AKASH SHIL

Indian Institute of Technology Tirupati, A.P-517619, India

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Nationality: Indian **D.O.B**: 06 / 12 / 2000

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RESEARCH OBJECTIVE

I am passionate about contributing to sustainable chemistry by developing eco-friendly, metal-free organic photoredox catalysts through computational methods like DFT & TDDFT. I aim to understand and enhance their photophysical and photochemical properties, aiming to create innovative solutions for efficient photocatalysis.

ACADEMIC DETAILS

Indian Institute of Technology Tirupati 2023-2025

M.Sc. - Chemistry | CGPA: 7.34 / 10

ICFAI University, Tripura 2020-2023

B.Sc. Hons. – Chemistry (Full time) | CGPA: 8.65 / 10

Udaipur English Medium Higher Secondary School 2020

12th | Tripura Board of Secondary Education | Percentage: 72 / 100

Holy Cross (South) English Medium H.S School, Tuikarmaw 2018

10th | Tripura Board of Secondary Education | Percentage: 78 / 100

ACADEMIC ACHIEVEMENTS

- Qualified IIT-JAM (Joint Admission Test for Master's) in Chemistry, 2023
- Gold medalist (Rank 1) for academic excellence in B.Sc. Chemistry

RESEARCH EXPERTISE

- Electronic structure calculations of ground & excited-state using DFT & TDDFT
- Optimal tuning of range-separated hybrid functional
- Predicting ground & excited-state redox potentials

RESEARCH INTERESTS

- Computational quantum chemistry
- Quantum algorithms for chemical systems
- Electronic structure theory & redox properties
- Photo-redox catalysis & excited-state dynamics
- Machine learning applications in computational chemistry
- AI-driven molecular design & reaction prediction

Developing computational methodologies:

- New DFT functionals
- New theoretical protocols

RESEARCH EXPERIENCE

Master's project:

Title: Tailored Ground and Excited-State Redox Potentials Through Halogenation and/or Extended π-Conjugation in BODIPY Dye: A Computational Perspective.

Guide: Dr. Arun K. Manna (Associate Professor, Department of Chemistry, IIT Tirupati)

Abstract: Focused on investigating redox potentials of functional BODIPY derivatives using DFT & TDDFT. The work emphasizes developing sustainable, visible-light absorbing metal-free organic photoredox catalysts.

SKILLS AND COMPETENCES

- **Laboratory skills**: a. Separation techniques – Chromatography (Column, TLC)
  b. Titrimetric methods – Redox, Iodometry, Conductometric
  c. Spectroscopic techniques – UV-visible, Infrared, Fluorescence

- **Software skills**: a. Language – Fortran, basic Python
  b. Use of Gaussian 16, GaussView 6, VESTA, ChemDraw, Linux and Windows 7, 8, 10 as operating systems, MS Office, LaTeX

RELEVANT COURSES

- Modern Electronic Structure Methods and Applications
- Principles of Spectroscopy
- Quantum Chemistry and Chemical Bonding
- Applications of Spectroscopy in Inorganic and Organic Chemistry
- Nanochemistry: Principles and Applications
- Computer Programming and Numerical Methods in Chemistry

REFERENCES

- **Dr. Arun K. Manna**
  Associate Professor
  Indian Institute of Technology Tirupati, E-mail: arun@iittp.ac.in

- **Dr. Rajib Biswas**
  Associate Professor
  Indian Institute of Technology Tirupati, E-mail: rajib@iittp.ac.in

- **Dr. Gouriprasanna Roy, HOD**
  Professor
  Indian Institute of Technology Tirupati, E-mail: gproy@iittp.ac.in

- **Dr. Tufan Singha Mahapatra**
  Assistant Professor
  ICFAI University, Tripura, E-mail: tsmahapatra@iutripura@edu.in