

Shreyas Malpathak

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Education

Cornell University, Department of Chemistry and Chemical Biology *Ithaca, USA*
PhD *Aug 2018-present*

Indian Institute of Science Education and Research (IISER) *Pune, India*
BS-MS *2013–2018*

Research Experience

Advisor: Prof. Nandini Ananth **Cornell University, USA**
Doctoral Research *Aug 2018–present*
Path-integral and semi-classical methods in real-time quantum dynamics

Advisor: Prof. William Hase **Texas Tech University, USA**
Master's Thesis *May 2017–April 2018*
Ab-initio dynamics of 1,2-dioxetane dissociation.

Advisor: Prof. Anirban Hazra **IISER Pune, India**
Undergraduate Research *May 2016–December 2016*
Electronic structure based mechanistic studies of organic reactions.

Research Interests

- o Development of real-time path-integral and semiclassical dynamic methods for condensed phase reactions — Filinov Filtered Path Integrals (FFPI), Mixed Quantum-Classical Initial Value Representation (MQC-IVR), Ring Polymer Molecular Dynamics (RPMD), Matsubara Dynamics.
- o Zero-point energy leakage in approximate quantum dynamic methods and connections to conservation of quantum boltzmann distribution.
- o Non-adiabatic dynamics within mapping formalisms – Meyer-Miller-Stock-Thoss (MMST) and spin-mapping. Applications to dynamics of population transfer and coherences in systems with strong vibronic coupling.
- o Open quantum dynamics with Generalized Quantum Master Equation (GQME) approaches – approximations to memory kernels using quasiclassical dynamics.
- o Strong light-matter coupling – applications to vibrational strong coupling (VSC).
- o Theories of chemical reaction rates – classical and quantum, transition state theory and beyond.

Publications

- *Non-Linear Correlation Functions and Zero-Point Energy Flow in Mixed Quantum-Classical Semiclassical Dynamics.* **Shreyas Malpathak** and Nandini Ananth, submitted.
- *A Semiclassical Framework for Mixed Quantum Classical Dynamics.* **Shreyas Malpathak**, Matthew S. Church, and Nandini Ananth, *J. Phys. Chem. A*, **2022**, 126, 6359-6375.
- *Is CH₃NC isomerization an intrinsic non-RRKM unimolecular reaction?* Bhumika Jayee, **Shreyas Malpathak**, Xinyou Ma, and William L. Hase, *J. Chem. Phys.*, **2019**, 151, 184110.
- *Unimolecular Rate Constants versus Energy and Pressure as a Convolution of Unimolecular Lifetime and Collisional Deactivation Probabilities. Analyses of Intrinsic Non-RRKM Dynamics.* **Shreyas Malpathak** and William L. Hase, *J. Phys. Chem. A*, **2019**, 123, 1923-28.
- *Addressing an Instability in Unrestricted Density Functional Theory Direct Dynamics Simulations.* **Shreyas Malpathak**, Xinyou Ma, and William L. Hase, *J. Comput. Chem.*, **2019**, 40, 933-936.
- *Direct Dynamics Simulations of the Unimolecular Dissociation of Dioxetane: Probing the non-RRKM Dynamics* **Shreyas Malpathak**, Xinyou Ma, and William L. Hase. *J. Chem. Phys.*, **2018**, 148, 164309.
- *Transition-Metal-Free C-H Hydroxylation of Carbonyl Compounds.* Moreshwar B. Chaudhari, Yogesh Sutar, **Shreyas Malpathak**, Anirban Hazra, and Boopathy Gnanaprakasam, *Org. Lett.*, **2017**, 19 (13), 3628-3631.

Conferences & Presentations

- CECAM Workshop - *Theories of Molecular Processes and Spectra based on the Quantum-Classical Synergy*, Sept. 2022.
- Cornell Chemistry & Chemical Biology Graduate and Postdoc Seminar Series, Nov. 2020. Seminar titled **Real-time Path Integral Dynamics**.
- Telluride Workshop - *Condensed Phase Dynamics*, July 2020.
- ACS Southwest Regional Meeting, Oct. 2017. Presented poster titled **Decomposition Dynamics of 1,2-dioxetane**.

Teaching Experience

- **CHEM 3890: Honors Physical Chemistry I** with Prof. Gregory Ezra, Fall 2021.
Recitation TA
- **CHEM 3900: Honors Physical Chemistry II** with Prof. Robert DiStasio, Spring 2021.
Recitation TA
- **CHEM 2870: Introductory Physical Chemistry** with Prof. Nozomi Ando, Fall 2020.
Head TA
- **CHEM 2090: Engineering General Chemistry** with Prof. John Marohn, Spring 2019.
Laboratory TA
- **CHEM 2070: General Chemistry I** with Prof. Kyle Lancaster, Fall 2018.
Laboratory TA

Awards and Fellowships

- o Howard Neal Wachter Memorial Prize, 2021
- o ACS Graduate (Covestro) Teaching Award, 2021
- o Cornell University Graduate Fellowship, 2019-20
- o Best MS Thesis Award in Chemistry, IISER Pune, 2018
- o S N Bose Scholar, 2017-18
- o Kishore Vaigyanik Protsahan Yojana (KVPY) Fellow, 2012-18