



# Arghyadeb Roy

Research Undergrad.

*I'm a research student pursuing the BS-MS int. dual degree and want to explore the fascinating field of theoretical chemistry & astrochemistry and its approaches to defining the atomic to the molecular basis of the physical and chemical phenomena that appear astonishingly.*

*My main research interest is molecular modelling and quantum mechanical and dynamical study.*

## Research Interests

- Theoretical and Computational Chemistry
- Quantum Chemistry and Information Theory
- Ab initio potential energy surfaces study
- Modelling of astrochemical gas grains in star-forming regions
- Theoretical reaction dynamics in astronomical environments
- Modelling astrochemistry in radiation-dominated environments
- Spectroscopy

## Participations

- DIG (Dust, Ice and Gas) Astrochemistry webinar organized by IASES, PRL, Europlanet Society, Niigata University, Quantum Research Center.
- Evening Course on Astronomy and Space Science organized by Institute of Astronomy Space and Earth Science(IASES).
- SICS 2023 seminar organized by IISER Kolkata

## Achievements

### Fellowship

Innovation in Science Pursuit for Inspired Research (INSPIRE) fellow sponsored by the "Department of Science & Technology (DST)," India

## Affiliation & Education

### Graduation Degree May'25 (Expected)

5 years BS-MS Int. Dual Degree  
Indian Institute of Science Education and Research (IISER) Kolkata, India  
4th Year Chemistry Major (DCS)

## Technical Skills

### Software/Tools

**Writeup:** MS Office, LaTeX

**Plotting:** Origin, GnuPlot

**MD:** VASP, CASTEP

**QM:** Gaussian, ORCA, Gamess, Qchem

**GUI:** Multiwfn, Avogadro

### Skills

Ubuntu (OS), Windows (OS), Python, Julia  
MATLAB, Fortran 95 (Basic), Shell Scripting

## Personal Details

**Address:** Tufanganj (PIN-736159),  
CoochBehar, West Bengal, India

**Nationality:** Indian

**Languages Known:** English, Bengali, Hindi

**Gender:** Male

**Marital Status:** Unmarried

**Religion or Belief:** Hindu

**Ethnic Origin:** Asian — Indian

**Disability:** No

## Contact Details

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