Dr. rer. nat. Raunak Farhaz

farhazraunak@proton.me | github.com/Raunak12775 | raunakfarhaz.com | Berlin, Germany

Computational Chemist and specialist in real-space numerical methods in quantum chemistry, algorithm design, and HPC simulation. Aspire to utilize deep-learning and frontier language models to accelerate molecular and materials simulations.

Technical Skills

- **Programming Languages:** Python (NumPy, SciPy, Pandas, Matplotlib), C++ (OOP), Julia, Fortran, Bash scripting, Wolfram Mathematica, Lua
- **High-Performance Computing (HPC):** SLURM/PBS queue managers, CMake, Ninja, fpm, custom scientific environment configurations (Conda, pip, uv), MPI, OpenMP
- **Data Engineering & ML:** Structured scientific data management, pipeline orchestration (Snakemake), JSON formatting, Git, GitHub/GitLab, PyTorch (Familiar)
- **Computational Chemistry Stack:** MADNESS, MRCPP / MRChem (wavelet-based solvers), PySCF, ORCA, ElemCo.jl, Gaussian, HUMMR
- **Languages:** English (Native), German (C1), Bengali (Native), Hindi (Bilingual)

Research & Software Engineering Experience

Ph.D. Researcher & Software Developer | *Humboldt-Universität zu Berlin* Berlin, Germany | 2020 – 2026

- Designed and coded a custom **Monte-Carlo simulated annealing global optimization framework** integrated with real-space Hartree-Fock theory to optimize structures of Helium molecules in extreme magnetic fields ($> 10^5\ T$). (manuscript in draft)
- Developed real-space Restricted Hartree-Fock methods, optimizing performance via combined shared-memory and distributed-memory parallel architectures (**MPI + OpenMP**).
- Quantified non-systematic basis set errors inherent in legacy atom-centered gaussian codes using wavelet-based numerical methods, culminating in a first-author publication.
- Configured, built, and compiled complex physical software packages and custom environments from source using **CMake, Ninja, and Fortran Package Manager (fpm)**.
- Spearheaded an independent collaboration with experimental researchers, utilizing Density Functional Theory (DFT) to validate physical measurements and model molecular properties (manuscript under review).

Visiting Doctoral Researcher | *Arctic University of Tromsø* Tromsø, Norway | 2023

- Authored automated scientific data pipeline extensions to read, write, and safely map multi-resolution wavelet-function datasets across heterogeneous computational chemistry software codebases.
- Standardized inter-process scientific data formats using robust, machine-readable schema structures to support reproducible multi-scale simulations.

Summer Research Fellow | *Indian Association for the Cultivation of Sciences* Kolkata, India | 2019

- Modeling complex structural bond breakages and hydrogen gas evolution catalysts using DFT funded by DST Govt. of India.

Leadership & Professional Contributions

- **Community Building:** Founded and coordinated the *Chemistry Coffee Talks*, a monthly *Doctoral Flash-talks & Networking Series* at Humboldt-Universität zu Berlin in partnership with Humboldt Innovation, driving interdisciplinary knowledge transfer.
- **Business Administration:** Operated as CEO/CFO of a online Edtech tutoring company (2020–2021) managing operations and curriculum development for 200+ students, highlighting financial, resource planning, and project management skills.
- **Academic Mentoring:** Guest lectured undergraduate mathematical foundations courses and instructed computational chemistry labs for Post-Graduate students in University level.

Education

Humboldt-Universität zu Berlin Berlin, Germany
Ph.D. / Dr. rer. nat. in Computational Chemistry *(Magna cum Laude)* Completed: 2026

- **Funding & Award**: Secured full four-year doctoral funding via the prestigious **DAAD Doctoral Fellowship** (2021–2025).

Jadavpur University Kolkata, India
M.Sc. in Chemistry (*Specialization in Physical Chemistry*) 2018 – 2020
B.Sc. in Chemistry (*Honors*) 2015 – 2018

- Recipient of the **DST-INSPIRE Scholarship** (Govt. of India) for high-potential (top 1% across country) natural science studies (2015–2020).

Publications

1. **R. Farhaz**, S. Stopkowicz, S. Blaschke, F. A. Bischoff. *Quantification of the basis set error for molecules in strong magnetic fields and general orientation*. **Journal of Chemical Physics** (2025)

2. R. Sardar, R. Banik, S. Ghosh, **R. Farhaz**. *Drug-Induced Micelle-to-Supermicelle Transition in CTAB: Comparative Study with Experimental and DFT Approaches*. **Langmuir - minor revision** (2026)

3. **R. Farhaz**, C. Rickert, F. A. Bischoff. *Geometry Optimization of Helium Dimers and Trimers in Extreme Magnetic Fields* **in preparation**