Sourav Mondal, PhD

AI/ML Scientist | Computational Chemist | Drug Discovery

Computational scientist with **10+ years of experience** in cross-disciplinary research spanning **Drug Discovery** and **Materials Modeling**. Currently at **Aganitha Cognitive Solutions**, leveraging quantum mechanical calculations and deep learning to accelerate small molecule research. Building end-to-end pipelines for crystal structure prediction, conformer generation, pKa estimation, and **ADMET property calculations**. Published in **Nature Computational Materials, JACS, and Nano Letters**. PhD from **JNCASR Bangalore** with postdoctoral research at **Trinity College Dublin**.

CONTACT

Hyderabad, India
+91 9740851654
souravchembwn@gmail.com
github.com/mondalsou
linkedin.com/in/soura1
Portfolio

Professional Experience

Scientist

Jan 2024 - Present

Aganitha Cognitive Solutions - Hyderabad

- Designing CSP pipeline using Graph Neural Networks for rapid polymorph screening of drug-like molecules
- Developing conformer generation methods for PROTACs across diverse environments & ligand conformers in protein pockets
- Creating predictive models for pKa values in non-aqueous conditions
- Building workflows for thermodynamics property estimation: solubility, logP, and solvation energy
- Project management, client communications, proposal writing & SoW implementation

Education

PhD, Computational Material Science

JNCASR - Bangalore

2015 - 2020

M.Sc, Chemistry

IIT Guwahati

2012 - 2014

Computational Scientist & Deep Learning Engineer

Aug 2023 - Dec 2023

QpiVolta Technologies - Bangalore

- Modeled thermodynamic properties using molecular dynamics and ML force fields
- Developed and refined machine learning force fields for solid-state electrolytes
- Led contract research on simulating complex biological systems

Postdoctoral Researcher

Mar 2021 - Jul 2023

Trinity College Dublin - Ireland

- Simulated spin dynamics using ab-initio methods and machine learning approaches
- Explored spin dynamics in systems from 0D to 3D structures (Co/Dy SMMs, NV defects in Diamond)
- Developed computational methodology for accurately predicting spin-relaxation times
- Built Neural Network models for predicting spin properties, replacing intensive QM calculations

PhD Researcher

Jan 2015 - Feb 2021

JNCASR - Bangalore

Thesis: "Tailoring the Properties of Two-dimensional Systems by Molecular Adsorption and Defect Engineering"

- Employed DFT to examine molecular adsorption behavior and defect impacts on 2D materials
- Investigated electronic and magnetic properties across diverse systems
- Built novel post-processing tools for STM spectroscopy analysis
- Research visits to University of Paris Diderot and CEA Saclay (CEFIPRA grant)

Technical Skills

AI/ML & DEEP LEARNING

Gen AI · PyTorch · TensorFlow · GNN · Transformers · AI-Agents · Scikit-learn

COMPUTATIONAL CHEMISTRY

CP2K · ORCA · psi-4 · PySCF · DFT/SAPT · ML Force Fields

CHEMINFORMATICS

RDKit · ASE · SMILES/SMARTS · ADMET · Docking

PROGRAMMING & TOOLS

Python · Fortran · n8n · Git · Docker · Azure

Achievements

- ✓ **Irish Research Council Ulysses Grant** - University of Rennes, France (2022)
- ✓ **Contributed Talk** at Psi-K 2022 Conference, Switzerland
- ✓ **CEFIPRA Travelling Grant** - University Paris Diderot (2016-2020)
- ✓ **8th European Conference on Molecular Magnetism** - Poster Presentation (2022)

Certifications

NET CSIR-UGC Junior/Senior Research Fellowship
Government of India, 2014

Selected Publications

Sourav Mondal, Julia Netz et al., "The spin phonon relaxation of single molecules magnet in the presence of strong exchange coupling"

ACS Cent. Sci. (2025)

Sourav Mondal and A. Lunghi, "Spin-phonon decoherence in solid-state paramagnetic defects from first principles"

npj Comput. Mat. (2023)

Sourav Mondal and A. Lunghi, "Unravelling the contributions to spin-lattice relaxation in Kramers single-molecule magnets"

J. Am. Chem. Soc. (2022)

R. Harsh, **Sourav Mondal***, et al., "Identification and Manipulation of Defects in Black Phosphorus"

J. Phys. Chem. Lett. (2022)

M. Bouatou, **Sourav Mondal***, et al., "Direct Observation of the Reduction of a Molecule on a Nitrogen pair in Doped Graphene"

Nano Lett. (2020)

C. Fourmental, **Sourav Mondal***, et al., "Importance of Epitaxial Strain at a Spin-Crossover Molecule Metal Interface"

J. Phys. Chem. Lett. (2019)