Sohang Kundu

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Academic Background

Aug, 2023 – Present	Postdoctoral Research Scientist Columbia University, New York, USA Advisor: Prof. Timothy C. Berkelbach
Aug, 2017- July, 2023	PhD in Chemistry University of Illinois, Urbana Champaign (UIUC), USA Advisor: Prof. Nancy Makri
Aug, 2015- Aug, 2017	Master of Science in Chemistry Indian Institute of Technology (IIT) Bombay, India Master's Thesis Advisor: Prof. Raghavan B. Sunoj
Jul, 2012- Jul, 2015	Bachelor of Science in Chemistry (Hons.) Presidency University, Kolkata, India & Project Oriented Chemical Education Fellow Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR), Bengaluru, India Research Advisor: Prof. Kanishka Biswas

Awards & Fellowships

2023-2024	Justin Jankunas Doctoral Dissertation Award in Chemical Physics by the American Physical Society
2022-2023	Physical Chemistry Dissertation Award, Department of Chemistry at UIUC
2022-2023	Finalist, Graduate Student Award in Theoretical Chemistry by the American Chemical Society
2020-2021	Peixin He and Xiaoming Chen Graduate Fellowship
2019-2020	Zumdahl Teaching Award, Department of Chemistry at UIUC for Graduate Quantum Mechanics, Fall 2018
2019-2020	Lester E. and Kathleen A. Coleman Graduate Fellowship
2018-2019	James R. Becke Graduate Fellowship
2017-2018	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	POCE Research Fellowship and Outstanding Student Award by JNCASR
2012	Gold Medal in Mathematics, International Assessment for Indian Schools, University of New South Wales (UNSW), Australia & Macmillan, India

Publications

[20] **S. Kundu** and T.C. Berkelbach, "Reaction Rate Theory for Electric Field Catalysis in Solution", arXiv preprint arXiv:2404.01455 (*in review*)

[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 Phenomena in Chemistry", Chemical Reviews (*in press*).

[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). # - authors contributed equally.

[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**, G.R. Fleming and N. Makri, "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 & Workshops

[12] Spring 2024 School on Electron-Phonon Physics, Many-Body Perturbation Theory, and Computational Workflows, University of Texas, Austin, TX.

[11]	Spring 2024	Invited prize talk, American Physical Society March Meeting, Minneapolis, MN. Justin Jankunas Award lecture.
[10]	Summer 2023	Talk, International Workshop on Nuclear Quantum Effects in Chemistry, Simons Center for Computational Physical Chemistry, New York Universit, NY.
[9]	Spring 2023	Talk, American Chemical Society National Meeting, Indianapolis, IN
[8]	Fall 2022	Invited prize talk, American Chemical Society Graduate Award Symposium
[7]	Fall 2022	Physical Chemistry Dissertation Award Seminar, UIUC.
[6]	Spring 2022	Theory Seminar, Department of Chemistry, UC Berkeley.
[5]	Fall 2021	Invited talk, American Chemical Society National Meeting, Atlanta, GA.
[4]	Spring 2021	Poster at the American Chemical Society National Meeting (virtual).
[3]	Spring 2020	Poster at 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
- Sohang Kundu wins the 2024 Justin Jankunas Doctoral Dissertation Award
- Quantum visualization technique gives insight into photosynthesis
- High-level simulations bring insights to quantum effects in photosynthesis

Teaching Assistantships

Fall, 2017	CHEM 442 Physical Chemistry I, Instructor – Prof. Renske M. van der Veen
Spring, 2018	CHEM 204 Accelerated Chemistry II, Instructor – Dr. Tina Huang
Fall, 2018	CHEM 540 Graduate Quantum Mechanics, Instructor – Prof. Nancy Makri
Fall, 2019	CHEM 540 Graduate Quantum Mechanics, Instructor – Prof. Nancy Makri

Undergraduate Research

2) Masters' Thesis Project – IIT Bombay May 2016 – June 2017

Advisor – Prof. Raghavan B. Sunoj, Computational Chemistry Group
Title – *Computational design of chiral N-heterocyclic carbenes for asymmetric catalysis using Multivariate Linear Free Energy Relationships.*

1) Project Oriented Chemical Education – JNCASR December 2013 and June-July 2014
Advisor – Prof. Kanishka Biswas, Materials Chemistry Group
Title – *Effect of Aliovalent Chlorine Doping on the Thermoelectric Properties of n-type AgBi0.5Sb0.5Se2.*

Declaration

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