Hao Tian

Location: Dallas, TX | Phone: 682-347-6392 | Email: hhaootian@gmail.com
Homepage: hhaootian.com | LinkedIn: linkedin.com/in/hhaootian

EDUCATION

Southern Methodist University, Dallas, TX — Aug. 2019 – May 2023

- Ph.D. in Theoretical and Computational Chemistry, GPA: 4.0 / 4.0
- Core courses: Statistical Thermodynamics, Advanced Computational Chemistry, Machine Learning and Neural Networks, Mathematical Statistics
- Thesis title: Exploring Protein Conformations and Functions Through Molecular Dynamics Simulations and Machine Learning

Georgia Institute of Technology, Atlanta, GA — Aug. 2020 – May 2023

- Online M.S. in Computer Science, GPA: 4.0 / 4.0
- Core courses: Database Systems Concepts and Design, Computer Networks, Graduate Introduction to Operating Systems, Introduction to Graduate Algorithms, Software Architecture and Design

Beijing University of Chemical Technology, Beijing, China — Aug. 2015 – Jun. 2019

- B.Eng. in Chemical Engineering, GPA: 3.49 / 4.33

TECH STACK

- **Languages**: Python, Java, C, C++, HTML, CSS, JavaScript, PHP
- **Toolkits & Frameworks**: Linux, Docker, Git, MySQL, Django, Bootstrap, RESTful API
- **Machine Learning**: Scikit-learn, Tensorflow (Keras), PyTorch

EXPERIENCE

Software Engineer Intern — **Meta** (Facebook), Menlo Park, CA — May 2022 – Aug. 2022

- Implemented a relay IP to real IP mapping service in Ads identity prediction for iOS 15 privacy mitigation.
- Wrote 3k+ lines of PHP codes for service implementation and 2k+ lines of SQL (Presto) for impact evaluation.
- Improved IP coverage by 2.5%, identity match rate by 11% in iOS 15.5 and 3% in the overall Meta Pixel traffic, leading to 1.7% offsite conversion gain and 0.08% of incremental revenue.
- Published one internal technical post about viewer context which leads to a team Better Engineering project.

Graduate Research Assistant — **Southern Methodist University**, Dallas, TX — Aug. 2019 – May 2023

- Developed machine learning models on high-performance computing (HPC) clusters with SLRUM scheduler.
- Launched a web server (40k+ visits) with Django for biology prediction, supporting job submission and protein visualization, with web pages written in HTML / CSS / Javascript and improved UI using Bootstrap.
- Act as the group's Tech Lead in leading and designing research directions and writing funding proposals.
- Initiated automated and customized development workflow with CI / CD via GitHub Actions.

PUBLICATIONS

Google Scholar link: https://scholar.google.com/citations?user=X7ZR8J0AAAAJ

15. **Tian, H.**, Xiao, S., Jiang, X., & Tao, P. (2023). PASSer: Fast and Accurate Prediction of Protein Allosteric Sites. *Nucleic Acids Research*, gkad303.
14. Li, H., **Tian, H.**, Chen, Y., Xiao, S., Zhao, X., Gao, Y., & Zhang, L. (2023). Analyzing and Predicting the Viscosity of Polymer Nanocomposites in the Conditions of Temperature, Shear Rate, and Nanoparticle Loading with Molecular Dynamics Simulations and Machine Learning. *Journal of Physical Chemistry B*, 127, 15, 3596–3605.
13. Xiao, S., Song, Z., **Tian, H.**, & Tao, P. (2023). Assessments of Variational Autoencoder in Protein Conformation Exploration. *Journal of Computational Biophysics and Chemistry*, 22, 1-13.
12. Yin, C., Song, Z., **Tian, H.**, Palzkill, T., & Tao, P. (2023). Unveiling the structural features that regulate carbapenem deacylation in KPC-2 through QM/MM and interpretable machine learning. *Physical Chemistry Chemical Physics*, 25(2), 1349-1362.
11. Krishnan, K., **Tian, H.**, Tao, P., & Verkhivker, G. M. (2022). Probing conformational landscapes and mechanisms of allosteric communication in the functional states of the ABL kinase domain using multiscale simulations and network-based mutational profiling of allosteric residue potentials. *The Journal of Chemical Physics*, 157(24), 245101.
10. **Tian, H.**, Jiang, X., Xiao, S., La Force, H., Larson, E. C., & Tao, P. (2022). LAST: Latent Space-Assisted Adaptive Sampling for Protein Trajectories. *Journal of Chemical Information and Modeling*, 63(1), 67-75.
9. **Tian, H.**, Ketkar, R., & Tao, P. (2022). ADMETboost: a web server for accurate ADMET prediction. *Journal of Molecular Modeling*, 28(12), 1-6.
8. Song, Z., Trozzi, F., **Tian, H.**, Yin, C., & Tao, P. (2022). Mechanistic insights into enzyme catalysis from explaining machine-learned quantum mechanical and molecular mechanical minimum energy pathways. *ACS Physical Chemistry Au*, 2(4), 316-330.
7. Xiao, S., **Tian, H.**, & Tao, P. (2022). PASSer2. 0: accurate prediction of protein allosteric sites through automated machine learning. *Frontiers in Molecular Biosciences*, 9.
6. **Tian, H.**, & Tao, P. (2021). Deciphering the protein motion of S1 subunit in SARS-CoV-2 spike glycoprotein through integrated computational methods. *Journal of Biomolecular Structure and Dynamics*, 39(17), 6705-6712.
5. **Tian, H.**, Jiang, X., Trozzi, F., Xiao, S., Larson, E. C., & Tao, P. (2021). Explore protein conformational space with variational autoencoder. *Frontiers in Molecular Biosciences*, 8, 781635.
4. **Tian, H.**, Jiang, X., & Tao, P. (2021). PASSer: Prediction of allosteric sites server. *Machine Learning: Science and Technology*, 2(3), 035015.
3. Song, Z., Zhou, H., **Tian, H.**, Wang, X., & Tao, P. (2020). Unraveling the energetic significance of chemical events in enzyme catalysis via machine-learning based regression approach. *Communications Chemistry*, 3(1), 134.
2. **Tian, H.**, Trozzi, F., Zoltowski, B. D., & Tao, P. (2020). Deciphering the allosteric process of the Phaeodactylum tricornutum Aureochrome 1a LOV domain. *The Journal of Physical Chemistry B*, 124(41), 8960-8972.
1. **Tian, H.**, & Tao, P. (2020). ivis Dimensionality Reduction Framework for Biomacromolecular Simulations. *Journal of Chemical Information and Modeling*, 60(10), 4569-4581.

PRESENTATIONS

Oral

- Prediction of Allosteric Sites Through Ensembled Learning
  ACS Spring 2021, Apr. 2021
- ivis Dimensionality Reduction Method for Macromolecular Simulations
  ACS Spring 2021, Apr. 2021
- Machine Learning Framework for Deciphering the Allosteric Process of Circadian Clock Protein
  Invited seminar talk, Department of Chemistry and Biochemistry, The University of Oklahoma, Nov. 2020

Poster

- LAST: Latent Space Assisted Adaptive Sampling for Protein Trajectories
  Machine Learning in Computational Biology, Nov. 2022
- Iterative expansion of protein conformational space with variational autoencoder
  ACS Fall 2022, Aug. 2022
- Exploration of protein conformational space with variational autoencoder
  ACS Spring 2022, Mar. 2022

AWARDS

- Research Achievement Award, Southern Methodist University, Dec. 2022
- Chemical Computing Group Excellence Award for Graduate Students, American Chemical Society, Computers In Chemistry division, Apr. 2022 (only 5 awardees in each meeting)
- Research and Innovation Week Dean's Award, Southern Methodist University, May 2021 & Apr. 2022
- Graduate Research Assistant Award, Southern Methodist University, May 2021
- Outstanding Teaching Assistant, Southern Methodist University, May 2020

SERVICES

Journal Reviewer

- BioMedInformatics
- Biomolecules
- Cancers
- Computational and Structural Biotechnology Journal
- Frontiers in Cardiovascular Medicine
- International Journal of Molecular Sciences
- Journal of Chemical Information and Modeling
- Living Journal of Computational Molecular Science
- Machine Learning: Science and Technology
- Molecules

Conference and Workshop Reviewer

- NeurIPS 2022 Workshop AI4Science