

# Sian Xiao (He/Him)

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## Education

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

<b>Southern Methodist University</b> , Dallas, TX	<b>Aug. 2020 – May. 2024</b>
<i>Graduate Research Assistant</i>	
• Assisted with establishment and maintenance of one <b>public website</b> in <b>Django</b> 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 <b>CI/CD</b> via GitHub Actions.	
<i>Graduate Teaching Assistant</i>	
• Responsible for <b>8 courses</b> (lectures/ labs) for <b>11 sections</b> in <b>4 academic terms</b> .	

## Projects and Research

<b>Deep Learning Aided Protein Conformation Exploration</b>	<b>Sep. 2021 – Present</b>
• Explored the feasibility of <b>variational autoencoder</b> model to explore protein conformational spaces.	
• Designed an efficient, open-source algorithm that is <b>3 times faster</b> than traditional method.	
• Publication was selected to <b>ICML 2022 AI4Science Workshop</b>	
<b>Protein Allosteric Sites Prediction Server</b>   <a href="http://passer.smu.edu">http://passer.smu.edu</a>	<b>Jun. 2021 – Jun. 2022</b>
• Advanced the state-of-the-art prediction accuracy of top 3 protein pockets to <b>82.7%</b> through <b>Automated machine learning (AutoML)</b> methods on larger datasets	
• Deployed the model to our web server Protein Allosteric Site Server (passer.smu.edu) built with <b>Django</b> and <b>JSmol</b> (a <b>JavaScript</b> framework)	
• The web server can handle job submission and protein visualization within web pages and already has <b>37,550</b> visits from more than <b>70</b> countries with more than <b>3,000</b> 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