Amit Kumar Upadhyay (Male)

Ph.D. Research Scholar
Department of Energy Science & Engineering
Indian Institute of Technology Bombay
Mumbai, Maharashtra, India (400076)

ORCiD: 0009-0004-4706-3399
LinkedIn: amit-upadhyay-2a3586124
Twitter: Amit_Upadhyay96
Email: upadhyay.amit@iitb.ac.in
Email: upadhyay.amit1996@gmail.com

Research interests

- Quantum dynamics of electronic excitation and charge transfer
- Light-matter interactions and cavity quantum electrodynamics
- Quantum information theory and computing
- Tensor network theory and applications
- Quantum phase transitions and heat transport

Technical skills

- **Modeling:** Spin-Boson, Frenkel-exciton, Jaynes-Cummings, classical and quantum coupled harmonic oscillators
- **Dynamics:** Marcus rate theory, Fermi Golden Rule, Bloch-Redfield equation, Lindblad master equation, coherent modified Redfield theory, non-Markovian master equation, hierarchical equations of motion (HEOM)
- **Simulations:** Unitary and dissipative quantum evolution, molecular spectra, molecular dynamics, RK4, simpson-3/8, Gaussian random sampling, Metropolis Monte-Carlo optimization
- **Programming:** Python, QuTiP, Mathematica, Fortran, LaTeX, Origin, Numpy, Pandas, Matplotlib, Gnuplot

Research experience

Ph.D. projects (2019-present)

- **Electronic Excitation Transfer in Multi-Site Systems**
  - Derived analytical expressions of site populations in 3-site uphill and downhill systems
  - Theoretical and numerical examination of tunability effects in 3-site systems through Lindblad equation and HEOM
- **Incoherent Born-Markov Rate Model for Excitation Transport**
  - Developed a population-coherence decoupled rate model in site-basis for strong coupling regime
  - Demonstrated negligible inter-site coherence effect on 3-site system's tunability
  - Observed both coherence-assisted and resisted energy transfer in multi-site systems
  - Optimized energy transfer efficiency of multisite systems using Born-Markov rate model
- **Extended Förster Theory for Coherent Energy Transfer**
  - Derived rate expressions beyond the Förster's regime in the weak coupling regime
  - Observed energy oscillations in resonance energy transfer

M.Sc. project (2018-19)

- **Resonance Energy Transfer via Classical Coupled Oscillators**
  - Established a classical analogy to dipole-dipole interactions
  - Validated Förster's theory using eigenmode analysis

Journal publications

- **Amit Kumar Upadhyay**, Karthik Sasihithlu. *Tunability in 3-Site Electronic Excitation Transfer Dynamics: Insights into the Role of Perturbative Coupling*. The Journal of Physical Chemistry B 128.17, 4047-4052 (2024)
- **Amit Kumar Upadhyay**, Karthik Sasihithlu. *Electronic excitation transfer dynamics in a 3-site system using an incoherent Born-Markov rate model*. ChemPhysChem 26.15, e202500029 (2025)
- **Amit Kumar Upadhyay**, Karthik Sasihithlu. *Analyzing Coherence Effects in Multisite Electronic Excitation Transport Using the Born-Markov Rate Model.* The Journal of Physical Chemistry B (accepted)
- **Amit Kumar Upadhyay**, Karthik Sasihithlu. *Extended Forster's theory to explain coherent effects in resonance energy transfer.* (under preparation)

Education

Examination	Department	College/University	Year
Ph.D.	Energy Science & Eng.	IIT Bombay	2019-present
Masters (M.Sc.)	Energy Science & Eng.	IIT Bombay	2017-19
Bachelors (B.Sc.)	Physics	A.R.S.D. College, University of Delhi	2014-17

Scholastic achievements

- First prize, **Energy Systems Modelling and Economics**, Energy Day 2021, IIT Bombay *(May'21)*

Conference presentations

- **Oral presentations:**
  - *Electronic Excitation Transfer in 3-site systems: Tunability and coherence effects*, **Youth Scientist Conclave on Topics in Quantum Dynamics, IIT Bombay** *(July'24)*
- **Poster Presentations:**
  - *Coherent Population Dynamics of the Correlated Spin System in the Markovian Limit*, **International Conference on Quantum, Atomic, and Molecular Physics, Glasgow (UK)** *(Sep'23)*
  - *Coherent Population Dynamics of the Correlated Spin System in the Markovian Limit*, **International Conference on Quantum Coherent Dynamics, Barcelona (Spain)** *(Sep'23)*
  - *Understanding the Validity of the Markovian Approximation in the Dynamics of Energy Transfer in the FMO Complex*, **International Conference on Photonics, IISc Bangalore** *(July'23)*
  - *Understanding the Validity of the Markovian Approximation in the Dynamics of Energy Transfer in the FMO Complex*, **International Conference on Progress in Quantum Science and Technologies, IIT Madras** *(Jan'23)*

Schools/Internships/Workshops

- **ICTS-TIFR (Online Winter Program, 2023):** Classical & Quantum Transport Processes *(Jan'23)*
- **ICONS (2023):** Quantum Science and Technology Workshop, IIT Bombay *(Feb'23)*
- **Advanced courses:** Light-matter interaction, Quantum optics, Simulation techniques in physics, Programming in chemistry, Chemical dynamics *(2019-23)*

Position of responsibilities & extra-curricular

- **Teaching Assistant:** Physics for energy science, Computer programming, Micro and nanoscale energy transport, Energy conversion lab, Thermodynamics and statistical mechanics *(2019-24)*
- **Outreach:** Organized Mumbai Science Talk, IIT Bombay *(2018-19)*
- **Conference Volunteer:** 7th Int. Conf. on Advances in Energy Research, IIT Bombay *(Dec'19)*

Referees

- **Prof. Karthik Sasihithlu** (M.Sc. & Ph.D. supervisor)
  Department of Energy Science and Engineering, IIT Bombay, India
  email: ksasihithlu@ese.iitb.ac.in
- **Prof. Amber Jain** (Research examiner)
  Department of Chemistry, IIT Bombay, India
  email: amberj@chem.iitb.ac.in
- **Prof. Gopal Dixit** (Research examiner)
  Department of Physics, IIT Bombay, India
  email: gdixit@phy.iitb.ac.in

Declaration: I certify that all information provided is accurate to the best of my knowledge.