Yihang Wang, Ph.D.

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INTERESTS **Biophysics, Complex System, Statistical Mechanics, Machine Learning, MD simulation.**

PROFESSIONAL EXPERIENCE

Schmidt AI in Science Fellow — University of Chicago
Supervisors: Profs. Aaron Dinner, Gregory Voth — January 2023—present

Post-doctoral fellow in theoretical chemistry — University of Chicago
The Chicago Center for Theoretical Chemistry
Supervisors: Profs. Aaron Dinner, Gregory Voth — June 2022— January 2023

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

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 (Oustanding thesis award)

University of California, Irvine (UCI) — Irvine, California
UCInspire Program — July 2016—September 2016

PUBLICATIONS

1. **Mechanism of Phosphate Release from Actin Filaments**, Y. Wang, J. Wu, V. Zsolnay, TD. Pollard, GA. Voth, PNAS, 121(29), e2408156121. (2024).
2. **From latent dynamics to meaningful representations**. D. Wang, Y. Wang, L. Evans and P. Tiwary, JCTC, 20 (9), 3503-3513 (2024).
3. **The Data-Driven Equation-Free Dynamics Method Applied to Large Many-Protein Complexes: The Example of the Microtubule (MT) Tip Relaxation**. J. Wu, S. Dasetty, D. Beckett, Y. Wang, W. Zhi, AJ Ferguson, GA Voth, Submitted to Biophysical Journal (2024).
4. **Bayesian Inference for Biochemical Networks Using Normalizing Flow Models**. Y. Wang, C. Chi, A. Dinner, Under preparation.
5. **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]**
6. **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).
7. **Understanding the role of predictive time delay and biased propagator in RAVE**, Y. Wang, P. Tiwary, J. Chem. Phys. 152, 144102–144109 (2020).
8. **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).
9. **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***

10. **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"
11. **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]**
12. **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
13. **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

Service

1. Organising committee member of Uchicago AI + Science Summer School (2023, 2024)
2. Organising committee of AAAI Workshop on Responsible Generative Models
3. Organising committee member of Uchicago Schmidt fellow journal club
4. Mentor at Uchicago AI+Science Hackathon 2024

Conferences & Workshops

1. **Mesilla Chemistry Workshop**
Talk: Towards Kinetic Accuracy in Coarse-Grained Models with Machine Learning (Invited) Mesilla, NM, March 2025

2. **Annual Conference on Neural Information Processing Systems**
New Orleans, LA, December 2023

3. **Molecular Machine Learning Conference**
Cambridge, MA, November 2023

4. **Convening of the Eric and Wendy Schmidt AI in Science Postdocs**
Poster: AI-enhanced MD simulation Toronto, Canada, May 2023

5. **The University of Chicago and Caltech Conference on AI+Science**
Chicago, IL, March 2023

6. **Gordon Research Conference/Seminar on Protein Folding Dynamics**
Poster: Mixing physics across temperatures with generative artificial intelligence
Ventura, CA, October, 2022

7. **BPS Conference, Molecular Biophysics of Membranes**
Tahoe , CA, June 2022

8. **Lorentz Center workshop: Accelerating the Understanding of Rare Events**
online

9. **NCI-UMD Partnership for Integrative Cancer Research**
Talk: Understanding RNA-small molecule interactions with chemical biology and AI augmented-molecular October, 2020

10. **PoLS-SRN student seminar**
Talk: How do proteins, nucleic acids and ligands talk to each other: Insights from AI augmented molecular simulations. May, 2020

11. **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, Octorber, 2019

12. **Machine Learning and Chemistry: Progress so far and Challenges on the Way Forward** College Park, MD

13. **Telluride School on Theoretical Chemistry** Telluride, CO

14. **International Physics of Living Systems Annual Meeting**
Talk: Predictive information bottleneck for sampling and driving rare events in biophysics
Houston, Texas, June, 2018

Review Activity: Journal of Chemical Theory and Computation, Journal of Physical Chemistry, Biomolecules, Proteins: Structure, Function and Bioinformatics

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

Gregory A. Voth, Ph.D.
Haig P. Papazian Distinguished Service Professor of Chemistry, University of Chicago
Phone: 773-702-9092
E-mail: gavoth@uchicago.edu

Aaron Dinner, Ph.D.
Professor of Chemistry, University of Chicago
Phone: 773-702-2330
E-mail: dinner@uchicago.edu

Pratyush Tiwary, Ph.D.
Millard and Lee Alexander Professor in Chemical Physics,
University of Maryland, College Park
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E-mail: ptiwary@umd.edu