Arghyadeb Roy

Master's Student
Department of Chemical Sciences
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Research Interests

- Theoretical and Computational Chemistry
- Astrochemical Modeling

Education

Indian Institute of Science Education and Research (IISER) Kolkata

- 5-year Integrated BS-MS Dual Degree *Expected May'25*
- 5th Year Chemistry Major and Physics Minor

Research Affiliations

QuantAct Group, IISER Kolkata (PI: Dr. Sangita Sen)

Master's Project Student *2023 – Present*

- Potential Energy Surfaces for Reactions of Astrochemical Importance.
- Computational study on molecular properties using ab initio methods.

Conferences and Seminars Attended

- PCAMC 2024 Conference, IISER Kolkata
- IINCM 2024 Conference, IISER Kolkata (*Best Poster Award from Royal Society of Chemistry*)
- SICS 2023 Seminar, IISER Kolkata

Technical Skills

Writeup: MS Office, LaTeX

Plotting: Origin, GnuPlot, Python

Quantum Chem: Gaussian, ORCA, Qchem, Avogadro, Multiwfn

Skills: Python, Julia, Shell Scripting

Fellowship

INSPIRE Fellow, Department of Science & Technology, India *2020 – Present*

Personal Details

Nationality: Indian

Languages Known: English (Proficient), Bengali (Native), Hindi (Proficient)

Gender: Male

Teaching Assistant

Teaching assistantship (TA) in CH4202 - Symmetry in Chemistry Course **Present**
This course explores the application of group theory and symmetry principles in molecular bonding, vibrations, and spectroscopy. It provides a foundation for understanding molecular orbital construction, vibrational modes and electronic transitions through symmetry-adapted methods and selection rules.

Teaching assistantship (TA) in CH1201 - Elements of Chemistry-II Course **Jan – May 2024**
This course provides a comprehensive overview of the states of matter, the laws of thermodynamics, and the kinetics of chemical reactions.

Teaching assistantship (TA) in CH2102 - Quantum Chemistry-I Course **Aug – Dec 2023**
This course covers the fundamental principles of Quantum Chemistry, focusing on the transition from classical to quantum mechanics and exploring various quantum systems.