Pratyush Tiwary **CURRICULUM VITAE**

Millard and Lee Alexander Professor
Department of Chemistry & Biochemistry
and Institute for Physical Science & Technology
University of Maryland at College Park

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Summary of research interests

Rare events in Chemistry, Biology and Materials Science; Drug Discovery; Thermodynamics, Statistical Mechanics and their connections with Artificial Intelligence

Education

Ph.D., California Institute of Technology 2008–2012
Department of Applied Physics & Materials Science Pasadena, CA
Supervisor: Prof. Axel van de Walle
Thesis: Atomistic simulations of materials - methods for accurate potentials and realistic time scales

M.S., California Institute of Technology 2007–2008
Department of Applied Physics & Materials Science Pasadena, CA

B.Tech., Indian Institute of Technology - Banaras Hindu University 2003–2007
Department of Metallurgical Engineering Varanasi, India
Thesis: Potts Model - Monte Carlo simulations of grain boundary effects on spinodal decomposition

Work experience

Professor and Millard and Lee Alexander Professor, Department of Chemistry & Biochemistry and Institute for Physical Science & Technology, University of Maryland, College Park 2023–present

Professor (Secondary Appointment), Department of Chemistry & Molecular Biology, School of Medicine, University of Maryland, Baltimore 2023–present

Lead, Therapeutic Discovery, Institute for Health Computing, University of Maryland Baltimore and College Park 2023–present

Associate Professor (with tenure), Department of Chemistry & Biochemistry and Institute for Physical Science & Technology, University of Maryland, College Park 2022–2023

Assistant Professor (tenure-track), Department of Chemistry & Biochemistry and Institute for Physical Science & Technology, University of Maryland, College Park 2017–2022

Affiliate Professor, Applied Mathematics & Statistics, and Scientific Computation (AMSC) program
Affiliate Professor, Biophysics program
Affiliate Professor, Chemical Physics program
Affiliate Professor, Department of Materials Science and Engineering

Post-doc with Prof. Bruce Berne, Department of Chemistry, Columbia University 2015–2017

Post-doc with Prof. Michele Parrinello, Department of Chemistry and Applied Biosciences, ETH Zurich 2013–2015

Awards

1. Nature Communications Editors' choice article in both "Applied physics and mathematics" and "AI and machine learning" categories (2024)
2. Board of Visitors Creative Educator Award, University of Maryland (2023)

3. Joseph O. Hirschfelder Distinguished Visitor, Theoretical Chemistry Institute, University of Wisconsin-Madison (2023)
4. Nature Communications Editors' choice article in "Applied physics and mathematics" category (2022)
5. Dean's Award for Excellence in Teaching, University of Maryland (2022; Nominated by students)
6. Sloan Research Fellow in Chemistry (2022)
7. "Rising Talent" Speaker, American Conference on Theoretical Chemistry (2022)
8. National Institutes of Health R35 Maximizing Investigators' Research Award (MIRA) (2021)
9. ACS OpenEye Outstanding Junior Faculty Award (2021)
10. National Science Foundation (NSF) CAREER award (2021)
11. Emerging Investigator, Journal of Chemical Physics (2021)
12. Nature Communications top-ten of the year article as Editors' choice in both "Applied physics and mathematics" and "AI and machine learning" categories (2020)
13. Philip Merrill Outstanding Faculty Mentor Award (2020)
14. Emerging Investigator, Royal Society of Chemistry's Molecular Systems Design and Engineering (2020)
15. Doctoral New Investigator Award from ACS-Petroleum Research Fund (2019)
16. "Future of Biochemistry", ACS journal Biochemistry (2019)
17. Emerging Investigator, Journal of Chemical Physics (2019)
18. Editors' choice award, Journal of Chemical Physics for manuscript titled "Predicting reaction coordinates in energy landscapes with diffusion anisotropy" (2018)
19. Research and Scholarship Award, University of Maryland Graduate School (2017)
20. Peter Salamon Award for Young Scientists, Telluride Science Research Center (2016)
21. NSF MCC-UIUC Travel Award for attending CECAM workshop in Vienna (2015)
22. Division of Engineering and Applied Sciences Fellowship, California Institute of Technology (2007–2008).
23. Certificate of merit for outstanding all-round achievement, Banaras Hindu University (2007).
24. First prizes in National Level Paper Presentation Contests, IIT-BHU (Multiple years 2005, 2006, 2007).
25. Summer Research Fellowship, Indian Academy of Sciences (2005)

Awards won by mentored Students and Research Associates

1. Dedi Wang – Finalist for American Chemical Society PHYS Division Outstanding Graduate Student Award (2024)
2. Eric Beyerle – American Chemical Society Wiley Outstanding Postdoc Award (2024)
3. Anurag Sodhi – Gold Medal, International Chemistry Olympiad (2023)
4. Bodhi Vani – Best Poster Prize, Gordon Research Conference on Protein Folding Dynamics (2022)
5. Pavan Ravindra – Churchill Scholarship to Cambridge University, UK; Goldwater Scholarship; Chemical Society of Washington Outstanding Undergraduate Researcher Award (2019–2021)
6. Yihang Wang – University of Chicago Centre for Theoretical Chemistry Independent Postdoctoral Fellowship; Ann Wylie Dissertation Fellowship; Outstanding Graduate Research Assistant Award (2018–2021)
7. Dedi Wang – Ann Wylie Dissertation Fellowship; Outstanding Graduate Research Assistant Award (2021–2023)
8. Zachary Smith – Ann Wylie Dissertation Fellowship; NSF COMBINE fellowship; Outstanding Graduate Research Assistant Award (2018–2021)
9. Luke Evans – Ann Wylie Dissertation Fellowship; Outstanding Graduate Research Assistant Award (2021)

Publications

1. *Inferring phase transitions and critical exponents from limited observations with Thermodynamic Maps*, L. Herron, K. Mondal, J. Schneekloth and P. Tiwary, **Proc. Natl. Acad. Sci.** (in press).
2. *Thermodynamics-inspired explanations of artificial intelligence*, S. Mehdi and P. Tiwary, **Nature Communications** (2024). ***Featured article as Editors' choice in both "Applied physics and mathematics" and "AI and machine learning" categories.***
3. *Atomic scale insights into NaCl nucleation in nanoconfined environments*, R. Wang and P. Tiwary, **Chemical Science** (2024).
4. *From latent dynamics to meaningful representations*, D. Wang, Y. Wang, L.A. Evans and P. Tiwary, **J. Chem. Theor. Comp.** (2024).
5. *Graph Attention Site Prediction (GrASP): Identifying Druggable Binding Sites Using Graph Neural Networks with Attention*, Z. Smith, M. Strobel, B.P. Vani and P. Tiwary, **J. Chem. Inf. Mod.** (2024).
6. *Thermodynamically Optimized Machine-learned Reaction Coordinates for Hydrophobic Ligand Dissociation*, E.R. Beyerle and P. Tiwary, **J. Phys. Chem. B.** (2024).
7. *Is the local ion density sufficient to drive NaCl nucleation in vacuum and in water?*, R. Wang, S. Mehdi, Z. Zou and P. Tiwary, **J. Phys. Chem. B.** (2024).
8. *Urea nucleation in water: Do long-range forces matter?*, R. Zhao, Z. Zou, J. D. Weeks and P. Tiwary, **J. Chem. Theor. Comp.** (2024).
9. *Exploring kinase DFG loop conformational stability with AlphaFold2-RAVE*, B.P. Vani, A. Aranganathan and P. Tiwary, **J. Chem. Inf. Mod.** (2024).
10. *Enhanced Sampling with Machine Learning: A Review*, S. Mehdi, Z. Smith, L. Herron, Z. Zou and P. Tiwary, **Ann. Rev. Phys. Chem. vol 75** (2023).
11. *Recent advances in describing and driving crystal nucleation using machine learning and artificial intelligence*, E.R. Beyerle, Z. Zou and P. Tiwary, **Curr. Op. Solid State Mat. Sci.** (2023).
12. *AlphaFold2-RAVE: From Sequence to Boltzmann Ranking*, B. Vani, A. Aranganathan, D. Wang and P. Tiwary, **J. Chem. Theor. Comp.** 19, 4351–4354 (2023).
13. *Good things take time: Tiwary-Seeliger collaboration for predictive pharmacodynamics*, P. Tiwary and M. Seeliger, **Angewandte Chemie** 62, e202303339 (2023). ***Invited Team Profile.***
14. *Driving and characterizing nucleation of urea and glycine polymorphs in water*, E.R. Beyerle, Z. Zou, S.-T. Tsai and P. Tiwary, **Proc. Natl. Acad. Sci.** 120, e2216099120 (2023).
15. *Computing committors in collective variables via Mahalanobis diffusion maps*, L.A. Evans, M.K. Cameron and P. Tiwary, **Applied and Computational Harmonic Analysis** 64, 62–101 (2023).
16. *Path sampling of recurrent neural networks by incorporating known physics*, S.T. Tsai, E. Fields, Y. Xuo, E. J. Kuo and P. Tiwary, **Nature Communications** 13, 7231–7240 (2022).
    Featured article as Editors' choice in "Applied physics and mathematics" category.
17. *Artificial Intelligence in computational materials science: overview*, H.J. Kulik and P. Tiwary **MRS Bulletin** 47, 927–929 (2022).
18. *Computing committors via Mahalanobis diffusion maps with enhanced sampling data*, L.A. Evans, M.K. Cameron and P. Tiwary, **J. Chem. Phys.** 157, 214107–214115 (2022).
19. *Molecular recognition of methylated amino acids and peptides by Pillar[6]MaxQ*, D. King, C. Wilson, L. Herron, C.-L. Deng, S. Mehdi, P. Tiwary, F. Hof and L. Isaacs, **Org. Biomol. Chem.** 20, 7429–7438 (2022).
20. *From data to noise to data for mixing physics across temperatures with generative artificial intelligence*, Y. Wang, L. Herron and P. Tiwary, **Proc. Natl. Acad. Sci.** 119, e2203656119 (2022).
21. *Protein flexibility and dissociation pathway differentiation can explain onset of resistance mutations in kinases*, M. Shekhar, Z. Smith, M. Seeliger and P. Tiwary, **Angewandte Chemie** 61, e202200983–e202200989 (2022).
    Featured as Hot Paper.

22. *Interrogating RNA-small molecule interactions with structure probing and AI augmented-molecular simulations*, Y. Wang, S. Parmar, J. Schneekloth Jr. and P. Tiwary, **ACS Cent. Sci.** 8, 741–748 (2022).

23. *Quantifying Energetic and Entropic Pathways in Molecular Systems*, E.R. Beyerle, S. Mehdi and P. Tiwary, **J. Phys. Chem. B**. 126, 3950–3960 (2022).

24. *Accelerating all-atom simulations and gaining mechanistic understanding of biophysical systems through State Predictive Information Bottleneck*, S. Mehdi, D. Wang, S. Pant and P. Tiwary, **J. Chem. Theor. Comp.** 18, 3231–3238 (2022).

25. *Influence of long range forces on the transition states and dynamics of NaCl ion-pair dissociation in water*, D. Wang, R. Zhao, J. D. Weeks and P. Tiwary, **J. Phys. Chem. B** 126, 545–551 (2022).

26. *Towards automated sampling of polymorph nucleation and free energies with SGOOP and metadynamics*, Z. Zou, S.T. Tsai and P. Tiwary, **J. Phys. Chem. B** 125, 13049–13056 (2021).

27. *SGOOP-d: Estimating kinetic distances and reaction coordinate dimensionality for rare event systems from biased/unbiased simulations*, S.T. Tsai, Z. Smith and P. Tiwary, **J. Chem. Theor. Comp.** 17, 6757–6765 (2021).

28. *Making high-dimensional molecular distribution functions tractable through Belief Propagation on Factor Graphs*, Z. Smith and P. Tiwary, **J. Phys. Chem. B**. 125, 11150–11158(2021).

29. *State Predictive Information Bottleneck*, D. Wang and P. Tiwary, **J. Chem. Phys.** 154, 134111–134119 (2021).

30. *On the distance between A and B in molecular configuration space*, S.T. Tsai and P. Tiwary, **Mol. Sim.** 46, 1-8 (2021).

31. *Confronting pitfalls of AI-augmented molecular dynamics using statistical physics*, S. Pant, Z. Smith, Y. Wang, E. Tajkhorshid and P. Tiwary, **J. Chem. Phys.** 153, 234118–234128 (2020).
Featured article; Journal cover and Editors' Choice

32. *Learning Molecular Dynamics with Simple Language Model built upon Long Short-Term Memory Neural Network*, S.T. Tsai, E.J. Kuo and P. Tiwary, **Nature Communications** 11, 5115–5125 (2020).
Featured article as Editors' choice in both "Applied physics and mathematics" and "AI and machine learning" categories.

33. *Discovering loop conformational flexibility in T4 lysozyme mutants through artificial intelligence aided molecular dynamics*, Z. Smith, P. Ravindra, Y. Wang, R. Cooley and P. Tiwary, **J. Phys. Chem. B** 124, 8221-8229 (2020). Special issue on "Machine Learning in Physical Chemistry"

34. *Understanding the role of predictive time delay and biased propagator in RAVE*, Y. Wang and P. Tiwary, **J. Chem. Phys.** Special issue on "Machine Learning Meets Chemical Physics", **J. Chem. Phys.** 152, 144102–144109 (2020).

35. *Automatic mutual information noise omission (AMINO): generating order parameters for molecular systems*, P. Ravindra, Z. Smith and P. Tiwary, **Mol. Sys. Des. Engg** 5, 339-348 (2020).

36. *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).

37. *Reaction coordinates and rate constants for liquid droplet nucleation: quantifying the interplay between driving force and memory*, S.T. Tsai, Z. Smith and P. Tiwary, **J. Chem. Phys.** 151, 154106-154113 (2019).

38. *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).

39. *Promoting transparency and reproducibility in enhanced molecular simulations*, Bonomi, Bussi, Camilloni et al, **Nature Methods** 16, 670–673 (2019).

40. *Can One Trust Kinetic and Thermodynamic Observables from Biased Metadynamics Simulations: Detailed Quantitative Benchmarks on Millimolar Drug Fragment Dissociation*, D. Pramanik, Z. Smith, A. Kells and P. Tiwary, **J. Phys. Chem. B** 123, 3672–3678 (2019).

41. *Towards Achieving Efficient and Accurate Ligand-Protein Unbinding with Deep Learning and Molecular Dynamics through RAVE*, J.M. Ribeiro and P. Tiwary, **J. Chem. Theor. Comp.** 15, 708-719 (2019).

42. *Ligand dissociation mechanisms from all-atom simulations: Are we there yet?*, J.M. Ribeiro, S.T. Tsai, D. Pramanik, Y. Wang and P. Tiwary, **Biochemistry**, invited perspective article in the special issue *Future of Biochemistry*, 58, 156-165 (2019).

43. *Multi-dimensional spectral gap optimization of order parameters (SGOOP) through conditional probability factorization*, Z. Smith, S.T. Tsai, D. Pramanik and P. Tiwary, **J. Chem. Phys.** 149, 234105-234113 (2018).

44. *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).

45. *Frequency adaptive metadynamics for the calculation of rare event kinetics* Y. Wang, O. Valsson, P. Tiwary, M. Parrinello and K. Lindorff-Larsen, **J. Chem. Phys.** 149, 072309-072315 (2018).

46. *Molecular determinants and bottlenecks in the dissociation dynamics of biotin-streptavidin*, P. Tiwary, **J. Phys. Chem. B** 121, 10841-10849 (2017).

47. *Kinetics of ligand binding through advanced computational approaches*, A. Dickson, P. Tiwary and H. Vashisth, **invited review article for Curr. Top. Med. Chem.** 17, 2626-2641 (2017).

48. *Predicting reaction coordinates in energy landscapes with diffusion anisotropy*, P. Tiwary and B.J. Berne, **J. Chem. Phys.: Special Topic Issue on Reaction Pathways** 147, 152701-152708 (2017).
Selected as Editors' Choice

49. *How does an anti-cancer drug molecule unbind?*, P. Tiwary, J. Mondal and B.J. Berne, **Science Advances** 3, e1700014-e1700019 (2017).

50. *Unbinding kinetics of a p38 MAP kinase type II inhibitor from metadynamics simulations*, R. Casasnovas, P. Tiwary, V. Limongelli, P. Carloni and M. Parrinello, **J. Amer. Chem. Soc.** 139, 4780-4788 (2017).

51. *Overcoming time scale and finite size limitations to compute nucleation rates from small scale well tempered metadynamics simulations*, M. Salvalaglio, P. Tiwary, M. Mazzotti and M. Parrinello, **J. Chem. Phys.** 145, 211925-211934 (2016).

52. *How wet should be the reaction coordinate for ligand unbinding?*, P. Tiwary and B.J. Berne, **J. Chem. Phys.** 145, 054113-054119 (2016).

53. *Prediction of protein-ligand binding poses via a combination of induced fit docking and metadynamics simulations*, A.J. Clark, P. Tiwary, K. Borrelli, S. Feng, E. Miller, R. Abel, R.A. Friesner and B.J. Berne, **J. Chem. Theor. Comp.** 12, 2990-2998 (2016).

54. *How a kinase inhibitor withstands gatekeeper residue mutations*, J. Mondal, P. Tiwary and B.J. Berne, **J. Amer. Chem. Soc.** 138, 4608-4615 (2016).

55. *Kramers turnover: from energy diffusion to spatial diffusion using metadynamics*, P. Tiwary and B.J. Berne, **J. Chem. Phys.** 144, 134103-134105 (2016).

56. *Spectral gap optimization of order parameters (SGOOP) for sampling complex molecular systems*, P. Tiwary and B.J. Berne, **Proc. Natl. Acad. Sci.** 113, 2839-2844 (2016).

57. *A New Approach for Investigating Reaction Dynamics and Rates with Ab Initio Calculations*, K. Fleming, P. Tiwary and J. Pfaendtner, **J. Phys. Chem. A** 120, 299-305 (2016).
Selected as ACS Editors' choice.

58. (Invited review article) *Enhancing essential fluctuations: Rare events and metadynamics*, O. Valsson, P. Tiwary and M. Parrinello, **Ann. Rev. Phys. Chem.** 67, 159-184 (2016). (Web of Science top 1 % cited paper)

59. *Role of water and steric constraints in the kinetics of cavity-ligand unbinding*, P. Tiwary, J. Mondal, J. Morrone and B.J. Berne, **Proc. Natl. Acad. Sci.** 112, 12015-12019 (2015).

60. *A perturbative solution to metadynamics ordinary differential equation*, P. Tiwary, J. Dama and M. Parrinello, **J. Chem. Phys.** 143, 234112-243115 (2015).

61. *De Broglie swapping metadynamics for quantum and classical sampling*, M.Nava, R. Quhe, F. Palazzesi, P. Tiwary, and M. Parrinello, **J. Chem. Theor. Comp.** 11, 5114-5119 (2015).
62. *Variationally optimized free energy flooding for rate calculation*, J. McCarty, O. Valsson, P. Tiwary and M. Parrinello, **Phys. Rev. Lett.** 115, 070601-070605 (2015).
63. *Path integral metadynamics*, R. Quhe, M. Nava, P. Tiwary, and M. Parrinello, **J. Chem. Theor. Comp.** 11, 1383-1388 (2015).
64. *Kinetics of protein-ligand unbinding: predicting pathways, rates and rate-limiting steps*, P. Tiwary, V. Limongelli, M. Salvalaglio and M. Parrinello, **Proc. Natl. Acad. Sci.** 112, E386-E391 (2015). (Web of Science top 1 % cited paper)
65. *A time-independent free energy estimator for metadynamics*, P. Tiwary and M. Parrinello, **J. Phys. Chem. B** 119, 736-742 (2015). (Web of Science top 1 % cited paper)
66. *Ab initio calculation of anisotropic interfacial excess free energies*, A. van de Walle, Q. Hong, L. Miljacic, C. B. Gopal, S. Demers, G. Pomrehn, A. Kowalski and P. Tiwary, **Phys. Rev. B** 89, 184101-184111 (2014).
67. *Assessing the reliability of dynamics reconstructed from metadynamics*, M. Salvalaglio, P. Tiwary and M. Parrinello, **J. Chem. Theor. Comp.** 10, 1420-1425 (2014).
68. *From metadynamics to dynamics*, P. Tiwary and M. Parrinello, **Phys. Rev. Lett.** 111, 230602-230606 (2013).
    Highlighted in the issue as exceptional research.
69. *Accelerated molecular dynamics through stochastic iterations and collective variable based basin identification*, P. Tiwary and A. van de Walle, **Phys. Rev. B** 87, 094304-094308 (2013).
70. *Efficient stochastic generation of special quasirandom structures*, A. van de Walle, P. Tiwary, M. de Jong, D.L. Olmstead, M. Asta, A. Dick, D. Shin and Y. Wang, **Calphad** 42, 13-18 (2013). (Web of Science top 1 % cited paper)
71. *Hybrid deterministic and stochastic approach for efficient atomistic simulations at long time scales*, P. Tiwary and A. van de Walle, **Phys. Rev. B (Rapid)** 84, 100301-100304 (2011).
72. *Interatomic potentials for mixed oxide and advanced nuclear fuels*, P. Tiwary, A. van de Walle, B. Jeon and N. Grønbech-Jensen, **Phys. Rev. B** 84, 094104-094109 (2011).
73. *Ab initio construction of interatomic potentials for uranium dioxide across all interatomic distances*, P. Tiwary, A. van de Walle and N. Grønbech-Jensen, **Phys. Rev. B** 80, 174302-174309 (2009).
74. *An analytical expression for the characteristic length scale for randomly faulted hexagonal close-packed structures*, P. Tiwary and D. Pandey, **Acta Cryst. Sec. A** 63, 481-482 (2007).
75. *Scaling behaviour of pair correlation functions for randomly faulted hexagonal close-packed structures*, P. Tiwary and D. Pandey, **Acta Cryst. Sec. A** 63, 289-295 (2007).
76. *Cluster variation investigation of phase equilibria in FeCo system using simulated annealing approach*, P. Tiwary and S.K. Ghosh, **Comp. Mat. Sci.** 39, 788-793 (2007).

Book Chapters

1. "Metadynamics: a unified framework for accelerating rare events and sampling thermodynamics and kinetics", in *Handbook for Materials Modeling.* Editors: Wanda Adreoni and Sidney Yip. Publisher: Springer.
2. "Extended time-scale atomistic simulations", in *Multiscale Modeling for Nanomechanics (Springer Series in Materials Science).* Editors: C.R. Weinberger, G. Trucker. Publisher: Springer.

Active External Grants (Net amount raised $4.7M, including $4.3M Tiwary's share)

1. Principal investigator for DOE-BES grant from Condensed Phase and Interfacial Molecular Science program titled "Modeling phase transitions in liquids with interfaces with Artificial Intelligence and Local Molecular Field theory", $1,427,010; Tiwary's share approx. $1,250,000 (2020–2026)
2. Sole investigator for NIH R35 MIRA grant from NIH/NIGMS titled "From atoms to mechanisms - Artificial Intelligence augmented molecular simulations for mechanistic ligand design", $1,868,775 (2021–2026)
3. Sole investigator for NSF CAREER grant from Chemical Theory, Models, and Computational Methods program (Chemistry Division) titled "Learning to learn - Artificial Intelligence Augmented Chemistry for Molecular Simulations and Beyond", $650,000 (2021–2026)
4. Sole investigator for Sloan Research Fellowship, $75,000 (2022–2024)
5. Principal investigator for grant titled "Quantifying human RNA targetability for small molecule drug discovery" from NCI-UMD Partnership for Integrative Cancer Research, approx. $160,000 (2022–2025)
6. Principal investigator for grant titled "Modeling structure, thermodynamics and kinetics of T cell activation by antigens" from NCI-UMD Partnership for Integrative Cancer Research, approx. $160,000 (2022–2025)
7. Gift from Schrodinger, LLC to support research activities in Tiwary lab, $75,000 (2019–2022)

Active Computing Grants

1. Principal investigator for net 25+ million CPU and GPU hours project (XSEDE/ACCESS, USA, 2018–current)

Completed Grants

1. Principal investigator for ACS-PRF "Doctoral New Investigator" grant to study nucleation mechanisms in zeolite materials, $110,000 (2019–2021)
2. Principal investigator for grant titled "Demystifying sequence-specific nucleic acids-ligand interactions with statistical mechanics and deep learning based all-atom simulations" from NCI-UMD Partnership for Integrative Cancer Research, approx. $150,000 (2018–2021)
3. Co-Principal investigator for Teaching Innovation Grant for Mathematics for Physical Chemistry, Tiwary's share $6,000 (2020)
4. Principal investigator for NSF-MolSSI grant for organizing workshop on 'Machine learning in chemistry: progress so far and challenges ahead', College Park, $22,000 (2019)
5. Co-principal investigator for Indo-US Science & Technology Forum grant for organizing workshop on 'Recent Advances in modeling Rare Events (RARE)', Agra, India, approx. $17,500 (2017)
6. Principal investigator for a 2.3 million CPU hours project (Swiss National Supercomputing Centre, Switzerland, 2014)
7. Co-principal investigator for a 1.1 million CPU hours project (Forschungszentrum Julich, Germany, 2014)
8. Principal investigator for CECAM grant for organizing workshop on 'Long time dynamics from short time simulations', Lugano, Switzerland, approx. $16,200 (2013)
9. Principal investigator for a 0.2 million CPU hours project (XSEDE, USA, 2012)

Mentoring activities

Current Postdoctoral researchers:

1. Da Teng
2. Xinyu Gu
3. Ruiyu Wang
4. Yunrui Qiu

Current PhD students:

1. Shams Mehdi, Biophysics
2. Akashnathan Aranganathan, Biophysics
3. Lukas Herron, Biophysics
4. Suemin Lee, Biophysics
5. Vanessa Meraz, Chemical Physics
6. Anjali Verma, Biophysics
7. Richard John, Physics
8. Sai Venkata Sreyas Adury, Chemical Physics
9. Mariadelia Argello-Acua, Biophysics

Alumni:
PhD students – 6

1. Dr. Dedi Wang (PhD in Biophysics), Postdoc at Genentech, San Francisco
2. Dr. Ziyue Zou (PhD in Chemistry), Postdoc with Prof. James Fraser, UCSF
3. Dr. Zachary Smith (PhD in Biophysics), Senior Scientist, Schrodinger
4. Dr. Luke Evans, (PhD in Applied Mathematics & Statistics, and Scientific Computation), Flatiron Institute Postdoctoral Research Fellow, New York
5. Dr. Yihang Wang (PhD in Biophysics), Eric and Wendy Schmidt AI in Science Postdoctoral Fellow, University of Chicago
6. Dr. Sun-Ting Tsai (PhD in Physics), Postdoctoral Fellow with Prof. Sharon Glotzer at University of Michigan, Ann Arbor

Postdoctoral – 4

1. Dr. Eric Beyerle, postdoc researcher, now Postdoc with Prof. Kresten Lindorff-Larsen, University of Copenhagen
2. Dr. Bodhi Vani, postdoc researcher, now Machine Learning Scientist at Prescient Design, San Francisco
3. Dr. Joao Ribeiro, postdoc researcher, now tenure-track Assistant Professor of Chemistry at St. Josephs College, New York
4. Dr. Debabrata Pramanik, postdoc researcher, now scientist at IIT Kanpur

Editorial service

1. Associate Editor, Journal of Chemical Theory and Computation, 2023–
2. Guest Editor (with Chaok Seok), Current Opinion in Structural Biology - Artificial Intelligence (AI) Methodologies in Structural Biology, 2025–
3. Co-editor (with Pilar Cossio and Francesca Grisoni), Journal of Chemical Physics (JCP) Special Issue on “Machine Learning for Biomolecular Modeling”, 2024
4. Member of Advisory Board, Nature Reviews Physics, 2023–2024
5. Member of Editorial Board, Proteins: Structure, Function and Bioinformatics, 2021–

6. Co-editor (with Christoph Dellago, Laura Filion, Frank Noe and Christine Peter), Journal of Chemical Physics (JCP) Special Issue on "Machine Learning hits molecular simulations", 2022
7. Co-editor (with Heather Kulik), Materials Research Society (MRS) Bulletin Special Issue on "Artificial Intelligence for Materials Science", 2022
8. Topic editor, Frontiers special issue on "Molecular Dynamics and Machine Learning in Drug Discovery", 2020

Other service and synergistic activities

1. Standing Member, NIGMS MRAB (R35) study section, 2024–2028
2. Lead Panelist on "AI algorithms, trustworthiness, and interpretability", Department of Energy Office of Science (SC) Roundtable on Transformational Science Enabled by Artificial Intelligence: Materials and Chemical Sciences, 2024
3. Member, Scientific Advisory Board, Schrödinger, Inc. 2023–
4. Member, Physician-Scientist Early Investigator Program Mentoring Committee for Dr. Andra Krauze, National Cancer Institute, 2023–
5. Member, Advisory Committee, Natural Sciences and Engineering (NSE) department, Prince George's Community College, Largo, Maryland, 2018–
6. Reviewer on continued basis for grant proposals from National Institutes of Health, US Department of Energy, National Science Foundation, Office of Naval Research, European Research Council, Canada Excellence Research Chairs, Centre Europen de Calcul Atomique et Molculaire (CECAM), ACS Petroleum Research Fund and others.
7. Member, Executive Council, Theory and Computation Sub-group of Biophysical Society (2022-2026)
8. Organizer, 3-day international workshop on "Machine learning in chemistry: are we there yet?", funded by NSF-MolSSI, College Park, June 2023 (forthcoming)
9. Organizer, 5-day international workshop on "Rare Events: Analysis, Numerics, and Applications", Brin Mathematics Research Centre, University of Maryland, February 2023
10. Co-organizer, International conference on "Recent Advances in modeling Rare Events (RARE)", virtual, December 2021
11. Organizer, 4-day session on "Predicting Rare-Event Kinetics in Complex Systems with Theory, Simulations, and Machine Learning" at APS March meeting, March 2021
12. Principal organizer, 3-day workshop on "Machine learning in chemistry: progress so far and challenges ahead", funded by NSF-MolSSI, College Park, November 2019
13. Principal organizer, 3-day international symposium on "Sampling conformations and pathways in biomolecular systems", ACS Spring Meeting, March 2019
14. Referee for Proceedings of National Academy of Sciences, Nature Communications, Nano Letters, Physical Review Letters, Journal of Physical Chemistry Letters, Journal of Chemical Physics, Journal of Chemical Theory and Computation, Biophysical Journal, Chemical Physics Letters, Physical Review B, Scientific Reports, Medicinal Chemical Communications, Philosophical Magazine, Intermetallics, Computational Materials Science, Biopolymers, Biochimica et Biophysica Acta, Cell Chemical Biology
15. Co-organizer, International conference on "Recent Advances in modeling Rare Events (RARE)", Agra, India, December 2017
16. Co-organizer, International CECAM conference on "Long time dynamics from short time simulations", Lugano, Switzerland, March 2014
17. Secretary, Materials Research Society Caltech Chapter, 2008-2012. I helped establish the chapter and initiated the first weekly journal club in the Department of Applied Physics and Materials Science, Caltech.
18. President, Caltech Alpine Club, 2011–2012.

Service to the University of Maryland

1. Member, College Appointment, Promotion and Tenure (APT) Committee, University of Maryland (2023–2025)
2. Chair, Mentoring Committee for Prof. Hong-Zhou Ye, Department of Chemistry and Biochemistry and IPST (2024–)
3. Faculty Advisory Committee, Department of Chemistry and Biochemistry (2019–2021, 2023–)
4. Member, Summer Research Fellowships Committee, University of Maryland (2023, 2024)
5. Chair, Search Committee for two open-rank tenured/tenure-track faculty positions, Department of Chemistry and Biochemistry, University of Maryland (2022–2023)
6. Member, Search Committee for Business Director of Institute for Physical Science and Technology, University of Maryland (2023)
7. Member, Merit, Pay and Awards Committee (MPAC), Department of Chemistry and Biochemistry, University of Maryland (2022–2023)
8. Member, Salary Committee, Institute for Physical Science and Technology, University of Maryland (2022–2023)
9. Member, Committee for funding high performance computing at University of Maryland, (2021–current)
10. Member, Allocations and Advisory Committee for high-performance computing, University of Maryland (2020-current)
11. Organizer, Physical Chemistry seminar series (2019–2022)
12. Statistical Physics seminar series, co-organizer with Chris Jarzynski (2017–current)
13. Curriculum Committee, Department of Chemistry and Biochemistry (2020–current)
14. Graduate Admissions Committee, Department of Chemistry and Biochemistry (2018–2020, 2021–current)
15. Graduate Admissions Committee, Biophysics program (2018–current)
16. Facilities and Services Committee, Institute for Physical Sciences and Technology (2017–current)
17. Problem setter and grader, qualifying exams for Chemical Physics (2018–current)
18. Faculty Advisory Committee, Department of Chemistry and Biochemistry (2019–2021)
19. Served on multiple PhD defense committees in Chemistry and Biophysics

Invited Talks and Presentations

1. Invited talk at CECAM workshop "Expanding the Impact of Molecular Simulations by Integrating Machine Learning with Statistical Mechanics", Sorrento, Italy (October 2024)
2. Seminar at Department of Chemistry and the Center for Applied Artificial Intelligence in Protein Dynamics, Vanderbilt University (September 2024)
3. Invited talk at CECAM workshop "Leveraging Machine Learning for Sampling Rare Events in Biomolecular Systems", Mainz, Germany (September 2024)
4. Plenary talk at FOMMS 2024, Snowbird, Utah (July 2024)
5. Invited talk at Montreal Summer School of ML for Drug Discovery (June 2024)
6. Seminar at Department of Chemistry, Cornell University (May 2024)
7. Invited talk at ECT workshop "Bridging scales: At the crossroads among renormalisation group, multi-scale modelling, and deep learning", Trento, Italy (April 2024)
8. Seminar at "Predictive Science Network" Series, AstraZeneca (virtual) (April 2024)
9. Seminar at Purdue University (March 2024)
10. Invited talks at ACS Spring Meeting, New Orleans (March 2024)
11. Seminar at Georgetown University (February 2024)

12. Seminar at Northeastern University (January 2024)
13. Institute Colloquium at IISER Kolkata, India (January 2024)
14. Seminar at IIT Delhi, India (January 2024)
15. Invited talk at Rutgers Stat Mech Meeting, Rutgers University (December 2023)
16. Frontiers in AI in theoretical chemistry mini-symposium, Caltech (November 2023)
17. Seminar at Department of Chemistry, University of Chicago (November 2023)
18. Invited talk at CECAM workshop on "Making the invisible protein life visible using integrative biophysical approaches", Lugano, Switzerland (October 2023)
19. Invited talk at DFG workshop on "Reducing complexity of nonequilibrium systems", Freiburg, Germany (September 2023)
20. Invited talk at student organized Biophysics 101: "Incorporating Bayesian and Artificial Intelligence Approaches into Biophysics" at Biophysical Society Annual Meeting, San Diego (February 2023)
21. Hirschfelder Visitor Seminar, Theoretical Chemistry Institute, University of Wisconsin-Madison (January 2023)
22. Seminar at Department of Chemistry, Texas A&M University (January 2023)
23. Colloquium at the Center for Computational Biology, Flatiron Institute, New York (January 2023)
24. AI4Science Seminar, Chalmers University of Technology, Sweden (November 2022)
25. Invited talk at Gordon Research Conference on Protein Folding Dynamics, Ventura Beach (October 2022)
26. Seminar at IBBR/NIST Biomolecular Measurement Division (October 2022)
27. Invited talk at CECAM Workshop "Machine Learning Meets Statistical Mechanics: Success and Future Challenges in Biosimulations", Sorrento, Italy (October 2022)
28. Invited talk at Erice school on exploring and quantifying free energy landscapes, Erice, Italy (September 2022)
29. Invited talk at Department of Atomic Energy - Board of Research in Nuclear Sciences Symposium on Current Trends in Theoretical Chemistry, Mumbai, India (September 2022)
30. Invited talk at CECAM Workshop "20 years of Metadynamics", Lausanne, Switzerland (September 2022)
31. Chemical Physics Seminar at California Institute of Technology, Pasadena (August 2022)
32. Invited talk at American Conference on Theoretical Chemistry, Palisades Tahoe (July 2022)
33. Invited talk at CECAM Workshop "Chasing collective variables using machine learning", Paris, France (June 2022)
34. Invited talk at Les Houches-TSRC Protein Dynamics workshop, Aussois, France (May 2022)
35. Invited talk at CECAM Workshop "Machine learning augmented sampling", Lausanne, Switzerland (May 2022)
36. Invited talk at New York Area Group for Informatics and Modeling (May 2022)
37. Invited talk at Deep Generative Models for Highly Structured Data (ICLR 2022 Workshop) (April 2022)
38. Invited talk at "Scientific Machine Learning: Foundations and Applications" conference, Translational AI Center (TrAC) at Iowa State University (April 2022)
39. Institute Seminar at Max Planck Institute for Polymer Research, Mainz (April 2022)
40. Data Institute for Societal Challenges and Department of Chemistry and Biochemistry Seminar at University of Oklahoma (April 2022)
41. Department of Chemistry seminar at University of Texas, Austin (March 2022)
42. Invited talk at NSF-workshop "AI Super Resolution Simulations - From Climate Science to Cosmology", Carnegie Mellon University (February 2022)

43. Invited talk at Theory and Computation Subgroup meeting, Biophysical Society, San Francisco (February 2022)
44. Co-organizer and speaker at RARE workshop, India, virtual, funded by Indo-US Science & Technology Forum (December 2021)
45. Invited talk at Theoretical Chemistry Symposium, IISER Kolkata, India, virtual (December 2021)
46. Department of Chemistry seminar at Columbia University (November 2021)
47. Department of Chemistry seminar at University of Florida (November 2021)
48. Colloquium at Penn Institute for Computational Science, University of Pennsylvania (November 2021)
49. Keynote speaker at "AI for Biomaterials and Drug Design symposium" in TechConnect meeting, Washington DC (October 2021)
50. University of Pittsburgh/Carnegie Mellon's Joint Molecular Biophysics/Structural Biology (MBSB) seminar (October 2021)
51. Invited talk at "Physical Chemistry and Chemical Biology - 2021" Conference, India (September 2021)
52. Invited talk at Lorentz Center workshop on "Accelerating the understanding of rare events", virtual (September 2021)
53. Theoretical and Computational Biophysics Group (TCBG) seminar at University of Illinois (August 2021)
54. Invited talk at "ACS COMP Awards" symposium at American Chemical Society meeting, virtual (August 2021)
55. Invited talk at "Sequence-Structure-Dynamics-Function Relationships of Proteins" symposium at American Chemical Society meeting, virtual (August 2021)
56. Seminar at Scientific Machine Learning Webinar Series, Carnegie Mellon University (August 2021)
57. Statistical Biophysics Seminar at Scuola Internazionale Superiore di Studi Avanzati, Trieste, Italy (July 2021)
58. Colloquium at AI4Science, University of Amsterdam (June 2021)
59. Invited talk at Machine Learning for Chemistry & Materials Science Focused Research Program Symposium, Boston University (June 2021)
60. Physical Chemistry Seminar at University of Oregon (June 2021)
61. Seminar at Laufer Center, Stony Brook University (June 2021)
62. Seminar at Free University, Berlin (May 2021)
63. Statistical Mechanics seminar at Cambridge University (May 2021)
64. Seminar at Department of Chemistry, New York University (May 2021)
65. Invited talk at "Machine Learning in Chemical and Materials Sciences" Conference, Center for Nonlinear Studies, Los Alamos National Laboratory (May 2021)
66. Invited talk at Frontiers in Chemistry and Biology Interface Symposium (FCBIS), University of Maryland (May 2021)
67. Seminar at Department of Chemistry, The Hong Kong University of Science and Technology (May 2021)
68. Seminar at Laboratory of Computational Biology, National Institute of Health (April 2021)
69. Seminar at Department of Chemistry, Pennsylvania State University (April 2021)
70. Seminar at Department of Chemistry, Rutgers University, Camden (April 2021)
71. Invited talk at "Kinetics of Macromolecular Systems: Methods and Applications" symposium at American Chemical Society meeting, virtual (April 2021)
72. Invited talk at "The Future of AI in Chemistry and Drug Discovery" symposium at American Chemical Society meeting, virtual (April 2021)

73. Seminar at Department of Chemistry and Biochemistry, University of California, San Diego (April 2021)
74. Seminar at Department of Chemistry, Massachusetts Institute of Technology (April 2021)
75. Seminar at Chicago Center for Theoretical Chemistry, University of Chicago (April 2021)
76. Invited talk at "AI and Statistical/Thermal Physics" symposium at American Physical Society Meeting, virtual (March 2021)
77. Biophysics seminar at University of Michigan (March 2021)
78. Center for Biological Physics seminar at Arizona State University (March 2021)
79. Invited talk at "Data driven models for non-linear systems" symposium at Society for Industrial and Applied Mathematics (SIAM) conference on computational science and engineering, virtual (March 2021)
80. Physical Chemistry seminar, Purdue University (December 2020)
81. Department of Department of Mechanical and Aerospace Engineering Seminar at University of Colorado Colorado Springs (December 2020)
82. Topical Data Science Group seminar for American Physical Society, virtual (May 2020)
83. "Statistics, optimization and machine learning" seminar at University of Colorado, Boulder (April 2020)
84. Keynote lecture at student-organized annual Biophysics symposium at University of Michigan (March 2020, cancelled due to COVID)
85. Department of Chemistry Colloquium at Rutgers University (March 2020)
86. Invited talk at "Computational Thermodynamics and Kinetics" (CTK) symposium at TMS 2020 annual meeting, San Diego (February 2020)
87. Department of Physics Colloquium at University of Vermont (November 2019)
88. Invited talk at IPAM workshop on "Interpretable Learning in Physical Sciences", as a part of the long program Machine Learning for Physics and the Physics of Learning, Los Angeles (October 2019)
89. Seminar at Department of Pharmacological Sciences at the Icahn School of Medicine at Mount Sinai in New York (September 2019)
90. Invited talk at CECAM workshop "Learning the Collective Variables of Biomolecular Processes", Paris, France (July 2019)
91. Invited talk at the annual symposium "Science at theInterface: machine learning as applied to biophysics" of Institute for Biophysical Dynamics, University of Chicago (June 2019)
92. Invited talk at "Exploring Complex Free Energy Landscapes: Structure/Function Formation, Multiscales, and Long-timescales" workshop at Max Planck for Polymer Research in Mainz, Germany (June 2019)
93. Invited talk at "Three decades in Free Energy methods" conference at Santa Fe, New Mexico (June 2019)
94. Invited talk at CECAM workshop "Network analysis to elucidate natural system dynamics, diversity and performance", Lyon, France (May 2019)
95. Machine Learning seminar at Michigan State University, East Lansing (March 2019)
96. Department Colloquium at Department of Physics, University of Maryland, Baltimore County (March 2019)
97. Invited talk at "Exploring Free Energy Landscapes in Biology and Materials Science with Advanced Algorithms" symposium at American Physical Society Meeting, Boston (March 2019)
98. Invited talk at "Role of Fluctuations and Dynamics in Biomolecular Function" workshop at Telluride, Colorado (January 2019)
99. Seminar at Department of Chemistry and Biochemistry, University of Delaware (November 2018)

100. Invited talk at CECAM/ECAM state-of-the-art workshop: Large scale activated event simulations, Vienna, Austria (October 2018)
101. Invited talk at Gordon Research Conference on Water and Aqueous Solutions, New Hampshire (July 2018)
102. Invited talk at "Exploring and quantifying rough free energy landscapes" symposium at International School of Statistical Physics, Erice, Sicily, Italy (May 2018)
103. Invited talk at "Workshop on free energy methods, kinetics and markov state models in drug design" at Novartis Institutes for Biomedical Research, Boston (May 2018)
104. Seminar at Computer-Aided Drug Design Center, School of Pharmacy, University of Maryland, Baltimore (April 2018)
105. Seminar at Department of Chemistry and Biochemistry, Montana State University, Bozeman (March 2018)
106. Seminar at Center for Scientific Computation and Mathematical Modeling, University of Maryland, College Park (March 2018)
107. Seminar at National Cancer Institute-University of Maryland annual symposium (February 2018)
108. Seminar at Laboratory of Computational Biology, National Institute of Health (February 2018)
109. Invited talk at "Data-driven Discovery and Design in Soft and Biological Materials" conference at Aspen Center for Physics 2018 Winter Conference, Aspen (January 2018)
110. Invited talk at "Modeling and measuring protein-ligand kinetics and residence time" symposium at American Chemical Society meeting, Washington D.C. (August 2017)
111. Invited talk at "Free energy calculations: Three decades of adventure in Chemistry and Biophysics" workshop at Telluride, Colorado (July 2017)
112. Seminar at Center for Biophysics & Computational Biology, Temple University (May 2017)
113. Physical Chemistry student seminar at Department of Chemistry, Columbia University (May 2017)
114. Invited talk at "Recent progress in biophysical applications of Molecular Dynamics" symposium at American Chemical Society meeting, San Francisco (April 2017)
115. Invited talk at "Exploring and quantifying rough free energy landscapes" workshop at International School of Statistical Physics, Erice, Sicily, Italy (October 2016)
116. Invited talk at "Bridging time scale techniques and their applications in atomistic computational science" workshop, Max Planck Institute for Complex Systems, Dresden, Germany (September 2016)
117. Invited talk at "Reaction coordinates from molecular trajectories" workshop, Leiden, Netherlands (August 2016)
118. Invited talk at "Hydrophobicity: From theory, Simulation, to experiment" workshop, Telluride (July 2016)
119. Invited talk at "Car-Parrinello Molecular Dynamics" conference, Chicago (May 2016)
120. Seminar at University of New Hampshire, Durham (March 2016)
121. Invited talk at "International Conference on Physics and Chemistries at Hydrophobic Interfaces" at KAUST, Saudi Arabia (February 2016)
122. Seminar at University of Colorado, Boulder (February 2016)
123. Seminar at University of Maryland (January 2016)
124. Seminar at Imperial College, London (November 2015)
125. Physical Chemistry Student Seminar at Columbia University (October 2015)
126. Seminar at Laufer Center for Physical and Quantitative Biology, Stony Brook University (October 2015)
127. Contributed talk at CECAM workshop on "From trajectories to reaction coordinates", Vienna (September 2015)
128. Invited talk at ACS Fall meeting, Boston (August 2015).

129. Seminar at Department of Chemical Engineering, University of Washington (May 2015)
130. Seminar at DE Shaw Research, New York (May 2015)
131. Seminar at Department of Chemistry, University of Louisville, Kentucky (February 2015)
132. Seminar at Computational Biomedicine Section, Forschungszentrum, Jülich (December 2014)

Teaching Experience at the University of Maryland

1. Sole instructor for CHM 481 "Physical Chemistry I", 3 credits (Fall 2018, fall 2020, fall 2021).
2. Created and was sole instructor for "Introduction to programming and AI for non-computer science students" (summer 2021, summer 2022). 6-day workshop (approximating 12+ hours of instruction) aimed at students from UMD, Prince George's Community College and Bowie State University who have no prior programming worksop.
3. Joint instructor for Machine Learning modules at "UMD Science Academy's Quantum Computing Bootcamp" (summer 2021).
4. Sole instructor for CHM 687 "Statistical Mechanics and Chemistry", 3 credits (Spring 2018, spring 2019, spring 2020, spring 2021, spring 2023).
5. Sole instructor for CHM 684 "Thermodynamics and Chemistry", 3 credits (Fall 2022, Fall 2023).
6. Joint instructor for BCHM 677 "Computational Tools in Biochemistry", 1 credit (Winter 2018, winter 2019, winter 2020, winter 2021).

Teaching Experience prior to the University of Maryland

1. (At Caltech) APh105: Graduate level course on thermodynamics and statistical mechanics, Teaching Assistant to Prof. William. L. Johnson, winter 2010–11. I gave around 20% of the lectures.
2. (At Caltech) MS131: Graduate level course on structure and bonding in materials, Teaching Assistant to Prof. Axel van de Walle, winters 2009–10 and 2008–09. I gave around 20% of the lectures.