Dhiman Ray

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Research Interest: The primary goal of my research is to understand the mechanistic details of biological processes of therapeutic relevance, using atomistic molecular dynamics simulation. To this end, I work on developing and applying path sampling and enhanced sampling techniques using statistical mechanics and machine learning to predict the free energy landscape and kinetics of biomolecular rare events, the timescales of which go beyond the capability of conventional simulation techniques. My areas of interest include drug-target interaction, antigen-antibody recognition, enzyme catalysis, and conformational transitions in proteins and nucleic acids.

Education:

March 2022	Ph.D. (Chemistry), University of California Irvine, USA Advisor: Prof. Ioan Andricioaei Dissertation Title: *Path Sampling and Machine Learning Approaches to Biomolecular Simulation*
June 2018	Integrated BS-MS (Chemical Sciences) Indian Institute of Science Education and Research (IISER) Kolkata, India Advisor: Prof. Ashwani K. Tiwari MS Thesis Title: *Quantum Dynamics of Water Dissociation on Copper-Nickel Bimetallic Alloy Surface*

Research Experience:

April 2022 - Present — Postdoctoral Researcher, Italian Institute of Technology, Genoa, Italy
Advisor: Prof. Michele Parrinello

- Development of enhanced sampling algorithms for calculating molecular kinetics
- Designing deep learning collective variables for ligand binding and protein folding.
- Employing dynamic time warping to explore and classify ligand unbinding pathways.

September 2018 - March 2022 — Graduate Research Assistant, University of California Irvine, USA
Advisor: Prof. Ioan Andricioaei

- Development of Weighted Ensemble Milestoning (WEM) algorithm for studying rare events in biophysics.
- Studying the kinetics and free energy of protein-ligand binding.
- Using unsupervised machine learning and graph theoretical models to study allosteric conformational transition in SARS-CoV-2 spike proteins and their antibodies
- Simulation of Hoogsteen base pairing in DNA and RNA using enhanced sampling and Markov state modeling

August 2016 - June 2018 — Masters' Thesis Research, Indian Institute of Science Education and Research (IISER) Kolkata, India. Advisor: Prof. Ashwani K. Tiwari

- Theoretical study of water dissociation on Cu-Ni bimetallic surface using time-dependent wave-packet dynamics

Awards and Achievements:

August 2023	Best Oral Presentation Award, European Conference on Theoretical and Computational Chemistry
May 2021	Wolfsberg Award in Theoretical Chemistry, University of California Irvine
November 2020	Best Poster Award, ChemSci2020, Royal Society of Chemistry
July-December 2020	NSF MolSSI Software Seed (COVID-19) Fellowship
2020	Graduate Student Travel Grant, University of California (awarded in 2022)
February 2020	Student Research Achievement Award (Best Poster), Biophysical Society, USA
June 2018	Directors Gold Medal, IISER Kolkata, India
June 2018	Best Master's Thesis Award in Chemistry, IISER Kolkata, India
May to July 2017	S.N. Bose (REU) Fellowship, University of Wisconsin Madison, USA
May to July 2016	DAAD WISE (REU) Fellowship, Max Planck Institute for Coal Research, Germany
2014	C.N.R. Rao Education Foundation Prize, India
2012 - 2018	KVPY Fellowship, Government of India (Bachelors and Masters)

Fellowship:

July 2020 - December 2020	MolSSI Software Seed Fellowship: NSF OAC-1547580 Project Title: *Development and Implementation of the Weighted Ensemble Milestoning (WEM) Scheme for Studying Rare Events in Molecular Biophysics*

Contribution to Successful Grant Application:

May 2020 - December 2022	NSF RAPID Grant: NSF MCB 2028443 Project Title: *RAPID: Computational studies of the structural dynamics, function and inhibition of the SARS-CoV-2 coronavirus spike protein* PI: Ioan Andricioaei

Publications: (reverse chronological order)

1. Michael Faran, **Dhiman Ray**, Shubhadeep Nag, Umberto Raucci, Michele Parrinello, and Gili Bisker. *A Stochastic Landscape Approach for Protein Folding State Classification.* **Journal of Chemical Theory and Computation** (2024)
2. **Dhiman Ray,** Sudip Das, and Umberto Raucci. *A Kinetic View of Enzyme Catalysis from Enhanced Sampling QM/MM Simulations.* **Journal of Chemical Information and Modeling** (2024)
3. **Dhiman Ray** and Michele Parrinello. *Data-Driven Classification of Ligand Unbinding Pathways.* **Proceeding of National Academy of Sciences** (2023)
4. **Dhiman Ray** and Michele Parrinello. *Kinetics from Metadynamics: Principles, Applications, and Outlook* **Journal of Chemical Theory and Computation** (2023) (Co-corresponding author)
5. **Dhiman Ray**, Enrico Trizio, and Michele Parrinello. *Deep Learning Collective Variables from Transition Path Ensemble* **The Journal of Chemical Physics** (2023) (Editor's Pick)
6. Praveen Ranganath Prabhakar, **Dhiman Ray**, and Ioan Andricioaei. *Predicting residue cooperativity during protein folding: A combined, molecular dynamics and unsupervised learning approach* **The Journal of Chemical Physics** (2023)
7. Anthony T. Bogetti*, Jeremy M. G. Leung*, John D. Russo*, She Zhang*, Jeff P. Thompson*, Ali S. Saglam*, **Dhiman Ray***, Barmak Mostofian, A. J. Pratt, Rhea C. Abraham, Page O. Harrison, Max Dudek, Paul A.

Torrillo, Alex J. DeGrave, Upendra Adhikari, James R. Faeder, Ioan Andricioaei, Joshua L. Adelman, Matthew C. Zwier, David N. LeBard, Daniel M. Zuckerman, Lillian T. Chong. (*=equal contribution) *A Suite of Tutorials for the WESTPA 2.0 Rare-Events Sampling Software [Article v2.0]* Living Journal of Computational Molecular Science (2022)

8. **Dhiman Ray***, Narjes Ansari*, Valerio Rizzi*, Michele Invernizzi, and Michele Parrinello. (*=equal contribution) *Rare Event Kinetics from Adaptive Bias Enhanced Sampling.* **Journal of Chemical Theory and Computation** (2022)
9. **Dhiman Ray**, Riley, N. Quijano, and Ioan Andricioaei. *Point Mutations in SARS-CoV-2 Variants Induce Long-Range Dynamical Perturbations in Neutralizing Antibodies* **Chemical Science** (2022) (Co-corresponding author)
10. Sharon E. Stone, **Dhiman Ray**, and Ioan Andricioaei. *Force-Field-Dependent DNA Breathing Dynamics: A Case Study of Hoogsteen Base Pairing in A6-DNA*. **Journal of Chemical Information and Modeling** (2022)
11. Sharon E. Stone, **Dhiman Ray**, and Ioan Andricioaei. *Studying the Association and Dissociation of Trypsin-Benzamidine Complex Using Enhanced Sampling Molecular Dynamics*. **Revue Roumaine de Chimie** (2022)
12. **Dhiman Ray**, Sharon E. Stone, and Ioan Andricioaei. *Markovian Weighted Ensemble Milestoning (M-WEM): Long Time Kinetics from Short Trajectories* **Journal of Chemical Theory and Computation** (2022) (Co-corresponding author)
13. **Dhiman Ray**, Ly Le, and Ioan Andricioaei. *Distant Residues Modulate the Conformational Opening in SARS-CoV-2 Spike Protein.* **Proceedings of the National Academy of Sciences** (2021)
14. **Dhiman Ray**, Trevor Gokey, David L. Mobley, and Ioan Andricioaei. *Kinetics and Free Energy of Ligand Dissociation Using Weighted Ensemble Milestoning*. **The Journal of Chemical Physics** (2020)
15. **Dhiman Ray**, and Ioan Andricioaei. *Free Energy Landscape and Conformational Kinetics of Hoogsteen Base-Pairing in DNA vs RNA.* **Biophysical Journal** (2020)
16. **Dhiman Ray**, and Ioan Andricioaei. *Weighted ensemble milestoning (WEM): A combined approach for rare-event simulations.* **The Journal of Chemical Physics** (2020) (Editor's Pick)
17. Dongyue Liang, Udaya Dahal, Yongqian Zhang, Christian Lochbaum, **Dhiman Ray**, Robert Hamers, Joel A. Pedersen, and Qiang Cui. *Interfacial water and ion distribution determine ζ potential and binding affinity of nanoparticles to biomolecules.* **Nanoscale** (2020).
18. Diptesh Dey, **Dhiman Ray**, and Ashwani K. Tiwari. *Controlling electron dynamics with carrier-envelope phases of a laser pulse.* **The Journal of Physical Chemistry A** (2019).
19. Smita Ghosh, **Dhiman Ray**, and Ashwani K Tiwari. *Effects of alloying on mode-selectivity in H2O dissociation on Cu/Ni bimetallic surfaces.* **The Journal of Chemical Physics** (2019).
20. **Dhiman Ray**, Smita Ghosh, and Ashwani K Tiwari. *Controlling heterogeneous catalysis of water dissociation using Cu-Ni bimetallic alloy surfaces: A quantum dynamics study.* **The Journal of Physical Chemistry A** (2018).

Invited Oral Presentations:

1. *Data-driven Enhanced Sampling for Biomolecular Simulation.* University of Oregon, USA (February 2024)
2. *Enhanced Sampling of Rare Events*. Bayes Comp 2023, Levi, Finland (March 2023)

3. *Markovian Weighted Ensemble Milestoning (M-WEM): Studying beyond millisecond protein-ligand interaction using sub-microsecond trajectories*. Inclusive Future Faculty Symposium (IFFS), Arizona State University, USA (March 2022)
4. *Probing the Kinetics of Protein Ligand Interaction using Molecular Dynamics Simulation*. Mathematical, Computational and Systems Biology Seminar, University of California Irvine, USA (March 2021)

Contributed Oral Presentations:

1. *Data Driven Classification of Ligand Unbinding Pathways and Kinetics*. European Conference on Theoretical and Computational Chemistry, Thessaloniki, Greece (August 2023) **(Best Oral Presentation Award)**
2. *OPES Flooding: Rare event kinetics from adaptive bias enhanced sampling*. CECAM Workshop on 20 years of Metadynamics, Lausanne, Switzerland (September 2022).
3. *Probing the dynamical couplings in the SARS-CoV-2 spike protein using unsupervised learning and protein graph connectivity network.* American Chemical Society (ACS) Fall Meeting (August 2021)
4. *Kinetics and Free Energy of Protein Ligand Interaction Using Weighted Ensemble Milestoning*. Hünfeld 2021: Workshop on Computer Simulation and Theory of Macromolecules. (April 2021)
5. *Kinetics and Free Energy of Protein Ligand Interaction Using Weighted Ensemble Milestoning*. American Chemical Society (ACS) Spring Meeting. (March 2021)
6. *Kinetics and Free Energy of Protein Ligand Interaction Using Weighted Ensemble Milestoning*. American Physical Society (APS) March Meeting. (March 2021)
7. *Kinetics and Free Energy of Protein Ligand Interaction Using Weighted Ensemble Milestoning*. 65th Biophysical Society (BPS) Annual Meeting (February 2021)

Poster Presentations:

1. Deep Learning Collective Variables from Transition Path Ensemble. Structure-Based Drug Design Conference (SBDD 2023), Sestri Levante, Italy. (June 2023)
2. Probing the dynamical couplings in the SARS-CoV-2 spike protein using unsupervised learning and graph network model. Molecular Simulations 2022, Past, Present, and Future, Erice, Sicily, Italy (June 2022)
3. Markovian Weighted Ensemble Milestoning (M-WEM): Studying beyond millisecond protein-ligand interaction using sub-microsecond trajectories. Recent Advances in Modelling Rare Events (RARE2021), IIT Kanpur, India (December 2021)
4. Probing the Dynamical Couplings in the SARS-CoV-2 Spike Protein Using Unsupervised Learning and Graph Network Model. Theoretical Chemistry Symposium, IISER Kolkata, India (December 2021)
5. Free Energy Landscape and Conformational Kinetics of Hoogsteen Base Pairing in DNA vs RNA: Enhanced Sampling and Markov State Modeling. ChemSci2020: Leaders in the Field Symposium, Royal Society of Chemistry. (November 2020)
6. Combining Weighted Ensemble with Milestoning (WEM) for Rare Event Simulations. Virtual Conference in Theoretical Chemistry, Stanford University (July 2020)
7. Hoogsteen Base Pairing in DNA vs RNA: Thermodynamics and Kinetics from Enhanced Sampling Simulation and Markov State Modeling. 64th Biophysical Society Annual Meeting, San Diego, USA (February 2020) **(Best Poster Award)**

Outreach Activities:

September 2021	Organized the Biophysical Society sponsored Virtual Networking Event on Computational Methods for Biomolecular Kinetics
February 2021	Virtual public talk to encourage undergraduates to do research in theoretical chemistry; organized by the IISER Kolkata Campus Radio, India
December 2020	Served as a panelist in the 2nd Annual Graduate Student Panel of the Chemistry Club of UC Irvine, to help undergraduate students in grad school (PhD) applications.

Teaching Experience: Graduate Teaching Assistantship at University of California Irvine, USA

Graduate Thermodynamics and Statistical Mechanics II (Spring 2020, Spring 2021)
Graduate Thermodynamics and Statistical Mechanics I (Winter 2020)
Undergraduate Chemical Thermodynamics and Kinetics (Fall 2021)
Undergraduate Scientific Computing Skills (Winter 2022)
Freshman General Chemistry Lecture (Fall 2019)
Freshman General Chemistry Laboratory (Spring 2019, Summer 2019)
Sophomore General Chemistry Laboratory (Fall 2018, Winter 2019, Summer 2019)

Research Mentorship:

Praveen Prabhakar, PhD Chemistry (expected 2026), University of California Irvine

Rodrigo Lozano, BS Chemistry (2023), University of California Irvine

Riley Quijano, BS Chemistry (2022), University of California Irvine

Sharon Stone, BS Chemistry (2021), University of California Irvine

Service:

September 2021	Organizer of the Biophysical Society sponsored Virtual Networking Event on Computational Methods for Biomolecular Kinetics
January 2020 - March 2022	Organizer of Molecular Dynamics Seminar at University of California Irvine
April 2020 - March 2022	Member of the UC Irvine Physical Sciences and Machine Learning Journal Club
August 2021 - Present	Member of the Trainee Advisory Committee of the Living Journal of Computational Molecular Science (LiveCoMS)
October 2022 - Present	Organizer of Informal Seminar Series, Atomistic Simulations, IIT Genoa, Italy
January 2024 - December 2025	Early Career Editorial Board Member of Journal of Chemical Information and Modeling, American Chemical Society

Peer Review: (ACS Reviewer Lab certification)

Journal of Chemical Information and Modeling (ACS), New Journal of Chemistry (RSC), Physical Chemistry Chemical Physics (RSC), Elife, ACS Omega (ACS), Journal of Chemical Theory and Computation (ACS)