TEJAS SHAH

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SUMMARY

- Interdisciplinary scientist with expertise in Molecular Dynamics and Protein Modeling, specializing in studying biomolecular systems and their interactions.
- Knowledgeable in AI/ML applications for molecular simulations, with a strong foundation in computational chemistry and statistical analysis.
- Proficient in Python and Bash for computational automation, data processing, and large-scale trajectory analysis, with experience in Gaussian calculations and structural modeling.

TECHNICAL SKILLS

Computational: Molecular Dynamics Simulations, Gaussian QM Calculations, Force Field Development, Structure-Property Relationship, Homology Modeling, Model Development, VMD
Programming and ML Awareness: Bash, Python - NumPy, Pandas, MatplotLib, Seaborn, Scikit learn libraries, Linux HPC clusters, Knowledge of PyTorch, TensorFlow
Data Science: Protein Data Bank (PDB), SWISS Modeler, Large-scale trajectory analysis, Data processing, MDAnalysis

WORK EXPERIENCE

Graduate Assistant Aug 2019 to Present
The University of Texas at Dallas *Richardson, TX*
- Applied homology modeling and molecular dynamics simulations to study nucleosome core particles to elucidate histone tail modifications and their impact on chromatin dynamics.
- Developed AMBER force field parameters for non-standard molecules to improve the accuracy of molecular dynamics simulations in protein-DNA systems.
- Investigated protein-DNA interactions by identifying non-covalent forces and applied principal component analysis to characterize protein functionality and dynamics.
- Leveraged Python (NumPy, Pandas, Matplotlib, Seaborn, SciPy) to process extensive molecular simulation datasets to analyze trajectories on high-performance Linux HPC clusters.

PROM Fellow Feb 2025 to Present
Dr. Jakub Rydzewski's Lab, Nicolaus Copernicus University *Torun, Poland*
- Selected as one of 16 international fellows for a prestigious program supporting advanced training in computational chemistry and scientific collaboration.
- Developing expertise in machine learning for molecular simulations, enhanced sampling techniques, and trajectory analysis to study rare events in complex biological systems.

ACADEMIC PROJECTS

Project 1: Elucidating the molecular mechanisms of histone lysine methyltransferase activity through comprehensive all-atom molecular dynamics simulations
Project 2: Computational Design to Experimental Validation: Molecular Dynamics-assisted Development of Polycaprolactone Micelles for Drug Delivery

EDUCATION

PhD, Computational Chemistry, University of Texas at Dallas, Richardson, TX Aug 2019 to Apr 2025 (Expected)

MENTORING AND LEADERSHIP EXPERIENCE

- Associate, Committee on Younger Chemists, ACS 2025 to Present
- Elected School Representative, Graduate Student Assembly - UTD 2020 to 2022

SELECTED PUBLICATIONS (2/11)

- **Shah, T.**, Stefan, M. C., Torabifard, H., *Journal of Physical Chemistry B*, **2024,** 128, 11981-11991.
- **Shah, T.**, Himanshu, P., Babanyunahm G., Bhadran, A., Wang, H., Cu Castillo, C., Grabowski, G., Biewer, M. C., Torabifard, H. Stefan, M. C., *Journal of Materials Chemistry B*, **2024.** *(Under Revision)*

SELECTED WORKSHOPS AND CONFERENCE (2/10)

- **Shah, T.**, Torabifard, H., Contributed poster at ACS National Meeting, Denver, CO. August 18-22, 2024. *(Finalist, NVIDIA GPU Poster Award)*
- AMBER Free Energy Workshop, San Diego Supercomputer Center, University of California San Diego, San Diego, CA. August 12 - 16, 2024. *(Selected through a competitive application process)*

SELECTED AWARDS

- Researcher and Travel Grant, Royal Society of Chemistry 2024
- Graduate Research and Cancer Education (GRACE) Fellowship, Office of Graduate Education, UT Dallas 2023