10.1021/acs.jcim.5c02002
- Kleiman, D. E., **Nadeem, H.**, & Shukla, D. (2023). Adaptive sampling methods for molecular dynamics in the era of machine learning. *The Journal of Physical Chemistry B*, *127*(50), 10669–10681. doi:10.1021/acs.jpcb.3c04843

[†]These authors contributed equally to this work.

Conference Presentations/Posters

- **Nadeem, H.**, & Shukla, D. (2026). Ensemble Adaptive Sampling Scheme: Identifying an Optimal Sampling Strategy via Policy Ranking. *ACS Spring 2026* (Oral Presentation), March 22–26, 2026, Atlanta, GA.
- **Nadeem, H.**, Samajdar, R., Schroeder, C. M., & Shukla, D. (2026). Towards Predictive Models of Charge Transport in Peptides. *US Army Center for Synthetic Biology 3rd Annual Review* (Poster Presentation), June 2, 2026, McCormick Auditorium.
- Samajdar, R., **Nadeem, H.**, Meigooni, M., Bansal, P., Jackson, N., Mosquera, M., Tajkhorshid, E., Shukla, D., & Schroeder, C. M. (2024). Active Learning to Understand and Predict the Electronic Behavior of Peptides. *2024 AIChE Annual Meeting*, October 29, 2024. AIChE.

Teaching

- Teaching assistant for BIOE-486 Computational Mathematics for Machine Learning and Imaging. UIUC, Fall 2024
- Teaching assistant for BIOE-210 Linear Algebra for Biomedical Data science. UIUC, Fall 2025

Skills

Programming: Python, C++, MATLAB, Shell; PyTorch, Keras, Sklearn
Molecular Dynamics: OpenMM, LAMMPS, Amber, GROMACS, NAMD
Molecular Visualization: VMD, ChimeraX, PyMol
Neutronics: OpenMC, MCRAC, WIMS
Operating Systems: Windows, MacOS, Unix, HPC
Version Control: Git, HuggingFace

Outreach

- Lab assistant for Exploring Your Options (EYO) summer camp, EYO is a week-long, residential program that introduces rising 9th - 12th graders to the varied disciplines of engineering at UIUC. (2023-2025)
- Lab assistant for CURIE(Catalyzing UR Interest in Chemical Engineering) summer camp, part of Worldwide Youth in Science and Engineering Program, organized by the Grainger College of Engineering, UIUC. (2023-2025)
- Volunteer teacher for *Teach for Pakistan* program. Teaching STEM courses to underprivileged children (ages 13-18), who could not afford formal school education. (2012-2015)