

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

Research Projects

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

- Development of novel adaptive sampling algorithms by leveraging insights from statistical mechanics, reinforcement learning, and generative machine learning. Computational design and study of peptide materials using molecular dynamics simulations and machine learning, with applications for peptide electronics and peptide polymers.

M.S. Nuclear Engineering – PI: Dr. Sikander Majid Mirza

- Multi-Objective Optimization of Core-Reload Pattern for Pressurized Water Reactors .
Techniques involved: Reactor Physics, Core Neutronics, Metaheuristic Optimization

Experience

Senior Scientist

Dec 2019 — Dec 2021

Pakistan Atomic Energy Commission

- Developed novel algorithms for core loading pattern optimization for Pressurized Light Water Reactors. Performed duties as QA Engineer for Quality Assurance audits, respective follow ups and coordination with relevant stakeholders for Corrective Action Plans. Instructor for Radiation Protection Training, Nuclear Safety Culture, Pressurized Light Water Reactor Organized different workshops, member missions, technical missions from PNRA, IAEA, WANO etc.

Junior Scientist

Nov 2017 — Dec 2019

Pakistan Atomic Energy Commission

- Instructor for basic mathematics/science courses for newly inducted engineers/scientists/technicians. Conducted Radiation Protection Training for nuclear power plant personnel. Shadow Nuclear Reactor Operator for Nuclear Island Systems.

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

- **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

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

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)