Sian Xiao (He/Him)

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Education

Southern Methodist University, Dallas, TX **Aug. 2020 – Dec. 2024**

- Ph.D. in Theoretical and Computational Chemistry GPA: 4.0/4.0
- Coursework: Machine Learning, Statistical Mechanics, Quantum Mechanics

Georgia Institute of Technology, Atlanta, GA **Aug. 2022 – Dec. 2024**

- M.S. in Computer Science GPA: 4.0/4.0
- Coursework: Software Dev Process, Database, Computer Network, Data and Visual Analytics, Machine Learning for Trading, etc.

Beijing University of Chemical Technology, Beijing, China **Sep. 2015 – Jul. 2019**

- B.Eng. in Polymer Materials and Engineering GPA: 88.0/100

Skills

- **Languages & Toolkits**: Python, Java, Bash, C, Scala; HTML, CSS; Linux, Git, Docker
- **Data Science & ML**: Scikit-learn, TensorFlow, PyTorch, Keras; Pandas, Spark, OpenRefine
- **Visualization**: Matplotlib, Tableau, D3.js
- **Platforms**: AWS, GCP, Azure ML Studio, DataBricks

Experience

Southern Methodist University, Dallas, TX **Aug. 2020 – May. 2024**

*Graduate Research Assistant – **AI for Science***

- 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.

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.
- One 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 through **Automated machine learning (AutoML)** and **Learn-to-Rank** 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 more than **54,000** visits from more than **70** countries with more than **7,500** 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).
- "PASSer2.0: Accurate Prediction of Protein Allosteric Sites Through **Automated Machine Learning**" *Frontiers in Molecular Biosciences* (2022).
- Others (co-authored 16 papers) could be found at my Google Scholar Website.

Major Awards

- Graduate Research Achievement Award, SMU May. 2023
- Computational Science and Engineering graduate fellowship (2023-2024), SMU Apr. 2023
- University Ph.D. Fellowship (extra funding, recurring 2020-2024), SMU Mar. 2020
- First Prize, Mathematical Contest in Modeling, BUCT May. 2017