Sohang Kundu

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Academic Background

Aug, 2023 – Present	Postdoctoral Research Scientist, Columbia University, New York Advisor: Prof. Timothy C. Berkelbach
Aug, 2017 – May, 2023	**PhD** in Chemistry, University of Illinois, Urbana Champaign (UIUC) Advisor: Prof. Nancy Makri
Aug, 2015 – Jul, 2017	**MSc** in Chemistry, Indian Institute of Technology (IIT) Bombay Advisor: Prof. Raghavan B. Sunoj
Aug, 2012 – Jul, 2015	**BSc** in Chemistry (Hons.), Presidency University, Kolkata

Awards & Fellowships

2025	ACS Physical Chemistry Young Investigator Award
2024	Justin Jankunas Doctoral Dissertation Award in Chemical Physics by APS
2023	UChicago Center for Theoretical Chemistry Postdoctoral Fellowship (declined)
2022	Physical Chemistry Dissertation Award, Department of Chemistry, UIUC
2022	Finalist, ACS PHYS Graduate Student Award in Theoretical Chemistry
2020	Zumdahl Teaching Award for Graduate Quantum Mechanics, UIUC
2018-2021	Lester E. and Kathleen A. Coleman, James R. Becke, and Peixin He-Xiaoming Chen Graduate Fellowships, Department of Chemistry, UIUC
2017-2018	Included in the List of Teachers Ranked Excellent by Their Students during Spring and Fall semesters, Center for Innovation Teaching and Learning, UIUC
2016	Junior Research Fellowship, Council of Scientific and Industrial Research, National Eligibility Test, India
2012-2015	Project Oriented Chemical Education (POCE) Summer Research Fellowship and Best Student Award by Jawaharlal Nehru Center for Advanced Scientific Research
2012	Gold Medal in Mathematics, International Assessment for Indian Schools, University of New South Wales (UNSW), Australia & Macmillan, India

Manuscripts in Preparation

* Denotes corresponding author(s). #Denotes authors contributed equally.

[23] **S. Kundu,** G.S. Schlau-Cohen, and T.C. Berkelbach, "Engineering Robust Timescales of Energy Transfer using Vibronic Coupling", to be submitted, 2025.

Publications (Updates may be found on Google Scholar and ResearchGate.)

[22] **S. Kundu*,** D. Chamaki, H.-Z. Ye, G. Agarwal, and T.C. Berkelbach*, "Reaction dynamics of lithium-mediated electrolyte decomposition using machine learning potentials", arXiv.2509.14067 (2025)

[21] **S. Kundu***, H.-Z. Ye, and T.C. Berkelbach*, "Diabatic States of Charge Transfer with Constrained Charge Equilibration", Journal of Chemical Theory and Computation **21**, 7, 3545–3551(2025).

[20] **S. Kundu** and T.C. Berkelbach*, "Reaction Rate Theory for Electric Field Catalysis in Solution", Journal of the American Chemical Society **146**, 38, 26041–26047 (2024).

[19] J. Schulz*, J. Yuly*, E. A. Arsenault, K. Parker, S. Chowdhury, R. Dani, **S. Kundu**, H. Nuomin, Z. Zhang, J. Valdiviezo, P. Zhang, K. Orcutt, S. J. Jang, G. R. Fleming, N. Makri, J. P. Ogilvie, M. J. Therien, M. R. Wasielewski, and D. N. Beratan*, "Coherence in Chemistry: Foundations and Frontiers", Chemical Reviews, **124**, 11641–11766 (2024).

[18] C. Zhang#, **S. Kundu#,** N. Makri*, M. Gruebele*, and P. Wolynes*, "Quantum Information Scrambling and Chemical Reactions", Proceedings of the National Academy of Sciences, **121**, 15) e2321668121 (2024).

[17] **S. Kundu** and N. Makri*, "PATHSUM: A C++ and Fortran Suite of Fully Quantum Mechanical Real-Time Path Integral Methods for (Multi-)System+Bath Dynamics", Journal of Chemical Physics, **158**, 224801 (2023).

[16] R. Dani, **S. Kundu**, and N. Makri*, "Coherence Maps and Flow of Excitation Energy in the Bacterial Light Harvesting Complex 2", Journal of Physical Chemistry Letters, **14**, 3835−3843 (2023).

[15] **S. Kundu**, R. Dani and N. Makri*, "Tight Inner Ring Architecture and Quantum Motion of Nuclei Enable Efficient Energy Transfer in Bacterial Light Harvesting", Science Advances, **8**, eadd0023 (2022).

[14] P.P. Roy, **S. Kundu**, N. Makri, and G.R. Fleming*, "Interference between Franck-Condon and Herzberg-Teller Terms in the Condensed-phase Molecular Spectra of Metal-based Tetrapyrrole Derivatives", Journal of Physical Chemistry Letters, **13**, 7413-7419 (2022).

[13] **S. Kundu**, R. Dani and N. Makri*, "B800-to-B850 Transfer of Excitation Energy in Bacterial Light Harvesting: All-State, All-Mode Path Integral Simulations", Journal of Chemical Physics **157**, 015101 (2022).

[12] **S. Kundu** and N. Makri*, "Small Matrix Quantum Classical Path Integral", Journal of Physical Chemistry Letters, **13**, 3492-3498 (2022).

[11] **S. Kundu**, P. P. Roy, G. R. Fleming and N. Makri*, "Franck-Condon and Herzberg-Teller signatures in molecular absorption and emission spectra", Journal of Physical Chemistry B, **126**, 15, 2899–2911 (2022).

[10] P.P. Roy, **S. Kundu**, J. Valdiviezo, G. Bullard, J.T. Fletcher, R. Liu, S-J. Yang, P. Zhang, D.N. Beratan, M.J. Therien, N. Makri* and G.R. Fleming*, "Synthetic Control of Exciton Dynamics in Bioinspired Cofacial Porphyrin Dimers", Journal of the American Chemical Society, **144**, 14, 6298–6310 (2022).

[9] **S. Kundu** and N. Makri*, "Intramolecular Vibrations in Excitation Energy Transfer: Insights from Real-Time Path Integral Calculations", Annual Review of Physical Chemistry, **73**, 349-375 (2022).

[8] **S. Kundu** and N. Makri*, "Electronic-Vibrational Density Evolution in a Perylene Bisimide Dimer: Mechanistic Insights into Excitation Energy Transfer", Physical Chemistry Chemical Physics, **23**, 15503 (2021).

[7] **S. Kundu** and N. Makri*, "Time Evolution of Bath Properties in Spin-Boson Dynamics", Journal of Physical Chemistry B, **125**, 8137 (2021).

[6] **S. Kundu** and N. Makri*, "Origin of vibrational features in the excitation energy transfer dynamics of perylene bisimide J-aggregates", Journal of Chemical Physics, **154**, 114301 (2021).

[5] **S. Kundu** and N. Makri*, "Exciton-Vibration Dynamics in J-Aggregates of a Perylene Bisimide from Real-Time Path Integral Calculations", Journal of Physical Chemistry C, **125**, 1, 201– 210 (2021).

[4] **S. Kundu** and N. Makri*, "Real-Time Path Integral Simulation of Exciton-Vibration Dynamics in Light Harvesting Bacteriochlorophyll Aggregates", Journal of Physical Chemistry Letters, **11**, 20, 8783–8789 (2020)

[3] **S. Kundu** and N. Makri*, "Efficient Matrix Factorization of the Modular Path Integral", Molecular Physics (2020), 10.1080/00268976.2020.1797200, Proceedings of the Sannibel Symposium.

[2] **S. Kundu** and N. Makri*, "Modular Path Integral for Finite-Temperature Dynamics of Extended Systems with Intramolecular Vibrations", Journal of Chemical Physics **153**, 044124 (2020)

[1] **S. Kundu** and N. Makri*, "Modular Path Integral for Discrete Systems with Non-Diagonal Couplings", Journal of Chemical Physics, **151**, 074110 (2019).

Conferences, Seminars, and Workshops

[18] Fall 2025	Prize Talk, American Chemical Society National Meeting, Washington, DC
[17] Fall 2024	Invited talk, Indian Institute of Technology Kanpur, India
[16] Fall 2024	Invited talk, Indian Institute of Science, Bengaluru, India
[15] Spring 2024	Deep Modeling for Molecular Simulation Workshop, Princeton University.
[14] Spring 2024	School on Electron-Phonon Physics, Many-Body Perturbation Theory, and Computational Workflows, University of Texas, Austin, TX.
[13] Spring 2024	Prize Talk, American Physical Society March Meeting, Minneapolis, MN.
[12] Summer 2023	Invited Talk, International Workshop on Nuclear Quantum Effects in Chemistry, Simons Center for Computational Physical Chemistry, NYU, New York, NY
[11] Spring 2023	Talk, American Chemical Society National Meeting, Indianapolis, IN
[10] Fall 2022	Invited Talk, New Chemistry Unit, JNCASR, Bengaluru, India
[9] Fall 2022	Invited Talk, Indian Association for the Cultivation of Sciences, Kolkata, India
[8] Fall 2022	Invited Talk, American Chemical Society Graduate Award Symposium
[7] Fall 2022	Physical Chemistry Dissertation Award Seminar, UIUC, Urbana, IL.
[6] Spring 2022	Theory Seminar, Department of Chemistry, UC Berkeley, Berkeley, CA.
[5] Fall 2021	Invited talk, American Chemical Society National Meeting, Atlanta, GA.
[4] Spring 2021	Poster, American Chemical Society National Meeting (virtual).
[3] Spring 2020	Poster, Virtual Conference on Theoretical Chemistry.
[2] Spring 2019	Talk, Midwest Theoretical Chemistry Conference Notre Dame, IN.
[1] Spring 2017	Recent Advances in Many-Electron Theory (RAMET) Workshop, Goa, India.

Press Releases

- Chemical reactions can scramble quantum information as well as black holes, by science springs.
- Sohang Kundu wins the 2024 Justin Jankunas Doctoral Dissertation Award, by the American Physical Society Newsletter
- Quantum visualization technique gives insight into photosynthesis, by Phys.org.
- High-level simulations bring insights to quantum effects in photosynthesis, by the Illinois Chemistry Newsletter.

Teaching Assistantships

Fall, 2017	CHEM 442 Physical Chemistry I
Spring, 2018	CHEM 204 Accelerated Chemistry II
Fall, 2018	CHEM 540 Graduate Quantum Mechanics
Fall, 2019	CHEM 540 Graduate Quantum Mechanics

Academic Service

Peer Reviewer, Scientific Reports, Journal of Chemical Physics, Journal of Organic Chemistry, and Bulletin of Material Science.

Convener, 2015 All India Chemiquiz: A quiz competition among undergraduate science institutions in India hosted by Presidency University, to encourage interactions among chemistry students across the country.

Mentorship

Diana Chamaki, Graduate Student, Chemical Physics, Columbia University: 2023-present, coauthored paper.
Alyssa Spencer, Graduate Student, Chemical Engineering, UIUC: 2022-2023
Karnika Purohit, Undergraduate Student, Chemistry, UIUC: 2022-2023

Pre-Doctoral Research

MSc Project – IIT Bombay, Advisor: Prof. Raghavan B. Sunoj
Title: Computational design of chiral N-heterocyclic carbenes for asymmetric catalysis using Multivariate Linear Free Energy Relationships.

Project Oriented Chemical Education – JNCASR, Advisor: Prof. Kanishka Biswas
Title: Effect of Aliovalent Chlorine Doping on the Thermoelectric Properties of n-type AgBi0.5Sb0.5Se2.

Outreach Activities

Co-Founder and Core Team Member, Fellowship for Research, Academic Mentorship and Exploration (FRAME), a not-for-profit organization providing academic and research fellowships and mentorship opportunities to students from under-represented backgrounds in West Bengal, India.

Declaration

I hereby declare that the information provided in this document is accurate and true to the best of my knowledge.