# **Hao Tian**

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#### **EDUCATION**

### Southern Methodist University, Dallas, Texas, USA

Aug 2019 – May 2023 (expected)

- Ph.D. in Theoretical and Computational Chemistry
- Adviser: Prof. Peng Tao
- Topic: Understanding protein allostery through molecular dynamics and artificial intelligence
- GPA: 3.9 / 4.0

## Georgia Tech, Atlanta, Georgia, USA

Aug 2020 – May 2022 (expected)

- M.S. in Computer Science, specialization: Computing Systems
- GPA: 4.0 / 4.0

### Beijing University of Chemical Technology, Beijing, China

Aug 2015 – Jun 2019

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

#### **PUBLICATIONS**

- [5] <u>Hao Tian</u>, Xi Jiang and Peng Tao. PASSer: Prediction of Allosteric Sites Server. *Machine Learning: Science and Technology*, 2021, 2, 035015.
- [4] Zilin Song, Hongyu Zhou, <u>Hao Tian</u>, Xinlei Wang and Peng Tao. Unraveling the energetic significance of chemical events in enzyme catalysis via machine-learning based regression approach. *Communications Chemistry*, 2020, 3, 134.
- [3] <u>Hao Tian</u>, Francesco Trozzi, Brian Zoltowski and Peng Tao. Deciphering the Allosteric Process of Phaeodactylum tricornutum Aureochrome 1a LOV Domain. *The Journal of Physical Chemistry B*, 2020, 124, 41, 8960–8972.
- [2] <u>Hao Tian</u> and Peng Tao. ivis Dimensionality Reduction Framework for Biomacromolecular Simulations. *Journal of Chemical Information and Modeling*, 2020, 60, 10, 4569-4581.
- [1] <u>Hao Tian</u> and Peng Tao. Deciphering the Protein Motion of S1 Subunit in SARS-CoV-2 Spike Glycoprotein Through Integrated Computational Methods. *Journal of Biomolecular Structure and Dynamics*, 2020.

### **SKILLS**

Programming languages: Python, Java, Bash

Front end: HTML, CSS, JavaScript

Back end: PHP, SQL

Machine learning packages: Scikit-learn, Keras, PyTorch

# CODING PROJECTS

## PASSer: Protein Allosteric Sites Server, passer.smu.edu

- •A public web server for protein calculations and predictions;
- •Implemented using Python Django framework and JSmol;
- •Integrated with machine learning models: XGBoost and graph convolutional neural network.

### getarticle, an open source Github repository, star: 23, downloads: 8k

- •A package written in Python to download scientific papers in one shot;
- •Web scrapy on Sci-Hub and Google Scholar;
- •Used as both Python module or command line.

## AWARDS & SCHOLARSHIPS

#### **Graduate Research Assisstant Award**

May 2021

Southern Methodist University

Research Days Dean's Award

Mar 2021

Southern Methodist University

**Outstanding Teaching Assistant** Southern Methodist University May 2020

	Meritorious Winner of Mathematical Contest in Modeling Beijing University of Chemical Technology	Mar 2018
	Outstanding Undergraduate Beijing University of Chemical Technology	Sep 2015
PRESENTATIONS	Prediction of Allosteric Sites Through Ensembled Learning Oral, ACS Spring 2021	Apr 2021
	ivis Dimensionality Reduction Method for Macromolecular Simulations Oral, ACS Spring 2021	Apr 2021
	Machine Learning Framework for Deciphering the Allosteric Process of Circadian Clock Protein Oral, The Virtual 2021 Meeting in Miniature at UT Dallas Oral, ACS Spring 2021 Invited talk, Department of Chemistry and Biochemistry, The University of Oklahoma	May 2021 Apr 2021 Nov 2020
	What is hidden behind allostery? An integrated framework to decipher key components in AuLOV dimerization Lightning presentation, 3rd RSC-BMCS/RSC-CICAG Artificial Intelligence in Chemistry	Nov 2020