Hassan Nadeem

Education

Ph.D. Bioengineering **Jan 2023 — present**
University of Illinois Urbana-Champaign

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 Bayesian statistics.
- 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 Systems.
- 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.**, and Shukla, D. "Ensemble Adaptive Sampling Scheme: Identifying an Optimal Sampling Strategy via Policy Ranking." *Journal of Chemical Theory and Computation*, 2025 https://doi.org/10.1021/acs.jctc.4c01488.
- Zhao, C., **Nadeem, H.**, and Shukla, D. "Structural Basis for Negative Regulation of ABA Signaling by ROP11 GTPase." *Journal of Chemical Information and Modeling*, under review, 2025.
- Kleiman, D. E., **Nadeem, H.**, and Shukla, D. "Adaptive Sampling Methods for Molecular Dynamics in the Era of Machine Learning." *The Journal of Physical Chemistry B* https://doi.org/10.1021/acs.jpcb.3c04843.

Teaching

- Teaching assistant for BIOE-486 Computational Mathematics for Machine Learning and Imaging. UIUC, Fall 2024

Skills

Programming

- Python, C++, MATLAB, Shell
- Pytorch, Keras

Molecular Dynamics Simulations

- OpenMM, LAMMPS, Amber, GROMACS, NAMD

Neutronics

- OpenMC, MCRAC, WIMS

OS

- 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. (2023,2024)
- Lab assistant for CURIE(Catalyzing UR Interest in Chemical Engineering) summer camp, part of World-wide Youth in Science and Engineering Program, organized by the Grainger College of Engineering, UIUC. (2023,2024)
- 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)