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 TaoCumulative GPA: 3.95 / 4.0

Georgia Tech, Atlanta, Georgia, USA

Aug 2020 - Now

- M.S. in Computer Science
 - Specialization: Computing Systems
 - Cumulative GPA: 4.0 / 4.0

Beijing University of Chemical Technology, Beijing, China

Aug 2015 - Jun 2019

- B.Eng. in Chemical Engineering
 - Cumulative 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 of biomacromolecules
- Decipher protein allostery through machine learning based methods
- · Machine learning and database based allostery development

PUBLICATIONS

- [5] <u>Hao Tian</u>, Xi Jiang and Peng Tao. PASSer: Prediction of Allosteric Sites Server. *ChemRxiv Preprint*, 2020.
- [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.

PROJECTS

getarticle, an open source Github repository, star: 22, downloads: 5k

- •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

- •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 network.

AWARDS & SCHOLARSHIPS

Outstanding Teaching Assistant

May 2020

Southern Methodist University

Meritorious Winner of Mathematical Contest in Modeling

Mar 2018

Beijing University of Chemical Technology

Outstanding Undergraduate Sep 2015

Beijing University of Chemical Technology

INVITED TALKS Machine Learning Framework for Deciphering

the Allosteric Process of Circadian Clock Protein Dec 2020

Department of Chemistry and Biochemistry, The University of Oklahoma

LEADERSHIP & Diversify Protein Science

SERVICES Member

Living Journal of Computational Molecular Sciences

Student reviewer

SKILLS Programming languages: Python, Java, Bash, JavaScript, PHP, SQL

Skill stacks: HTML, CSS, jQuery, Git

Machine learning packages: Scikit-learn, Keras, PyTorch

[Last updated on 2020-12-12]