Department of Chemical Sciences
Tata Institute of Fundamental Research,
Mumbai – 400005, Maharashtra, India

Curriculum Vitae

Amartya Bose

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Work Experience

2022 –	Assistant Professor, Tata Institute of Fundamental Research, Mumbai, India
2019 – 2022	Postdoctoral Research, Princeton University, Princeton, USA
2018 – 2019	Research Associate, University of Illinois at Urbana-Champaign, USA

Education

2012 – 2018	Ph. D. Chemistry, University of Illinois at Urbana-Champaign, USA	G. P. A. : 3.91/4
2007 – 2012	Integrated Master's in Chemistry, Indian Institute of Technology, Kanpur	G. P. A. : 9.30/10

Publications

Independent Work After Joining TIFR

(* indicates corresponding author)

[23] **A. Bose***, "Adaptive kink filtration: Achieving asymptotic size-independence of path integral simulations utilizing the locality of interactions", The Journal of Chemical Physics **162**, 114105 (2025).

[22] D. Sharma and **A. Bose***, "Non-hermitian state-to-state analysis of transport in aggregates with multiple endpoints", Journal of Chemical Theory and Computation **21**, 5858–5866 (2025).

[21] **A. Bose***, "Incorporation of Empirical Gain and Loss Mechanisms in Open Quantum Systems through Path Integral Lindblad Dynamics", The Journal of Physical Chemistry Letters **15**, 3363–3368 (2024).

[20] D. Sharma and **A. Bose***, "Impact of Loss Mechanisms on Linear Spectra of Excitonic and Polaritonic Aggregates", Journal of Chemical Theory and Computation **20**, 9522–9532 (2024).

[19] **A. Bose***, "Quantum correlation functions through tensor network path integral", The Journal of Chemical Physics **159**, 214110 (2023).

[18] **A. Bose***, "QuantumDynamics.jl: A modular approach to simulations of dynamics of open quantum systems", The Journal of Chemical Physics **158**, 204113 (2023).

[17] **A. Bose*** and P. L. Walters*, "Impact of Solvent on State-to-State Population Transport in Multistate Systems Using Coherences", Journal of Chemical Theory and Computation **19**, 4828–4836 (2023).

[16] **A. Bose*** and P. L. Walters*, "Impact of Spatial Inhomogeneity on Excitation Energy Transport in the Fenna–Matthews–Olson Complex", The Journal of Physical Chemistry B **127**, 7663–7673 (2023).

Independent Work Before Joining TIFR

(* indicates corresponding author)

[15] **A. Bose***, "Pairwise connected tensor network representation of path integrals", Physical Review B **105**, 024309 (2022).

[14] **A. Bose***, "Zero-cost corrections to influence functional coefficients from bath response functions", The Journal of Chemical Physics **157**, 054107 (2022).

[13] **A. Bose*** and P. L. Walters*, "A multisite decomposition of the tensor network path integrals", The Journal of Chemical Physics **156**, 024101 (2022).

[12] **A. Bose*** and P. L. Walters, "Effect of temperature gradient on quantum transport", Physical Chemistry Chemical Physics **24**, 22431 (2022).

[11] **A. Bose*** and P. L. Walters*, "Tensor Network Path Integral Study of Dynamics in B850 LH2 Ring with Atomistically Derived Vibrations", Journal of Chemical Theory and Computation **18**, 4095–4108 (2022).

Earlier Work

(* indicates corresponding author)

[10] **A. Bose** and N. Makri*, "Quantum-classical path integral evaluation of reaction rates with a near-equilibrium flux formulation", International Journal of Quantum Chemistry **121**, 10.1002/qua.26618 (2021).

[9] **A. Bose** and S. Torquato*, "Quantum phase transitions in long-range interacting hyperuniform spin chains in a transverse field", Physical Review B **103**, 014118 (2021).

[8] **A. Bose** and N. Makri*, "All-Mode Quantum–Classical Path Integral Simulation of Bacteriochlorophyll Dimer Exciton-Vibration Dynamics", The Journal of Physical Chemistry B **124**, 5028–5038 (2020).

[7] **A. Bose** and N. Makri*, "Coherent State-Based Path Integral Methodology for Computing the Wigner Phase Space Distribution", The Journal of Physical Chemistry A **123**, 4284–4294 (2019).

[6] **A. Bose** and N. Makri*, "Quasiclassical Correlation Functions from the Wigner Density Using the Stability Matrix", Journal of Chemical Information and Modeling **59**, 2165–2174 (2019).

[5] **A. Bose** and N. Makri*, "Wigner Distribution by Adiabatic Switching in Normal Mode or Cartesian Coordinates and Molecular Applications", Journal of Chemical Theory and Computation **14**, 5446–5458 (2018).

[4] **A. Bose** and N. Makri*, "Non-equilibrium reactive flux: A unified framework for slow and fast reaction kinetics", The Journal of Chemical Physics **147**, 152723 (2017).

[3] **A. Bose** and D. Goswami, "Investigating the science of few-cycle pulses on simple model systems", in *Advances in Laser Physics and Technology*, edited by M. Mohan, A. K. Maini, A. B. Bhattacharjee, and A. K. Razdan (Cambridge University Press, New Delhi, India, 2015), pp. 37–52.

[2] **A. Bose** and N. Makri*, "Wigner phase space distribution via classical adiabatic switching", The Journal of Chemical Physics **143**, 114114 (2015).

[1] **A. Bose** and D. Goswami, "Insignificance of Relative Time Delay between Photons for a Ultrafast Two-Photon Process", in 2012 International Conference on Fiber Optics and Photonics (PHOTONICS) (2012), pp. 1–3.

Teaching Experience

Spring 2025 **Computational Science: A Hands-On Approach** covering basics of programming, numerically modeling 1D quantum systems and calculating eigenstates, time-dependent Schrödinger equation, Feit-Fleck or split operator method, imaginary time propagation, etc.

Fall 2024 **Introduction to Thermodynamics and Statistical Mechanics** covering postulates of thermodynamics, equivalence of entropy maximization and energy minimization, equations of state, Euler relations for energy and entropy, Gibbs-Duhem relation, Legendre transform and equivalent representations, Maxwell's relations, microcanonical ensemble, canonical ensemble, partition function, ergodic hypothesis, etc.

Fall 2023 **Quantum Mechanics I** covering introduction to classical mechanics, basic postulates of quantum mechanics, linear vector spaces and conversions between position and momentum eigenbasis, 1D solvable problems like particle-in-a-box and harmonic oscillators, time-independent and time-dependent perturbation theory, etc.

Spring 2023 **Chemical Dynamics** covering Time-dependent perturbation theory, Born-Oppenheimer approximation and beyond, Gaussian wavepacket dynamics, quantum thermodynamics, trajectory surface-hopping, etc.

Research Group

Current Members

PhD Students Devansh Sharma (3rd year Int-PhD)
Project Students Arshdeep Kaur (1st year Int-PhD)

Former Members

Masters Students Devansh Sharma (Aug 2023 – Feb 2025)
Project Students Gnana Maheswar (Feb 2023 – Mar 2023); Swarnadeep Manna (Apr 2023 – May 2023); Harsh Arya Jalan (May 2023 – Jul 2023); Suman Bhadra (Feb 2024 – Mar 2024); Sriram Vignesh (Jun 2024 – Jul 2024)

Academic and Administrative Services

2023 – **Departmental Seminar Coordinator:** Organize departmental seminars by external visitors to the department. Schedule and coordinate the annual seminars given by students.

2024 – **Member of the Subject Board of Chemistry:** Participate in graduate school and subject board meetings and contribute to the discussions and decisions regarding academic issues in the department.

Conference Talks and Posters

February 2025 Invited talk on "Path Integral Methods for Spectra and Dynamics of Open Quantum Systems: Two Short Stories" at the Spectroscopy and Dynamics of Molecules and Clusters conference

November 2024 Invited talk on "Exciton Transport in Molecular and Polaritonic Aggregates" at the Optics Within Life Sciences conference

November 2024 Invited talk on "Analysing Routes of Exciton Transport from Path Integral Simulations" at the TIFR Annual Chemistry Conference

August 2024 Talk on "Exciton Transport in Open Quantum System: A Path Integral Perspective" at the American Chemical Society Annual Meeting

July 2024 Talk and poster on "Exciton Transport in Open Quantum System: A Path Integral Perspective" at the Molecular Interactions and Dynamics Gordon Research Conference

June 2024 Invited talk on "Quantum Transport in Biology: a Path Integral Perspective" at the Physics Colloquium of the Institute of Mathematical Sciences

February 2024 Invited talk on "Excitation Energy Transfer: Quantum Transport in Biological Systems" at the TIFR Institute Colloquium series

November 2023 Invited talk on "Quantum Correlation Functions using Tensor Networks" at the TIFR Annual Chemistry Conference

October 2023 Invited poster on "Exciton Transfer: Path Integral Approaches" in the inaugural Physical Chemistry Symposium organized by the Society of Physical Chemistry

August 2023 Invited talk on "Dynamics of Extended Open Quantum Systems — Tensor Network Path Integral Approaches" at Harish-Chandra Research Institute as a part of their Physics Colloquium series

July 2023 Invited talk on "Excitonic Dynamics: Path Integrals and Tensor Networks" at Kaleidoscope, 2023 at Udaipur

September 2022 Invited talk on "Non-Equilibrium Quantum Dynamics: Tensor Network Path Integral Formalism" at QMat 2022 hosted by Indian Institute of Technology Kanpur

Spring 2021 Talk on "Nuclear Quantum Effects in *ab initio* Water Dynamics" at American Physical Society's March Meeting

Summer 2019 Poster on "Classical and Path Integral Methods for Computing the Wigner Distribution" at American Conference of Theoretical Chemistry

Summer 2019 Poster on "Quantum-Classical Path Integral: Harmonic Backreaction & Blip Decomposition" at American Conference of Theoretical Chemistry

Summer 2017	Poster on "Quantum Mechanical Rate Calculations in Condensed Phase Reactions" at American Conference of Theoretical Chemistry
Summer 2017	Talk on "Quantum Mechanical Rate Calculations in Condensed Phase Reactions" at Midwest Theoretical Chemistry Conference
Spring 2016	Talk on "Wigner Phase Space Distribution via Classical Adiabatic Switching" at American Chemical Society's Annual Meeting

Posters and Oral Presentations by Group Members

February 2025	Poster on "Impact of Loss Mechanism on Linear Spectra and Transport" by Devansh Sharma & **Amartya Bose*** at the Spectroscopy and Dynamics of Molecules and Clusters conference
November 2024	Poster on "Impact of Loss Mechanism on Linear Spectra and Transport" by Devansh Sharma & **Amartya Bose*** at the TIFR Annual Chemistry Conference
November 2023	Poster on "Impact of Vibronic Coupling on Excitonic-Polaritonic Dynamics" by Devansh Sharma & **Amartya Bose*** at the TIFR Annual Chemistry Conference

Honors and Awards

2018	Certificate of Graduate Specialization in Computational Science and Engineering, UIUC
2017	Center for Advanced Theory and Molecular Simulation Travel Award, Department of Chemistry, UIUC
2016	Eastman Travel Award, Department of Chemistry, UIUC
2015 – 2016	Harry G. Drickamer Fellowship, Department of Chemistry, UIUC
2014 – 2015	Robert Carr Fellowship, Department of Chemistry, UIUC
2013 – 2014	Walter Brown Fellowship, Department of Chemistry, UIUC
2007 – 2012	KVPY Fellowship, Department of Science and Technology, Government of India: Fellowship instituted to promote excellence in pure science
2012	IIT Kanpur, Best Master's Thesis Dissertation
2008 – 2009	IIT Kanpur, Academic Excellence Award
2006	All India Rank 82 in the 5th National Cyber Olympiad
2004	Qualified for the Indian National Mathematical Olympiad with qualifying rank 18; among 3 students from 10th standard to qualify
2004	All India Rank 31 in Senior Mathematical Olympiad
2003	All India Rank 28 in Junior Mathematical Olympiad

Services to the Scientific Community

- Reviewer in the Journal of Chemical Physics, the Journal of Chemical Theory and Computation, and the Journal of Physical Chemistry
- Sole designer, developer, and maintainer of QuantumDynamics.jl and QuantumDynamicsCLI.jl open-source packages for simulation of dynamics in open quantum systems.

Research Experience

Assistant Professor — TIFR

- Developed a method for making the scaling of path integral simulations asymptotically independent of the system size.[23]
- Developed an approach for incorporating empirical loss mechanisms in numerically exact path integral simulations.[21,20]
- Developed new tensor network algorithm for non-perturbatively simulating thermal correlation functions of open quantum systems.[19]
- Designed and developed an **open-source Julia package** for simulations of dynamics in quantum non-adiabatic systems.[18]
- Developed a rigorous technique for identification of dynamical pathways in quantum transport processes in complex systems.[22,17,16]

Postdoctoral Research — Princeton University

- Explored quantum effects of transverse field on spin chains with long-range interactions that have disordered stealthy hyperuniform ground states using density matrix renormalization group (DMRG) with Prof. Salvatore Torquato.[9] Showed the possibility of generating order from disorder through quantum fluctuations in these spin systems.

Independent Work

- Established a novel pairwise connected tensor network representation for path integrals. This work generalizes the ideas from the MPS representation to a more flexible custom tensor network that manifestly captures the structure of the Feynman-Vernon influence functional, further illustrating the deep fundamental ties between tensor networks and path integrals.[15]
- Derived a series representation for the coefficients that capture the influence of the solvent on to the system in terms of the Kubo transform of the so-called "bath response function."[14]
- Developed a new multisite tensor network formalism for simulating extended quantum systems coupled to local dissipative environments like exciton transfer and charge transfer chains coupled with local vibrations. This MS-TNPI is a two-dimensional structure that, when evaluated yields the time propagated reduced density matrix of the entire extended system in the form of a matrix product state.[13]
- Explored the impact of thermal gradients on quantum transport in the Frenkel-Holstein model. Demonstrated for the first time, the possibilities of control using spatially inhomogeneous temperature profiles.[12]
- Studied the excitonic dynamics and absorption spectrum of a B850 ring using MS-TNPI accounting for the effects of atomistically derived protein and vibrational environments.[11]

Ph. D. Research — UIUC

- Derived an approach to approximating the thermal correlation functions for mixed quantum-classical methods. It is shown that this method can exactly calculate rates of reactions for systems in atomistic environments.[10]
- Simulated exciton transfer in a chlorophyll dimer with all local vibrations present. The effects of static disorder on the resultant dynamics were analyzed.[8]
- Formulated a new exact numerical method for calculating multidimensional Wigner distributions for thermalized operators.[7]
- Derived a method for calculating correlation functions using stability matrices under the quasiclassical approximation. A very simple yet accurate approximation which is applicable for multidimensional systems is proposed.[6]
- Applied the adiabatic switching based Wigner method to atomistic Hamiltonians in normal mode coordinates and Cartesian coordinates. Calculated quasiclassical correlation functions and explored the importance of Zero-Point Energy and quantization of the thermal density.[5]
- Constructed a nonequilibrium reactive flux based method for calculating rates of reactions. This method is shown to unify slow and fast reaction dynamics.[4]
- Described an efficient classical trajectory based method for calculating the quantum Wigner phase-space distribution.[2]

Master's Research Projects — IITK

- Investigated a simple model of two-photon processes using non-relativistic quantum electrodynamics.[1]
- Modelled and studied the impact of the shape of the envelope of a few-cycles laser pulse on the nature of the breakdown of rotating wave approximation in the dynamics of two-level systems.[3]
- Learned ultrafast spectroscopy with Prof. Debabrata Goswami. Worked on the instrumentation of a 2D nonlinear optical spectroscope using an acousto-optical modulator pulse shaper with colinear pulses.
- Worked with Prof. Martin Gruebele on expressing PGK-FRET proteins for subsequent study of protein dynamics in presence of gold nanorods during the Summer, 2011.