

RESEARCH INTEREST

Modelling chemical reactions using electronic structure calculations.
Development of machine learning potentials for condensed phase reactive systems.

EDUCATION

Indian Institute of Technology Delhi

Ph.D. (Computational Chemistry)

2023-Present

Advisor Prof. Tarak Karmakar

CGPA: 9.75/10.00

Indian Institute of Technology Delhi

M.Sc. (Chemistry)

2020-2022

Advisor Prof. Anil J. Elias

CGPA: 9.15/10.00

Rajdhani College, University of Delhi

B.Sc. Honors (Chemistry)

2017-2020

CGPA: 8.78/10.00

PUBLICATIONS

- Davas, D. S.; Gopalakrishnan, D. K.; Kumar, S.; **Anmol**; Karmakar, T.; Vaitla, J. Visible Light-Promoted Regioselective Benzannulation of Vinyl Sulfoxonium Ylides with Ynoates. *JACS Au* **2024**, 4 (3), 1073–1080.
- Yadav, R.; Das, B.; Singh, A.; **Anmol**; Sharma, A.; Majumder, C.; Kundu, S. Bicyclic (Alkyl)(Amino) Carbene (BICAAC)-Supported Phosphinidenes. *Dalton Transactions* **2023**, 52 (45), 16680–16687.
- Jain, S.; **Anmol**; Sharma, R.; Karmakar, T.; Yadav, M. R. Cu(I)/N,N-Imine Ligand Catalyzed C(Sp³)–C(Sp) Coupling of Alkyl Bromides with Alkynes: Scope and Mechanistic Investigation. *Organic Letters* **2023**, 25 (29), 5437–5442.
- Tyagi, A.; Mondal, S.; **Anmol**; Tiwari, V.; Karmakar, T.; Kundu, S. Understanding Cyclic(Alkyl)(Amino) Carbene–Copper Complex Catalysed N–H and O–H Bond Addition to Electron Deficient Olefins. *Chem. Commun.*, **2023**, 59, 110–113.

Conferences & Workshops

- Quantum2 on machine learning enhanced sampling (Organised by CECAM in hybrid format attended online).

KEY SKILLS

Programming Language Software

Python, Bash
Gaussian, CP2K, LAMMPS, GROMACS, Plumed, DeepMD, VMD