

Yihang Wang

Gordon Center for Integrative Science, University of Chicago, Chicago, Illinois 60637

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INTERESTS **Biophysics, Complex System, Statistical Mechanics, Machine Learning, Soft Condensed Matter.** In particular, I'm interested in using ideas in theoretical physics and machine learning to understand collective behavior of biophysical and chemical systems.

RESEARCH EXPERIENCE **Post-doctoral fellow in theoretical chemistry** University of Chicago
The Chicago Center for Theoretical Chemistry
Supervisors: Profs. Aaron Dinner, Benoît Roux, Gregory Voth June 2022—present

Research assistant UMD
Supervisor: Prof. Pratyush Tiwary September 2017—May 2022

Lab Rotation UMD
Supervisor: Prof. Christopher Jarzynski January 2018—April 2018

Research Internship UCI
Supervisor: Prof. Elizabeth Read July 2016—September 2016

Undergraduate Researcher SUSTC
Supervisor: Prof. Jiansheng Wu September 2015—June 2017

EDUCATION **University of Maryland, College Park (UMD)** College Park, Maryland
Ph.D in Biophysics August 2017—May 2022
Supervisor: Prof. Pratyush Tiwary

South University of Science and Technology of China (SUSTC) China
B.Sc. in Physics September 2013—June 2017
Thesis: Phase transition in biological tissues (Outstanding thesis award)
Cumulative GPA: 3.81/4.00 Rank: Top 3

University of California, Irvine (UCI) Irvine, California
UCInspire Program July 2016—September 2016
Cumulative GPA: 4.00/4.00

PUBLICATIONS

1. **From data to noise to data for mixing physics across temperatures with generative artificial intelligence**, Y. Wang, L Herron, P. Tiwary, PNAS. 119(32), p.e2203656119. (2022). [Code]
2. **Interrogating RNA–Small Molecule Interactions with Structure Probing and Artificial Intelligence-Augmented Molecular Simulations**, Y. Wang, S. Parmar, J. Schneekloth Jr, P. Tiwary, ACS Central Science. (2022).
3. **Introducing dynamical constraints into representation learning**. D. Wang, Y. Wang, L. Evans and P. Tiwary, arXiv:2209.00905. (2022).
4. **Understanding the role of predictive time delay and biased propagator in RAVE**, Y. Wang, P. Tiwary, J. Chem. Phys. 152, 144102–144109 (2020).
5. **Machine learning approaches for analyzing and enhancing molecular dynamics simulations**, Y. Wang, J.M. Ribeiro and P. Tiwary, Curr. Op. Struc. Bio. 61, 139-145 (2020).
6. **Confronting pitfalls of AI-augmented molecular dynamics using statistical physics**, S Pant, Y Wang, Z Smith, E Tajkhorshid, P Tiwary, J. Chem. Phys. 153, 234118–234128 (2020). *Featured article; Journal cover and Editors' Choice*

7. **Discovering loop conformational flexibility in T4 lysozyme mutants through Artificial Intelligence aided Molecular Dynamics**, Z. Smith, Y. Wang, P. Ravindra, R. Cooley, P. Tiwary, *J. Phys. Chem. B* 124, 8221-8229 (2020). Special issue on “Machine Learning in Physical Chemistry”
8. **Past–future information bottleneck framework for simultaneously sampling biomolecular reaction coordinate, thermodynamics and kinetics**, Y. Wang, J.M. Ribeiro and P. Tiwary, *Nature Communications* 10, 3573–3580 (2019). [Code]
9. **Kinetics of Ligand-Protein Dissociation from All-Atom Simulations: Are We There Yet?**, J.M. Ribeiro, P. Collado, S.Tsai, Y. Wang and P. Tiwary, *Biochemistry*, 58, 156-165 (2019). Invited perspective article in the special issue Future of Biochemistry
10. **Reweighted Autoencoded Variational Bayes for Enhanced Sampling (RAVE)**, J.M. Ribeiro, P. Collado, Y. Wang and P. Tiwary, *J. Chem. Phys.* 149, 072301-072308 (2018).

HONORS & AWARDS	Ann G. Wylie Dissertation Fellowship	2020-2021
	Outstanding Research Assistant(2%)	2019-2020
	UMD-NCI Partnership for Integrative Cancer Research	2018-2020
	Dean’s Fellowship, UMD	2017
	Overseas Research Project Funding	2016

**OTHER
ACADEMIC
ACTIVITIES**

Talks and posters

1. **Gordon Research Conference/Seminar on Protein Folding Dynamics**
Poster: Mixing physics across temperatures with generative artificial intelligence
Ventura, CA, October, 2022
2. **NCI-UMD Partnership for Integrative Cancer Research**
Virtual Informal Talk Session
Talk: Understanding RNA-small molecule interactions with chemical biology and AI augmented-molecular
October, 2020
3. **PoLS-SRN student seminar**
Talk: How do proteins, nucleic acids and ligands talk to each other: Insights from AI augmented molecular simulations.
May, 2020
4. **IPAM’s Workshop on “Interpretable Learning in Physical Sciences.”**
Machine Learning for Physics and the Physics of Learning
Poster: Past–future Information Bottleneck for Sampling Molecular Reaction Coordinate Simultaneously with Thermodynamics and Kinetics
Los Angeles, CA, October, 2019
5. **International Physics of Living Systems Annual Meeting**
Talk: Predictive information bottleneck for sampling and driving rare events in biophysics
Houston, Texas, June, 2018

Summer schools & Workshops:

1. **BPS Conference, Molecular Biophysics of Membranes**
Tahoe , CA, June 2022
2. **Lorentz Center workshop: Accelerating the Understanding of Rare Events**
online
3. **Machine Learning and Chemistry: Progress so far and Challenges on the Way Forward**
College Park, MD
4. **Telluride School on Theoretical Chemistry**
Telluride, CO

Reviewer for *Proteins: Structure, Function and Bioinformatics* 2021-present

TEACHING EXPERIENCE	PHYS261 General Physics II Laboratory	University of Maryland, College Park
	Teaching Assistant	August 2017—May 2018
	PHYS371 Modern Physics	University of Maryland, College Park
	Teaching Assistant	January 2018—May 2018