Raunak Farhaz

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EDUCATION

Humboldt-Universität zu Berlin 2021 — present
Dr. Rer. Nat. Computational Chemistry *Berlin, Germany*
- **Thesis** : Multiresolution Analysis in extreme magnetic fields

Jadavpur University 2018 — 2020
M.Sc. Chemistry with specialization in Physical Chemistry *Kolkata, India*
- **Thesis** : Theoretical study of adsorption of carbon monoxide on ZnO clusters

Jadavpur University 2015 — 2018
B.Sc. Chemistry *Kolkata, India*

RESEARCH EXPERIENCE

Arctic University of Tromsø, Norway 2023
Collaborated on portable binary file format for MRA wavelets with cross-codebase applications

Humboldt-Universität zu Berlin, Germany 2020
Quantum model systems in Multiresolution Analysis using Wolfram Mathematica

Indian Association for the Cultivation of Sciences, India 2019
Computational Catalytic study on Al-S bond breaking with hydrogen evolution

SKILLS

- **Quantum Chemistry**: MADNESS, MRCPP/MRChem, PySCF, ORCA, ElemCo.jl, HUMMR
- **Programming Languages**: Python, C++, Wolfram Mathematica, Julia, Fortran
- **HPC**: Git, Linux, Docker, SLURM/PBS, CMake, MPI/OpenMP, snakemake
- **AI/ML**: Pytorch, JAX
- **Data Science**: numpy, pandas, matplotlib, scipy

PUBLICATIONS

1. Bischoff, F. A.; Stopkowicz, S.; Blaschke, S.; **Farhaz, R.**
   Quantification of the basis set error for molecules in strong magnetic fields and general orientation
   *(**2025**) Journal of Chemical Physics, 163(3):034308*

2. Sardar, R.; Banik, R.; Ghosh, S.; **Farhaz, R.**
   Drug-Induced Micelle-to-Supermicelle Transition in CTAB: Comparative Study with Acetylenic Gemini Surfactant via Experimental and DFT Approaches
   *(**2026**) submitted*

FUNDING AND FELLOWSHIPS

Deutscher Akademischer Austauschdienst (DAAD) 2021 — 2025
Doctoral Programmes in Germany 2021/22

DST-INSPIRE Scholarship, Govt. of India 2015 — 2020
Scholarship for higher studies in natural sciences

CONFERENCES AND ACADEMIC ACTIVITIES

5 international conferences (e.g. WATOC, STC, QBIC, Numerical Methods in Quantum Chemistry) and 5 posters, 1 contributed talk and 2 workshops

TEACHING AND MENTORING

- Guest Lecturer **International University of Applied Sciences** for Math foundations
- M.Sc. practical course instructor **Humboldt-Universität zu Berlin** for theoretical molecular spectroscopy

updated on 2026-03-10

REFERENCES

- **PD Dr. Florian A. Bischoff** (Ph.D. supervisor) : florian.bischoff@hu-berlin.de
- **Prof. Dr. Luca Frediani** : luca.frediani@uit.no
- **PD Dr. Denis Usvyat** : denis.usvyat@hu-berlin.de

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