Tejas Shah

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Professional Summary

A passionate, adaptive, fast-learning, and inquisitive PhD Candidate with a broad and acute interest in academic research in Computational Chemistry, Simulations, and developing machine learning models to understand protein function and dynamics. Hands-on training and experience in literature search, experiment design, data collection, and interpretation. Comprehensive knowledge with demonstrated proficiency in Gaussian QM calculations, force field development, molecular dynamics, homology modeling, GNUPLOT, Python NumPy, Pandas, and Matplot libraries, as well as instrumental analysis. Transferable skills in AI/ML, Statistical Analysis, team management, and communication. Actively participated and presented at national conferences, international symposiums, and local workshops and seminars, enthusiastically interacted with academicians and scientists from various scientific disciplines to exchange and absorb ideas and develop new professional skills. A highly motivated team player who is always willing to take on new responsibilities. Excellent ability to work independently as well as in a group. Ability to apply out-of-the-box thinking to solve scientific problems. Ongoing academic quest to incorporate enhanced sampling methods and ML algorithms to develop novel therapeutics. Professional ambition is to eventually have a career in computational chemistry in a research and development setting.

Education

The University of Texas at Dallas Richardson, TX
Doctor of Philosophy (Ph.D.), Computational and Organic Chemistry Aug 2019 - Jul 2025 (Expected)
Advisor: Dr. Mihaela C. Stefan, Co-advisor: Dr. Hedieh Torabifard
Tentative Dissertation Title: *"Multiscale Investigation of Highly Dynamic Systems: All-Atom Molecular Dynamics Simulations of Polymeric Micelle for Drug Delivery Applications and Histone Tail Modifications"*
Committee: Dr. Michael C. Biewer, Dr. Gabriele Meloni

Gujarat University Ahmedabad, India
Master of Science (M.Sc.), Organic Chemistry Jul 2014 - Jun 2016
Recipient of the Gold medal for obtaining the highest score in the class

Gujarat University Ahmedabad, India
Bachelor of Science (B.Sc.), Chemistry Aug 2011 - Jun 2014

Experience

Graduate Assistant (Teaching/Research Assistant) Aug 2019 - Present
The University of Texas at Dallas Richardson, TX

- Led independent teams, designed experiments, and collaborated with cross-functional teams, resulting in 13 research articles.
- Conducted quantum mechanical calculations (Gaussian 16) to develop force field parameters for non-standard molecules, enabling accurate simulations of material properties.
- Identified chemical descriptors and non-covalent interactions in polymer systems, providing atomistic insights into material development.
- Implemented simulation-based screening to develop anticancer drug formulation and achieved 30% higher drug loading capacity without compromising stability.

- Synthesized, purified, and characterized three novel caprolactone monomers and two amphiphilic block copolymers for drug delivery applications.
- Optimized and characterized polymer-drug formulation with spectroscopic and microscopic techniques.
- Applied homology modeling and molecular dynamics simulations to study nucleosome core particles to elucidate histone tail modifications and their impact on chromatin dynamics.
- Leveraged Python (NumPy, Pandas, Matplotlib, Seaborn, SciPy) to process extensive molecular simulation datasets to analyze trajectories on high-performance Linux HPC clusters.
- Developed methodologies to investigate materials via NMR, MS, TEM, DLS, CLSM, UV-VIS, IR, and mass spectroscopy.
- Mentored six undergraduate students and a high school student for independent research and trained them on high-tech instruments.
- Prepared and organized course resources, helped 500+ undergraduate students in introductory organic chemistry I and II labs (20 classes), led discussions, graded assignments, and exams.
- Participated and presented the data obtained from the experiments in local, regional, and national conferences.
- Maintained and updated the laboratory website, ensuring accurate and timely information for researchers, prospective students, and collaborators.

PROM Fellow Feb 2025 - Mar 2025
Nicolaus Copernicus University Toruń, Poland Advisor – Dr. Jakub Rydzweski, Assistant Professor, Faculty of Physics, Astronomy and Informatics
- Awarded the PROM Fellowship (Polish National Agency for Academic Exchange - NAWA) as one of 16 international fellows supporting advanced training in Science and Technology.
- Applied machine learning techniques (PCA, tICA, spectral maps) and free energy calculations to analyze rare biological events.
- Utilized enhanced sampling methods in molecular dynamics simulations to improve rare-event detection and pathway exploration.
- Developed computational workflows to integrate machine learning for large-scale trajectory analysis to enhance the efficiency of classical simulations.

Intern, R&D Materials Engineering May 2023 - Aug 2023
Alcon Laboratories Ltd Fort Worth, TX
Manager – Dr. Huayun Yu, Surgical Devices Materials Engineering
- Optimized monomer formulation and synthesized cross-linkable polymers for the Intraocular Lens (IOL) application.
- Carried out literature search as required to design or modify ongoing experiments to solve a research problem.
- Worked collaboratively with analytical laboratory as well as intrateam personnel to obtain NMR, GPC, and GC analysis of the prepared samples.
- Carried out mechanical testing of the resultant polymer using mechanical and thermal analysis.

Teaching Assistant Jan 2017 - Jun 2019
Gujarat University Ahmedabad, India
- Taught synthetic organic chemistry and qualitative organic chemistry labs to 150+ graduate-level students.
- Instructed an introductory polymer chemistry class for 25 graduate-level students.
- Assisted graduate students in conducting literature searches, designing experiments, and performing UV-Vis and FT-IR spectroscopy analysis.

Trainee, Analytical Development Laboratory Jul 2016 - Sep 2016
Dishman Pharmaceuticals and Chemicals Ltd Ahmedabad, India

- Prepared and analyzed R&D samples using liquid and gas chromatography
- Conducted thermal properties of developing active pharmaceutical ingredients using DSC and metal residue analysis using ICP-AES
- Developed, validated and prepared standard operating procedures for analyzing samples at the Quality Control department using UV-Vis, FT-IR, XRD, and chromatographic analysis

Undergraduate and High School Students Mentoring

Alexandra Goldmann, Currently Graduate Student, UTD	2022 - 2024
Gerik Gebrowski, Currently Research Assistant, UTSW	2022 - 2023
Sofia Dai (Welch Scholar), Currently Undergraduate Student, UT Austin	2021 - 2021
Amal Patel, Currently Graduate Student, UCSD	2020 - 2021
Justin Sujith, Currently Program Specialist III, Texas Department of State Health Services	2019- 2021
Maria Kiesewetter, Currently Medical Student, TTUHSC EP PLFSOM	2019 - 2021
Karen Meija, Currently Scientist I, Pace Analytical Services	2019 - 2020

Publications

1. **Shah, T.**, Torabifard, H., Investigating trans-histone pathway of H3K36 methylation by histone-N-methyltransferase from Molecular Dynamics Simulations. (*Under Preparation*)

2. Babanyinah, G., Bhadran, A., Polara, H., **Shah, T.**, Biewer, M. C., Stefan, M. C., Fluorescent Poly(ε-Caprolactone)s Micelles for Anticancer Drug Delivery and Bioimaging, *Biomacromolecules*, **2025,** 26, 3213–3223.

3. Polara, H., **Shah, T.**, Babanyinah, G., Wang, H., Bhadran, A., Biewer, M. C., Torabifard, H., Stefan, M. C., Improved Drug Delivery through Amide-Functionalized Polycaprolactones: Enhanced Loading Capacity and Sustained Drug Release, *Biomacromolecules*, **2025,** 26, 3213–3223.

4. **Shah, T.**,† Polara, H.,† Bhadran, A., Babanyinah, G., Wang, H., Gerik, G., Biewer, M. C., Torabifard, H., Stefan, M. C., Computational Design to Experimental Validation: Molecular Dynamics-assisted Development of Polycaprolactone Micelles for Drug Delivery, *Journal of Materials Chemistry B*, **2025,** 13, 4166-4178. (†equally contributed)

5. **Shah, T.**, Stefan, M. C., Torabifard, H., Dynamics of amphiphilic poly(ε-caprolactone) micelles with doxorubicin and transition temperature predictions using all-atom molecular dynamics simulation, *Journal of Physical Chemistry B*, **2024,** 128, 11981–11991.

6. Goldman, A., **Shah, T.**, Torabifard, H., Histone H3 orchestrates the ubiquitination of nucleosomal H2A by BRCA1/BARD1-UbcH5c complex, *BioRxiv*, **2024**.

7. Abbas, M., Murtaza, D., Joy, M., Sheybani, S., **Shah, T.**, Balkus, K., Synthesis and Characterization of Two New Holmium Metal-Organic Frameworks, *CrystEngComm,* **2024,** 26, 5567-5573.

8. Babanyinah, G., Bhadran, A., Wang, H., Polara, H., **Shah, T.**, Biewer, M., Stefan, M. C., Maleimide functionalized polycaprolactone micelles for glutathione quenching and doxorubicin delivery, *Chemical Science,* **2024,** 15, 9987-10001. (*Featured on Journal Cover*)

9. Wang, H., Polara, H., Bhadran, A., **Shah, T.**, Babanyinah, G., Ma, Z., Miller, J., Biewer, M., Stefan, M., Effect of aromatic substituents on thermoresponsive functional polycaprolactone micellar carriers for doxorubicin delivery, *Frontiers in Pharmacology,* **2024,** 15, 1356639.

10. Bhadran, A., Polara, H., Calubaquib, E., Wang, H., Babniyinah, G., **Shah, T.**, Anderson, P., Saleh, M. Biewer, M., Stefan, M. C., Reversible cross-linked thermoresponsive polycaprolactone micelles for enhanced stability and controlled release, *Biomacromolecules,* **2023,** 24, 12, 5823-5835.

11. Mistry, H., Thakor, R., Polara, H., **Shah, T.**, Bariya, H., Biogenically efficient production and characterization of silver nanoparticles using the marine fungus Hamigera Terricola along with their antimicrobial and antioxidative efficacy. *Nanotechnology and In Silico Tools*, **2024,** 89–96.

12. Bhadran, A., Polara, H., **Shah, T.**, Babanyinah, K, G., Taslimy, S., Biewer, M, C., Stefan, M, C., Functional polycaprolactones for drug delivery applications, *Pharmaceutics,* **2023,** 15, 7, 1977. (*Invited Perspective*)

13. Stefan, M. C., Soltantabar, P., Wang, H., Bhadran, A., Polara, H., **Shah, T.**, Organ Chips in Safety Pharmacology Springer Nature, Accepted December 2022. (*Corresponding Author, Invited Book Chapter*)

14. **Shah, T.**, Vasava, D. V., A glimpse of biodegradable polymers and their biomedical applications. *e-Polymers*, **2019,** 19, 1, 385-410.

Conference, Symposium and Workshop Participation

1. **Shah, T.**, Polara, H., Bhadran, A., Babanyinah, G., Wang, H., Gerik, G., Biewer, M. C., Torabifard, H., Stefan, M. C., Contributed poster at The American Chemical Society national meeting, San Diego, CA. Mar 22-27, 2025. (Sci-Mix, POLY Outstanding Poster Award)

2. **Shah, T.**, Stefan, M. C., Torabifard, H., Contributed poster at The American Chemical Society national meeting, San Diego, CA. Mar 22-27, 2025. (Finalist NVIDIA GPU Poster Award)

3. **Shah, T.**, Torabifard, H., Contributed poster at The American Chemical Society national meeting, Denver, CO. Aug 18-22, 2024. (Sci-Mix, Finalist NVIDIA GPU Poster Award)

4. **Shah, T.**, Polara, H., Babanyinah, G., Bhadran A., Wang, H., Biewer, M., Stefan, M. C., Contributed poster at The American Chemical Society national meeting, Denver, CO. Aug 18-22, 2024. (Sci-Mix)

5. AMBER Free Energy Workshop, San Diego Supercomputer Center, San Diego, CA. Aug 11-16, 2024. (Selected through a competitive application process)

6. **Shah, T.**, Torabifard, H., Contributed poster at The American Chemical Society national meeting, New Orleans, LA. Mar 16-21, 2024.

7. **Shah, T.**, Torabifard, H., Contributed Poster at ACS Southwest regional meeting, Oklahoma City, OK. Nov 15 - 18, 2023

8. **Shah, T.**, Stefan, M. C., Torabifard, Hedieh, Contributed lecture at Annual Meeting-in-Miniature, The American Chemical Society, DFW section, Stephenville, TX. Apr 23, 2023. (Awarded 3^{rd} prize in polymer section)

9. **Shah, T.**, Stefan, M. C., Torabifard, Hedieh, at The American Chemical Society national meeting, Indianapolis, IN. Mar 26 - 30, 2023

10. **Shah, T.**, Stefan, M. C., Contributed Poster at ACS Southwest regional meeting, Baton Rouge, LA. Nov 06 - 09, 2022.

11. National Workshop on Characterization Techniques for Materials, Sardar Patel University, V. V. Nagar, INDIA. Mar 06 - 07, 2017.

12. **Shah, T.**, Vasava, D. V., Review Poster at International Science Symposium on Recent Trends in Science & Technology, Rajkot, INDIA. Feb 26 - 27, 2017.

13. **Shah, T.**, Contributed talk at Gujarat University Science Excellence Symposium, Ahmedabad, GJ, INDIA. Sep 26, 2015.

Leadership Experience

Younger Chemist Committee, American Chemical Society Jan 2025 - Present
Associate Member USA

UT Dallas Graduate Student Association Oct 2019 - May 2022
Natural Science and Mathematics School Representative Richardson, TX

- Served as a liaison between graduate students and university administration to voice the concerns of graduate students
- Pitched in monthly executive meetings and quarterly general meetings about ongoing efforts of GSA and new ideas for campus events
- Worked closely with the Office of Emergency Management & Continuity Planning (OEMCP) during the Coronavirus pandemic to ensure student's safe return to the campus
- Member of the nomination committees and reviewed, discussed, and suggested suitable applicants for the positions
- Member of the working groups to identify, voice, discuss, and resolve the concerns of the current and prospective graduate students, thereby helping them to enrich their graduate life experience at the UTD
- Organized events with other offices to enrich student campus life experience, discuss the importance of mental health in graduate school and campus-wide diversity, equity, and inclusion through discussion panels and community service events

Awards and Honors

Finalist, NVIDIA GPU Poster Award - American Chemical Society National Meeting Spring 2025 2025
POLY Outstanding Poster Award - American Chemical Society National Meeting Spring 2025 2025
PROM Fellow, National Academy of Academic Exchange (NAWA), Poland 2025
Finalist, NVIDIA GPU Poster Award - American Chemical Society National Meeting Fall 2024 2024
Research and Travel Grant Award – Royal Society of Chemistry 2023
School of Natural Science and Mathematics Travel Award – UTD 2023
Graduate Research and Cancer Research Fellowship – Office of Research and Innovation, UTD 2023
Awarded third prize for oral presentations 55^{th} meeting in miniature – ACS DFW section 2023
Betty and Gifford Johnson Travel Grant Award – Office of Graduate Education, UTD 2023
Orator 2020 award on departmental seminar talk – Department of Chemistry, UTD 2020
Financial support to apply for admission for PhD in chemistry at USA – Dr. Rohitkumar Vora 2019
Gold Medal for highest marks among all the students – Bhavan's Sheth R. A. College of Science 2016
Awarded second prize for the presentation at the Science Excellence Symposium 2015
Monetary support for graduate education – Shree Modasa Ekda Dasha Khadayta Kelvani Mandal 2014
Scholarship for Undergraduate Education – Shree Modasa Ekda Dasha Khadayta Kelvani Mandal 2012

Professional Affiliations

American Chemical Society 2021 - Present
Royal Society of Chemistry 2021 - Present

Volunteering and Community Services

Graduate Recruiting, Department of Chemistry, UTD	Mar 2023, Mar 2024
Grand Award Judge - Dallas Regional Science and Engineering Fair	Feb 2024
Grand Award Judge - Plano ISD Science and Engineering Fair	Feb 2024
Grand Award Judge - Regeneron International Science and Engineering Fair	May 2023
Graduate Recruiting, Department of Chemistry, UTD	Nov 2023
Panel member – Discussion for incoming TA/RA Students, UTD	Aug 2022
Award Judge – Chemists Celebrate Earth Week, ACS meeting in miniature, UTD	Apr 2022
Student Committee member – 54^{th} ACS meeting in miniature, UTD	Apr 2022
Volunteered at ACS National Chemistry Week	Aug 2021, Feb 2022
Workshop leader Organic Chemistry Success Workshop	Jan 2021, Aug 2021
Organizer – UTD Blood Donation Drive Campaign	Jul 2020

Technical Skills

Computational:

- Molecular Dynamics Simulations: AMBER, CPPTRAJ, tLeap, Antechamber, Packmol, VMD
- Force Field Development: Gaussian16, PyRED
- Homology Modeling: Swiss Modeller, PyMOL
- Programming Languages and Packages: Bash, Python NumPy, Panda, Matplotlib, Seaborn, SciPy, SciKit learn, GNUPLOT, MDTraj, MDAnalysis, knowledge of PyTorch, TensorFlow packages

Characterization Techniques:

- Advance Materials Characterization: DSC, TGA, and DLS
- Spectroscopic Techniques: NMR, UV-Vis, FT-IT, ATR-IR, MS, and Fluorescence Spectroscopy
- Chromatography Techniques: Column chromatography, HPLC, GC and SEC
- Microscopy Techniques: TEM, SEM, CLSM, and Optical Microscopy

Wet-lab Skills:

- Organic Synthesis: Small Molecule Synthesis, Purification, Compound isolation, Reaction optimization
- Polymerization: Ring Opening Polymerization, Free radical polymerization, *living* polymerization, cross-linked polymers, post-polymer modifications
- Drug Delivery: Drug encapsulation, 2D cell culture and in vitro drug release studies

Professional Reference Providers

Dr. Hedieh Torabifard
Assistant Professor, Department of Chemistry and Biochemistry
The University of Texas at Dallas
Email: Hedieh.Torabifard@UTDallas.edu

Dr. Mihaela C. Stefan
Professor, Department of Chemistry and Biochemistry
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Dr. Michael Biewer
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The University of Texas at Dallas
Email: BiewerM@UTDallas.edu