Yihang Wang, Ph.D.

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

PROFESSIONAL EXPERIENCE

Malcolm E. and Betty C. Kenney Distinguished Assistant Professor
Case Western Reserve University , Department of Chemistry — July 2025—present

Schmidt AI in Science Fellow — University of Chicago
Supervisors: Profs. Aaron Dinner, Gregory Voth — January 2023—June 2025

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

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

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

PUBLICATIONS

1. **Thermally Activated Snap-through Transitions Controlled by Tunable Metastability**, R. Zhao, Y. Zhang, C. Luo, Y. Wang, arXiv:2508.14658. (2025)
2. **Adversarial Training for Dynamics Matching in Coarse-Grained Models**, Y. Wang, G.A. Voth, J. Chem. Phys. 163, 104105. (2025)
3. **Mitigating mode collapse in normalizing flows by annealing with an adaptive schedule: Application to parameter estimation**, Y. Wang, C. Chi, A. Dinner, arXiv:2505.03652. (2025)
4. **Reaching the full potential of cryo-EM reconstructions with molecular dynamics simulations at 310 K: Actin filaments as an example**, S.S. Iyer, K.M. Hermana, Y. Wang, T.D. Pollard, G.A. Voth, PNAS 122.48 (2025): e2521421122. (2025)
5. **Mechanistic Insights into Lenacapavir-Induced Off-Pathway HIV-1 Capsid Assembly**, M. Gupta, C. Waltmann, N. Renner, Y. Wang, L. James, D.A. Jacques, T. Bocking, G.A. Voth, bioRxiv 2025.08.13.670175. (2025)
6. **Mechanism of phosphate release from actin filaments**, Y. Wang, J. Wu, V. Zsolnay, TD. Pollard, GA. Voth, PNAS, 121(29), e2408156121. (2024).
7. **From latent dynamics to meaningful representations**. D. Wang, Y. Wang, L. Evans and P. Tiwary, JCTC, 20 (9), 3503-3513 (2024).

8. **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, T. Skora, T. Bidone, AJ Ferguson, GA Voth, Biophysical Journal (2025).
9. **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**]
10. **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).
11. **Understanding the role of predictive time delay and biased propagator in RAVE**, Y. Wang, P. Tiwary, J. Chem. Phys. 152, 144102–144109 (2020).
12. **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).
13. **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***
14. **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"
15. **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**]
16. **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
17. **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

Schmidt AI in Science Postdoctoral Fellowship	2023-2026
Chicago Center for Theoretical Chemistry Postdoctoral Fellowship	2022-2023
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

Invited Talks, Conferences, & Workshops

1. **Breaking Boundaries in AI & Biology**
Talk: Beyond Boundaries: AI and the Future of Scientific Discovery in Biology (Invited) Cleveland, OH, November 2025

2. **Rocky Mountain Regional Meeting (RMRM)**
Talk: Generative AI for Molecular Simulations: From Coarse-Graining to Rare Event Discovery (Invited) Albuquerque, NM, October 2025

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

4. **Makerere University, Uganda**
Talk: Artificial Intelligence Augmented Molecular Dynamics Methods for Probing Ligand Dissociation from Nucleic Acids (Invited) By Zoom, December 2024

5. **University of Tennessee, Knoxville**
Talk: Integrating AI with Molecular Simulations: Enhancing Sampling and Coarse-Grained Modeling (Invited) Knoxville, TN, December 2024

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

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

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

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

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

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

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

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

14. **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

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

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

17. **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, Physical Review B, Biomolecules, Proteins: Structure, Function and Bioinformatics

TEACHING

CHEM 352/452 AI in Chemistry
Case Western Reserve University January 2026-present

CHEM 113 Principles of Chemistry Laboratory
Case Western Reserve University August 2025—December 2025

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