SOURAV MONDAL

AI/ML SCIENTIST | COMPUTATIONAL CHEMIST | DRUG DISCOVERY EXPERT

CONTACTS

+919740851654

souravchembwn@gmail.com

https://mondalsou.github.io/mondalsou/

Hyderabad, India

FIND ME ONLINE

- **Portfolio**
  https://mondalsou.github.io/mondalsou/
- **Github**
  https://github.com/mondalsou
- **LinkedIN**
  https://www.linkedin.com/in/soura1/

SUMMARY

AI/ML Scientist | 10+ years in drug discovery, computational chemistry, and deep learning. Core contributor to Igniva™ Agentic AI platform at Aganitha, building production GNN pipelines, AI Agents, and QM tools for CSP, conformer generation, pka, and ADMET. PhD (JNCASR) + Postdoc (Trinity College Dublin). Published in Nature Comput. Mat., JACS, Nano Letters. PyTorch, GNNs, RDKit, DFT, Azure.

KEY ACHIEVEMENTS

- **6+ Top-Tier Publications**
  Published in Nature Computational Materials, JACS, ACS Cent. Sci., and Nano Letters as first or equal-contribution author.

EXPERIENCE

Aganitha's Agentic AI platform for biopharma R&D — Hyderabad, India

Aganitha Cognitive Solutions Scientist — 01/2024 - Present

- Core contributor to Igniva™ - Aganitha's Agentic AI platform for biopharma R&D, developing multiple production tools for the small molecule design and CMC pipeline
- Developed Crystal CleanPro and Crystal LatticeAI - Crystal Structure Prediction (CSP) pipelines leveraging Graph Neural Networks for rapid polymorph screening of drug-like molecules
- Built MolConSUL Pro - AI-driven platform for 3D molecular conformer generation, enabling environment-aware drug discovery applications
- Engineered Sitepka - site-specific pka prediction tool using dual-graph cross-attention GNN architecture for non-aqueous conditions
- Developed QM-based pKa estimation pipeline using first-principles quantum chemistry methods, complementing the GNN approach for high-accuracy predictions
- Created physics-based QM platform for ADMET property prediction including solubility, logP, and solvation energy with production-grade deployment on Azure
- Managed client communications, project proposals, and end-to-end delivery of computational chemistry solutions for pharmaceutical partners

QpiVolta Technologies — Bangalore, India

Computational Scientist & Deep Learning Engineer — 2023 - 08/2023

- Developed machine learning force fields (MLFF) for solid-state electrolyte materials, enabling rapid molecular dynamics simulations
- Modeled thermodynamic properties of electrolyte systems using molecular dynamics and ML-augmented simulations
- Led contract research on complex biological system simulations, delivering actionable insights to stakeholders

Trinity College Dublin — Dublin, Ireland

Postdoctoral Researcher — 03/2021 - 07/2023

- Built neural network models for quantum property prediction of paramagnetic defects, published in Nature Computational Materials (npj Comput. Mat., 2023)
- Developed first-principles computational methods for spin-phonon dynamics simulation, published in JACS (2022)
- Combined ab-initio quantum chemistry methods with machine learning to model spin-lattice relaxation in single-molecule magnets
- Collaborated with experimental groups across Europe on quantum computing and molecular magnetism research

KEY ACHIEVEMENTS

- **6+ Production Pipelines in Igniva™**
  Built CrystalCleanPro, CrystalLatticeAI, MolConSUL Pro, SitepKa, QM-pKa, and ADMET platforms — shipped as part of Aganitha's commercial Agentic AI product.
- **AI Agent for Lead Optimization**
  Developed autonomous medicinal chemistry agent using Claude AI with iterative propose-score-compare loops for drug lead optimization.
- **End-to-End Drug Discovery Platform**
  Built and deployed full-stack triage app(React, FastAPI, RDKit) with real-time ADMET, QED, and PAINS screening on Vercel.

SKILLS

AI/ML & Deep Learning

AI/ML & Deep Learning · Graph Neural Networks (GNN) · PyTorch · TensorFlow · Transformers · AI Agents · Neural Networks · Transfer Learning · Hyperparameter Tuning · MLOps · CI/CD · Reinforcement Learning · Multi-tasking Learning · LSTM

Drug Discovery & Cheminformatics

ADMET Prediction · Molecular Property Prediction · Conformer Generation · pKa Prediction · CADD · RDKit · SMILES/SMARTS · Molecular Docking · QED Scoring · Lead Optimization · Binding Affinity Prediction

Computational Chemistry

DFT · Quantum Chemistry · CP2K · ORCA · Psi4 · PySCF · SAPT · ML Force Fields · MD · First-Principles Calculations

PERSONAL PROJECTS

Lead Optimization Agent

AI Agents · Claude AI · RDKit · Streamlit

- Built AI-powered medicinal chemistry sandbox using Claude for autonomous iterative lead optimization with propose-score-compare agent loop
- Tracks BBB permeability, CNS MPO, QED, and molecular flexibility per iteration with highlighted 2D structural changes
- Deployed on HuggingFace Spaces with local run persistence for cost-efficient multi-session workflows

https://huggingface.co/spaces/mondalsou/lead_optimization_agent

GNNBindOptimizer

PyTorch · HGTConv · REINFORCE · SQL Server · MLflow · Docker

- Heterogeneous GNN (HGTConv) for protein-ligand binding affinity prediction using multi-task learning with Kendall uncertainty-weighted loss across affinity, pose classification, and selectivity objectives.
- Reinforce-based molecular generator targeting EGFR kinase pocket, with generated candidates scored and benchmarked against AutoDock Vina docking.
- End-to-end deployment via Docker Compose with SQL Server persistence, MLflow experiment tracking, and Streamlit UI covering binding prediction, RL generation, and live GNN-vs-Vina comparison.

https://github.com/mondalsou/gnn-bind-optimizer

Drug Discovery Triage Platform

React · FastAPI · RDKit

- Full-stack application for real-time ADMET prediction, QED scoring, PAINS alerts, and interactive molecular visualization
- Dockerized deployment with CI/CD pipeline, deployed on Vercel with production-ready error handling

https://drug-discovery-triage.vercel.app

Solubility Dual-Graph GNN

PyTorch · MPNN · Cross-Attention · MLflow

- Dual-graph interaction GNN predicting molecular solubility (logS) from solute-solvent SMILES pairs using bidirectional cross-attention
- Trained on 100K+ pairs from BigSolDB 2.0 achieving R^2 = 0.90, RMSE = 0.388, MAE = 0.290

https://github.com/mondalsou/solubility-dual-graph-gnn

Quantum Property Prediction

Neural Networks · Materials Science

- Neural network models for predicting quantum properties of Nitrogen Vacancy centers in diamond, bridging ML with quantum materials science

https://github.com/mondalsou/quantum-property-prediction-nn

EDUCATION

Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR) — Bangalore, India

PhD in Computational Materials Science — 01/2015 - 02/2021

- Thesis: Tailoring Properties of 2D Systems via Molecular Adsorption and Defect Engineering

SKILLS

Programming & Tools

Python · Fortran · NumPy · Pandas · Scikit-learn · ASE · Docker · Microsoft Azure · Git · MLflow · n8n · Streamlit · SQL Server

EDUCATION

Indian Institute of Technology (IIT) Guwahati Guwahati, India

M.Sc in Chemistry 01/2012 - 12/2014

- Qualified NET CSIR-UGC Junior/Senior Research Fellowship

PUBLICATIONS

The spin phonon relaxation of single molecules magnet in the presence of strong exchange coupling 2025

ACS Cent. Sci.

S. Mondal, J. Netz et al.

Spin-phonon decoherence in solid-state paramagnetic defects from first principles 2023

Nature Computational Materials

S. Mondal and A. Lunghi

Unravelling the contributions to spin-lattice relaxation in Kramers single-molecule magnets. 2022

JACS

S. Mondal and A. Lunghi