

Sian Xiao (He/Him)

Location: Dallas, TX | Phone: (214)-597-9256 | Email: sxiao67@gatech.edu
LinkedIn: linkedin.com/in/sianxiao | Job preference: SDE/MLE/DS internship

Education

Southern Methodist University, Dallas, TX	Aug. 2020 – May. 2024
• Ph.D. in Theoretical and Computational Chemistry	GPA: 4.0/4.0
Georgia Institute of Technology, Atlanta, GA	Aug. 2022 – May. 2024
• M.S. in Computer Science, online	GPA: 4.0/4.0
Beijing University of Chemical Technology, Beijing, China	Sep. 2015 – Jul. 2019
• B.Eng. in Polymer Materials and Engineering	GPA: 88.0/100

Skills

- **Languages:** Python, Bash, Java, C, HTML, CSS, object-oriented design
- **Toolkits & Frameworks:** Linux, Git, MySQL, Django, Pandas
- **Machine Learning:** TensorFlow, PyTorch, Scikit-learn, Keras

Experience

Southern Methodist University, Dallas, TX	Aug. 2020 – May. 2024
<i>Graduate Research Assistant</i>	
<ul style="list-style-type: none">• Assisted with establishment and maintenance of one public website in Django on high computing center for protein allosteric site prediction.• Developed, assessed, and benchmarked machine learning models to explore protein conformational spaces.• Initiated automated and customized development workflow with CI/CD via GitHub Actions.	
<i>Graduate Teaching Assistant</i>	
<ul style="list-style-type: none">• Responsible for 8 courses (lectures/ labs) for 11 sections in 4 academic terms.	

Projects and Research

Deep Learning Aided Protein Conformation Exploration	Sep. 2021 – Present
<ul style="list-style-type: none">• Explored the feasibility of variational autoencoder model to explore protein conformational spaces.• Designed an efficient, open-source algorithm that is 3 times faster than traditional method.• Publication was selected to ICML 2022 AI4Science Workshop	
Protein Allosteric Sites Prediction Server http://passer.smu.edu	Jun. 2021 – Jun. 2022
<ul style="list-style-type: none">• Advanced the state-of-the-art prediction accuracy of top 3 protein pockets to 82.7% through Automated machine learning (AutoML) methods on larger datasets• Deployed the model to our web server Protein Allosteric Site Server (passer.smu.edu) built with Django and JSmol (a JavaScript framework)• The web server can handle job submission and protein visualization within web pages and already has 37,550 visits from more than 70 countries with more than 3,000 executions	

Publications

- "Assessments of Variational Autoencoder in Protein Conformation Exploration" *Journal of Computational Biophysics and Chemistry* (2023).
- "Machine learning and protein allostery" *Trends in Biochemical Sciences* (2022).
- "LAST: Latent Space Assisted Adaptive Sampling for Protein Trajectories" *Journal of Chemical Information and Modeling* (2022).
- "PASSer2.0: Accurate Prediction of Protein Allosteric Sites Through Automated Machine Learning" *Frontiers in Molecular Biosciences* (2022).
- "Explore protein conformational space with variational autoencoder" *Frontiers in Molecular Biosciences* (2021).

Major Awards

• Runner Up, Three Minute Thesis Competition, SMU	Nov. 2021
• University Ph.D. Fellowship (extra funding besides stipends, recurring), SMU	Mar. 2020
• First Prize, Mathematical Contest in Modeling, BUCT	May. 2017
• Outstanding student of Beijing University of Chemical Technology, BUCT	Sep. 2015