

ANISH CHAKRABORTY, PHD

☎ (+91) 6296680171, (+49) 17688031494 | ✉ anish.saheb41@gmail.com | inLinkedIn GitHub GitHub Portfolio

SUMMARY

- Computational Chemist with PhD and 6+ years of data-driven scientific research, molecular modeling, resulting in nine peer-reviewed high-impact publications.
- Skilled in both oral and written communication skills, adept at conveying scientific ideas to varied audiences, demonstrated by participation in 10+ scientific conferences leading to three national as well as international recognitions.
- Forward-thinking, interdisciplinary problem solver with a keen inclination towards collaboration, adept at working independently as well as within teams, demonstrated through mentoring 4 junior lab members and a successful collaboration in Germany.

EDUCATION

- PhD, Computational & Theoretical Chemistry, Indian Institute of Technology Bombay, 2023
- MSc, Chemistry, National Institute of Technology Rourkela, 2018
- BSc, Chemistry, Jadavpur University, Kolkata, 2016

PROFESSIONAL EXPERIENCE

Junior Quantum Chemist

Qclairvoyance Quantum Labs Pvt. Ltd., India

Apr'25 - Present

- Responsible for the development of an automated **Python-based CADD pipeline** for virtual screening, molecular docking, and cheminformatics scoring to accelerate structure based drug discovery (SBDD)
- Leading the development of **scalable algorithms** for predictive modeling of molecular interactions, improving early-stage drug screening efficiency.

Humboldt Postdoctoral Researcher, Chemistry

University of Heidelberg, Heidelberg, Germany

Aug'24 - March'25

- Led the development of **quantum chemistry-based methodologies** and softwares towards accurate quantification of energetics and associated properties of chemical systems, through an extensive use of **data handling**
- Extensive utilization of programming languages like Python and C++, as well as computational tools e.g. **Density Functional Theory (DFT)**, **Molecular Dynamics (MD)** towards the efficient implementation of the computational model

Postdoctoral Researcher, Chemistry

Rice University, Houston, Texas, USA

Feb'24 - July'24

- Development of a computationally efficient stochastic formulation (**Auxiliary Field Quantum Monte Carlo**) (**AFQMC**) to accelerate the calculations of various strongly correlated chemical systems
- Gained expertise in the domain of **Graphical Processing Units (GPUs)** and efficient implementations of C++ programs optimized for GPU architectures

TECHNICAL SKILLS & DOCUMENTATION

- **Programming languages:** Python, Fortran, C++, SQL, R and **Shell scripting (BASH)**
- **Computational Methods:** Coupled Cluster, Density Functional Theory, Quantum Monte Carlo, Molecular Dynamics
- **Computational Packages:** Gaussian, ORCA, Dalton, Q-CHEM, GAMESS, Gromacs, Diffdock, Haddock, OpenMM, PySCF, acpype
- **Python Libraries:** Numpy, Scipy, Pandas, Tensorflow, Keras, Scikit-learn
- **Data Visualization:** Gauss View, VMD, Power BI, Excel
- **Advanced Technologies:** Machine Learning, GPU coding, Quantum Computing, Qiskit
- **Data Analysis and Plotting:** Origin, GNUplot, Matplotlib, MySQL
- **Version Control:** GitHub
- **Presentation:** Microsoft Powerpoint, Latex Beamer, and Adobe platforms
- **Documentation:** Latex, MS Word, Adobe
- **Operating Systems:** Windows10/11, Linux/Ubuntu
- **Other soft Skills:** Project Management, Time Management, Reasoning skills, Analytical reasoning, Cross-functional Collaboration, Leadership & Mentoring, Efficient problem solver, Communication skills, Interdisciplinary Research

WORK EXPERIENCE

R&D and Project Management Expertise

Indian Institute of Technology Bombay, National Institute of Technology Rourkela

2017 - 2023

- Executed 3 primary and 2 collaborative projects involving extensive hands-on expertise in Python and basic proficiency in Fortran and C++ programming languages leading to nine high-impact peer-reviewed publications and two in the pipeline.
- Established a cohesive scientific team and guided four junior team members facilitating the transfer of technical knowledge resulting in the successful completion of a Master's thesis and two research projects.
- Optimize challenging scientific problems through high-level strategic planning, demonstrated by leading 4+ high-throughput methodologies and contributing to 4 high-impact first author publications.
- Gained expertise in several computational chemistry packages regarding DFT, culminating in the publication in an international peer-reviewed journal during Master's thesis.

Chemist and Research Teaching Assistant

Indian Institute of Technology Bombay

2019 - 2022

- Executed collaborative research with multi-disciplinary teams showcasing a robust capacity to investigate the current state of art scientific methodologies evidenced through the completion of three research projects.
- Gained leadership, teaching, and mentoring experience by instructing, supervising, and grading 60+ Engineering bachelor's students and 20+ master's students resulting in the successful completion of a teaching assistant program.
- Acquired adept oral and written communication abilities through the delivery of 10+ impactful poster presentations and talks at various national and international scientific conferences as evidenced by several award-winning presentations.

HONORS AND AWARDS

- 2024: Received the prestigious **Humboldt Research Award** for conducting research in Germany
- 2022: Received **Best Poster Award** in **25th International Workshop on Quantum Systems in Chemistry, Physics and Biology (QSCP)** held in Torun, Poland
- 2021: Received **Best Poster Award** in **Theoretical Chemistry Symposium (TCS)** held in IISER Kolkata, India

PUBLICATIONS

A full list of publication is available on my Google scholar page

OTHER SKILLS

Software Microsoft Word, Excel, and PowerPoint

Languages English: professional proficiency. Bengali: native. Hindi: conversational.

INTERESTS

Photography, Occasional sketching, Football aficionado, avid film buff