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**

Graduate Research Assistant

- 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.

Graduate Teaching Assistant

- 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**

- 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**

- 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

- "Machine learning and protein allostery" *Trends in Biochemical Sciences* (2022).

- "Assessments of Variational Autoencoder in Protein Conformation Exploration" *ChemRxiv-2022-g2c00* (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