

# Hao Tian

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## EDUCATION

**Southern Methodist University**, Dallas, Texas, USA

Aug 2019 – Now

- Ph.D. in Theoretical and Computational Chemistry
  - Adviser: Prof. Peng Tao
  - GPA: 3.97 / 4.0

**Georgia Tech**, Atlanta, Georgia, USA

Aug 2020 – Now

- 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

## RESEARCH EXPERIENCE

**Center for Research Computing,  
Center for Drug Discovery, Design, and Delivery (CD4)**

Aug 2019 – Now

Department of Chemistry, Southern Methodist University  
Graduate Research Assistant

Focus:

- Molecular dynamics simulations of biomacromolecules
- Decipher protein allostery through machine learning based methods
- Machine learning and database based allostery development

## PUBLICATIONS

- [5] [Hao Tian](#), Xi Jiang and Peng Tao. PASSer: Prediction of Allosteric Sites Server. *Machine Learning: Science and Technology*, 2021.
- [4] Zilin Song, Hongyu Zhou, [Hao Tian](#), 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] [Hao Tian](#), 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] [Hao Tian](#) and Peng Tao. iVis Dimensionality Reduction Framework for Biomacromolecular Simulations. *Journal of Chemical Information and Modeling*, 2020, 60, 10, 4569-4581.
- [1] [Hao Tian](#) 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.

## PROJECTS

getarticle, an open source Github repository, star: 22, downloads: 6k

- A package based on SciHub and Google Scholar that can download articles given DOI, website address or keywords;
- Imported in Python or used as command line.

PASSer: Protein Allosteric Sites Server, [passer.smu.edu](http://passer.smu.edu)

- A web server to predict allosteric sites given protein PDB ID or PDB file;
- Implemented using Django framework and JSmol;
- Learn both physical properties through XGBoost model and pocket topology through graph convolutional neural network.

## AWARDS & SCHOLARSHIPS

**Outstanding Teaching Assistant**  
Southern Methodist University

May 2020

**Meritorious Winner of Mathematical Contest in Modeling**  
Beijing University of Chemical Technology

Mar 2018

	<b>Outstanding Undergraduate</b> Beijing University of Chemical Technology	Sep 2015
<b>INVITED TALKS</b>	<b>Machine Learning Framework for Deciphering the Allosteric Process of Circadian Clock Protein</b> Department of Chemistry and Biochemistry, The University of Oklahoma	Dec 2020
<b>LEADERSHIP &amp; SERVICES</b>	<b>Diversify Protein Science</b> Member  <b>Living Journal of Computational Molecular Sciences</b> Student reviewer	
<b>SKILLS</b>	Programming languages: Python, Java, Bash, JavaScript, PHP, SQL Skill stacks: HTML, CSS, jQuery, Git Machine learning packages: Scikit-learn, Keras, PyTorch	

*[Last updated on 2021-02-13]*