

# Raunak Farhaz

Doctoral Student

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Department of Chemistry  
Faculty of Mathematics and Natural Sciences  
Humboldt-Universität zu Berlin  
Brook-Taylor-Str 2  
12489 Berlin  
Germany

Doctoral candidate in theoretical chemistry at Humboldt-Universität zu Berlin with expertise in computational chemistry, quantum mechanics, and multi-resolution analysis (MRA). Research focuses on molecules in extreme magnetic fields, with a strong background in high-performance computing and numerical simulations. Experienced in developing computational tools (C++, Python, Julia), expert in handling data (numpy and pandas) and working with advanced quantum chemistry software. Interested in integrating AI/ML approaches for data-driven modeling, molecular simulations, and scientific discovery.

## Education

- **Institut für Chemie, Humboldt-Universität zu Berlin, Germany**
  - **Expected Graduation Time:** October 2025
  - **Status:** Doctoral Studies [2021 - ongoing]
  - **Thesis:** Molecules in extreme magnetic fields using Multi-Resolution Analysis (MRA)
  - **Advisor:** PD Dr. Florian A. Bischoff
- **Department of Chemistry, Jadavpur University, India**
  - **Status:** Master of Sciences with specialization in Physical Chemistry [2018 - 2020]
    - **Thesis:** Theoretical study of adsorption of carbon monoxide on ZnO clusters
    - **Advisor:** Prof. Kalyan Kumar Das
  - **Status:** Bachelor of Sciences [2015 - 2018]

## Research Experience

- **Research visit at UiT Tromsø, Norway [2023]**
  - Developed functions and classes in MRCP for printing wavelet information of wavefunctions
  - Ongoing work on serialization of MRA wavelets into a portable binary file format with potential cross-codebase applications.
- **Research internship (remote) at HU Berlin, Germany [2020]**
  - Implementation of quantum model systems in MRA using Wolfram
  - Implementation of symmetry operators using OOP - C++
- **Research internship at IACS Kolkata, India [2019]**
  - Computational study of catalysis of Al-S bond breaking with H<sub>2</sub> evolution using Gaussian09
  - Scholarship provided by Department of Science and Technology (DST), Govt. of India

## Publications in Preparation

- **Farhaz R.**, Bischoff F. A., Stopkowicz S., Blaschke S. *Quantification of Basis Set Errors in Strong Magnetic Fields*
- **Farhaz R.**, Rickert C., Bischoff F. A. *Helium Dimers and Trimers in Extreme Magnetic Fields : A Geometry Optimization Study*
- Sardar R., Banik R., **Farhaz R.**, Ghosh S. *The drug induced micelle to super-micelle transition of cetyltrimethylammonium bromide(CTAB) and compares it with acetylenic gemini surfactant: an experimental and DFT study*

## Grants and Fellowships

- **Research Grants - Doctoral Programmes in Germany, 2021/22** from **Deutscher Akademischer Austauschdienst (DAAD)** for pursuing doctoral studies in Germany (**4 years**)
- **INSPIRE scholarship** from **Department of Science and Technology (DST), Govt. of India** for pursuing studies in natural sciences for top 10 percentile nationwide students (**5 years**)
- **Haji Mohd. Mahsin Scholarship, Govt. of West Bengal** (10<sup>th</sup> standard) for securing a position among the top 50 students within West Bengal

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## Skills

### Computational Tools

MADNESS ●●●●●

MRCPP ●●●●●

MRChem ●●●●○

PySCF ●●●●○

ORCA ●●●●○

Gaussian09 ●●●●○

ElemCo.jl ●●●●○

### Programming Languages

Python ●●●●●

C++ ●●●●●

Wolfram ●●●●○

Julia ●●●●○

Fortran77 ●●●○○

### Typesetting

Typst ●●●●●

Quarto ●●●●○

LaTeX ●●●●○

## Academic Contributions

- **Hylleraas Annual meeting 2023**, UiT Tromsø, Norway (*Contributed Talk*)
- **Numerical Methods in Quantum Chemistry conference (NMQC) 2023**, UiT Tromsø, Norway (*Poster*)
- **Symposium for Theoretical Chemistry conference (STC) 2022**, Heidelberg University, Germany
- **DFTK Workshop 2022**, Sorbonne University, France (*Poster*)

## Teaching Activities

- Instructor, Theoretical Molecular Spectroscopy (2022, Masters Level Practical, HU Berlin)
- Private Tutor in Physical Chemistry (2018 - 2020, Bachelors and Masters Level)

## Community Contributions

- Conference Organizer of Numerical Methods in Quantum Chemistry (NMQC 2025), HU Berlin
- Organizer of ChemistryCoffeeTalks at HU Berlin, creating networking platform for PhD students
- Provided quantum chemistry tutoring to economically backward students during COVID [2019 - 2021]
- Volunteer teaching at NGO for below-poverty-level school students [2016]

## Languages

Bengali *Mother Tongue*

English *Native Level*

Deutsch *Good*

Hindi *Fluent*

## Hobbies

Books (reading and writing), Music (playing guitar), Computer (building and setting up) and Cooking (various cuisines)