Atreyee Majumdar

PhD Student in Chemistry (2023–)
Tata Institute of Fundamental Research, Hyderabad, India

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Current Group: MolDis Group (Big Data Analytics for Molecular Discovery)

LinkedIn Google Scholar Twitter GitHub

Personal Details

Date of Birth: 09 September 1999
Nationality: Indian
Gender: Female
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Field of Interest

Computational chemistry, Chemical space, Excited states dynamics

Education

- **PhD in Chemistry**, Tata Institute of Fundamental Research, Hyderabad (India), 2023–present
  Supervisor: Prof. Raghunathan Ramakrishnan
- **M.Sc. in Chemistry**, Central University of Rajasthan, India, 2020–2022
  Grade: 7.73 / 10
- **B.Sc. in Chemistry**, Scottish Church College, Calcutta University, 2017–2020
  Percentage: 79.15%
- **ISC**, The Future Foundation School, 2015
  Percentage: 93.5%
- **ICSE**, The Future Foundation School, 2013
  Percentage: 95%

Publications on Thesis Work

1. *Leveraging the Bias-Variance Tradeoff in Quantum Chemistry for Accurate Negative Singlet-Triplet Gap Predictions: A Case for Double-Hybrid DFT*, A. Majumdar, R. Ramakrishnan, **J. Comput. Chem.**, Accepted (2025). DOI: 10.48550/arXiv.2502.09330
2. *Unlocking Inverted Singlet-Triplet Gap in Alternant Hydrocarbons with Heteroatoms*, A. Majumdar, S. Das, R. Ramakrishnan, **Chem. Sci.**, 16, 14392–14407 (2025). DOI: 10.1039/D5SC02309B
3. *Influence of Pseudo-Jahn–Teller Activity on the Singlet-Triplet Gap of Azaphenalenes*, A. Majumdar, K. Jindal, S. Das, and R. Ramakrishnan, **Phys. Chem. Chem. Phys.**, 26, 26723 (2024). DOI: 10.1039/D4CP02761B

4. *Resilience of Hund's rule in the chemical space of small organic molecules*, A. Majumdar and R. Ramakrishnan, **Phys. Chem. Chem. Phys.**, 26, 14505 (2024). DOI: 10.1039/D4CP00886C

Other Collaborative Publications

1. *Comment on "Designing potentially singlet fission materials with an anti-Kasha behaviour"* by R. Pino-Rios, R. Báez-Grez, DW Szczepanik, and M. Solá, K. Jindal, A. Majumdar, R. Ramakrishnan, **Phys. Chem. Chem. Phys.**, 27, 4968–4972 (2025).

Posters Presented

1. *"In Pursuit of Hund's-rule Violating Organic Molecules"*
   Presented at the **20th edition of the Spectroscopy and Dynamics of Molecules and Clusters (SDMC 2025)**, February 20–23, 2025.

2. *"A Tale of True & False Positives in Search of Hund's-rule Violating Organic Molecules"*
   Presented at **ChemSci 2024: Leaders in the Field Symposium**, organized by the **Royal Society of Chemistry** and **IISER Thiruvananthapuram**, 2024.

Research Projects

- **Graduate Student Lab Rotation I (Jan–Feb 2024)**: Computational Investigation of Hund's Rule Violating Organic Molecules, under the guidance of Dr. Raghunathan Ramakrishnan, Associate Professor, TIFR Hyderabad.
- **Graduate Student Lab Rotation II (Nov–Dec 2023)**: Theoretical Study of the Spectra of Diatomic Molecules, under the guidance of Dr. Pranav R. Shirhatti, Associate Professor, TIFR Hyderabad.
- **M.Sc. Dissertation Project (Feb–May 2022)**: Investigation of the Effects of Through-Bond and Through-Space Interactions on Thermally Activated Delayed Fluorescence in Organic Molecules, under the guidance of Dr. S. Rajagopala Reddy, Professor, Department of Chemistry, Central University of Rajasthan.

Software Skills

- **Programming:** Python, Fortran 90/95, Java
- **Quantum Chemistry Packages:** ORCA, Gaussian, Q-Chem, Molpro

Languages

- English — Fluent
- Hindi — Fluent
- Bengali — Native

Referees

Prof. Raghunathan Ramakrishnan
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