Manish Chandra

+91 7897914523 · manish.sia.mc@gmail.com · 26th June 2002
Khalilabad, Uttar Pradesh, India
LinkedIn https://linkedin.com/in/monees007/
GitHub https://github.com/monees007

Profile Summary

Chemistry researcher with hands-on experience in DFT-based electronic structure analysis, QM/MM simulations, and metal-organic framework characterization, supported by a strong computational and programming background.

Research Interests

Computational Quantum Chemistry | Machine Learning | Metal Organic Frameworks
Electronic Structure Theory | QM/MM

Research Experience

Research Intern *(May 2026 - present)*
under supervision of ***Dr. Krishna Kishore Inampudi***

- Performing QM/MM simulations to characterize enzymes–substrate interactions and compute free energy profiles using CP2K.

Masters Researcher *(Jul 2025 - May 2026)*
under supervision of ***Dr. Supriya Sabbani***

- Quantitatively correlating solvent induced reversible color change in Co(ina) metal organic frameworks (MOF) with gate-opening mechanism supported by DFT data.
- Study of Solvent-induced Redox Reactions in Copper Coordination Polymer: Catalysis Property, and Electrochemical H2 Evolution.

Laboratory Teaching Assistant *(May 2024 - present)*
Indian Institute of Technology Madras Chennai, TN (Remote)

- Assisted in laboratory sessions, guided students in command-line operations including grep, awk, vim, tmux, ssh, os installation, management and scripting fundamentals for the online laboratory component of course Introduction to Linux Shell (CS1102)

Research Intern *(Oct 2021 - June 2022)*
under supervision of ***Prof. Satyen Saha***

- UV-Visible Spectroscopic Analysis based determination of Isosbestic point of Bromocresol Green.

Publications

Manuscript in preparation: *Phase-Induced Chromatic Transition in [Co(INA)x] MOFs: DFT based study of Gate-Controlled Solvent Interaction*

Skills

Computational Chemistry: DFT, TD-DFT, Geometry Optimization, Frequency Analysis, Electronic Structure Analysis, Molecular Docking.
Software: ORCA, Quantum ESPRESSO, CP2K, AutoDock, ChemCraft, Avogadro
Programming & Computing: Python, Java, Kotlin, JavaScript, Dart, Linux, Git, Bash, HPC, MPI
Development: Cross-Platform Application Development using Flutter, Web Development.

Education

M.Sc. Chemistry *(Sep 2024 - May 2026)*
Jawaharlal Nehru University, New Delhi, India
Comprehensive training in organic, inorganic, physical, and analytical chemistry with strong emphasis on quantum chemistry, spectroscopy, and X-ray Diffraction, complemented by intensive laboratory work.

Diploma in Computer Programming *(May 2022 - May 2023)*
Indian Institute of Technology Madras, Chennai, India
Computer programming and data science foundations with courses in Python, Database Management, Data Structures & Algorithms, Machine Learning Techniques, Tools in Data Science, and project work.

B.Sc (Hons.) Chemistry *(July 2019 - August 2022)*
Banaras Hindu University, Varanasi, India
Rigorous honours chemistry curriculum covering core theory (organic, inorganic, physical, analytical), accompanied with biology courses, including genetics, biochemistry, cell biology, etc, with their accompanied laboratory courses.

Achievements

- Qualified GATE Chemistry 2026
- NPTEL — Computational Quantum Chemistry (12-week course), 2026
  Quantum chemistry methods, electronic structure theory, Hartree–Fock, DFT, basis sets, molecular properties, ORCA
- Qualified CSIR NET Chemistry 2025
- **REST API Intermediate**, HackerRank, 2023
- Qualified GATE Chemistry 2022
- **Functional Programming in Python**, Linkedin Learning, 2021
- **Python Object-Oriented Programming**, Linkedin Learning, 2021

Projects

- **Structure-Based Virtual Screening of BACE1 Inhibitors**
  Developed a machine learning pipeline to predict BACE1 inhibitor activity using molecular descriptors and supervised regression models for structure–activity relationship analysis.
- **AI-Based Assistive Vision System**
  Developed an AI-powered mobile system for real-time obstacle detection with audio and haptic feedback.
- **Secure Offline Mobile Wallet**

  Designed an encrypted mobile storage system with biometric/PIN authentication for secure data management.

Workshops and Conferences

- Attended the **TNQ Distinguished Lectures** on Quorum Sensing featuring Bonnie Bassler, New Delhi, February 2026.
- **Workshop on Physics of Living Systems**, School of Physical Sciences, Jawaharlal Nehru University (JNU), March 2025
- **Workshop on Breakthrough in Drug Design**: The Synergy of Machine Learning and High-Performance Computing, Prescience Insilico, 2024
- **Hands - on workshop on Single - Cell Transcriptomics** Centre for Integrative Biology and System Medicine, IIT Madras, 2022

Recommendations

Dr. Supriya Sabbani
Assistant Professor at Jawaharlal Nehru University
Masters Research Supervisor

Prof. Satyen Saha
Institution: Banaras Hindu University, Varanasi
Research Mentor

Dr. Deenbandhu Das
Assistant Professor at Jawaharlal Nehru University
Course Instructure

Languages

English (Level: Fluent, Native Language: No)
Hindi (Level: Fluent, Native Language: Yes)

Extracurricular

Lead, Technical Club – Coordinated technical events and workshops, fostering peer learning and collaborative problem-solving.

Member, Literary Club, Jawaharlal Nehru University – Contributed to organizing literary and academic events.