

Yihang Wang

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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 computational sciences to understand collective behavior of biophysical and chemical systems.

EDUCATION **University of Maryland, College Park (UMD)** College Park, Maryland
Ph.D in Biophysics August 2017—2022(expected)

South University of Science and Technology of China (SUSTC) Shenzhen, China

B.Sc. in Physics September 2013—June 2017

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

RESEARCH EXPERIENCE **Research assistant** UMD
Supervisor: Prof. Pratyush Tiwary September 2017—Present

Lab Rotation UMD

Supervisor: Prof. Christopher Jarzynski

January 2018—April 2018

Information processing in biological system

Research Internship UCI

Supervisor: Prof. Elizabeth Read

July 2016—September 2016

Analyzing oscillatory behavior of gene networks

Undergraduate Researcher SUSTC

Supervisor: Prof. Jiansheng Wu

September 2015—June 2017

Simulation of topological phase in classical system

PUBLICATIONS

1. **Interrogating RNA-small molecule interactions with structure probing and AI augmented-molecular simulations**, Y. Wang, S. Parmar, J. Schneekloth Jr, P. Tiwary, *bioRxiv*, 2021
2. **Denoising diffusion probabilistic models for replica exchange**, Y. Wang, P. Tiwary, *arXiv:2107.07369*, 2021.
3. **Understanding the role of predictive time delay and biased propagator in RAVE**, Y. Wang, P. Tiwary, *J. Chem. Phys.* 152, 144102–144109 (2020).
4. **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).
5. **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*
6. **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"
7. **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).

8. **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
9. **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
	Mathematical Contest in Modeling (leader of the team)	2016
	Honorable Mention	
	Outstanding Student of Shuren College (5%)	2014
	Start-up University Scholarship, SUSTC	2013–2016

**OTHER
ACADEMIC
ACTIVITIES**

Talks:

1. **NCI-UMD Partnership for Integrative Cancer Research** Virtual Informal Talk Session
Understanding RNA-small molecule interactions with chemical biology and AI augmented-molecular
October, 2020
2. **PoLS-SRN student seminar**
How do proteins, nucleic acids and ligands talk to each other: Insights from AI augmented molecular simulations.
May, 2020
3. **International Physics of Living Systems Annual Meeting** Predictive information bottleneck for sampling and driving rare events in biophysics
Houston, Texas, June, 2018

Summer schools & Workshops:

1. **Lorentz Center workshop: Accelerating the Understanding of Rare Events**
online
2. **Machine Learning and Chemistry: Progress so far and Challenges on the Way Forward**
College Park, MD
3. **IPAM's Workshop on "Interpretable Learning in Physical Sciences."**
Machine Learning for Physics and the Physics of Learning
Los Angeles, CA
4. **Telluride School on Theoretical Chemistry**
Telluride, CO

Reviewer for Proteins 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	Janurary 2018—May 2018

REFERENCES: Available Upon Request