



Amit Kumar Upadhyay (Male)
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Research interests

- Energy and charge transfer dynamics in molecular aggregates
- Light-matter interactions and cavity quantum electrodynamics
- Quantum information theory and computing
- Tensor network based computations
- Quantum phase transitions and heat transport
- Quantum thermodynamics

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, Github

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). [Link](#)
- **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). [Link](#)
- **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 129.44, 11387-11394 (2025). [Link](#)
- **Amit Kumar Upadhyay**, Karthik Sasihithlu. *Extended Forster's theory to explain coherent effects in resonance energy transfer*. (in preparation)

Education

Examination	Department	College/University	Year
Research Associate	Energy Science & Eng.	IIT Bombay	May-Nov'25
Ph.D.	Energy Science & Eng.	IIT Bombay	2019-25
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)
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Declaration: I certify that all information provided is accurate to the best of my knowledge.