Gurjot **Singh**

PhD Candidate, Computational Chemistry

Interests

- Quantum Chemistry
- Computational Chemistry
- Electronic Structure Theory
- Ab Initio Methods

Contact and Links

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Personal

Nationality: Indian
Year of birth: 1996

Languages

English

Hindi

Modelling & Scientific Software

ORCA

HUMMR

PySCF

Gaussian

Avogadro | Chemcraft

Programming Skills

C++

Python

Bash / Shell scripting

Version Control & Dev Tools

Git

GitHub Actions

GitLab CI

Education

2020-present **PhD in Chemistry**
Humboldt-Universität zu Berlin — Berlin, Germany

2017-19 **MSc in Chemistry**
Indian Institute of Technology Bombay — Mumbai, India

2014-17 **BSc (Hons.) in Chemistry**
Hansraj College, University of Delhi — Delhi, India

Research Experience

PhD Thesis

2020-present **Ab Initio Insights into Molecular Magnetism: A Multireference Study of Transition Metal Complexes**
Humboldt-Universität zu Berlin — Berlin, Germany
Supervisor: Prof. Dr. Michael Roemelt
In this PhD thesis, the electronic structure and magnetic properties of several transition metal complexes were explored using multireference methods, over three sub-projects:

- Studied magnetic exchange coupling of two copper dimers with methods such as CASSCF/DMRGSCF + NEVPT2, DDCI, and BS-LPNO-CCSD.
- Investigated the electronic structure of an ambiguous cobalt-oxo intermediate through a collaborative theoretical and experimental study.
- Developed a new methodology to calculate spin-orbit coupling and g-tensors by combining QD-NEVPT2 with selected CI references, and tested it on benchmark systems.

Master's Thesis

2018-19 **A Theoretical Investigation of Hetero Binuclear Diamond-shaped-core Complexes**
Indian Institute of Technology Bombay — Mumbai, India
Supervisor: Prof. G. Rajaraman
This project was a theoretical study of hetero-binuclear inorganic molecules with a diamond-shaped core of $[\mathrm{M}^1(\mathrm{III})(\mu-O)_2\mathrm{M}^2(\mathrm{III})]$.

- Investigated electronic structure, energetics, and spectral properties of $[\mathrm{L}^1\mathrm{Ni}(\mu-\mathrm{O})_2\ \mathrm{CuL}^2]^{2+}$ molecule using density functional theory.
- Explored the nucleophilicity of the $[\mathrm{L}^1\mathrm{M}^1(\mu-\mathrm{O})_2\mathrm{M}^2\mathrm{L}^2]^{n+}$ system (M = Fe, Ni, Co, and Cu) towards cyclohexanecarbaldehyde.

Projects

2020-25 **HUMMR Program**
Roemelt Group at Humboldt-Universität zu Berlin — Berlin, Germany

- Worked as a developer on the HUMMR program, devoted to conducting accurate and efficient multireference electronic structure calculations.
- Implemented Angeli et. al.'s QD-NEVPT2 method in the program.
- Wrote the spin-orbit coupling module for calculation of spin-orbit coupling and g-tensors.

Design & Documentation

LaTeX

Markdown

Quarto

Office Suites

Inkscape

MkDocs

Typst

Beamer | Matplotlib | RevealJs | MkDocs-Material | Chemdraw

Grants and Scholarships

2020–24 **Doctoral Research Fellowship**

Deutsche Forschungsgemeinschaft (DFG) — Berlin, Germany

- Supported through a DFG-funded research project in the group of Prof. Dr. Michael Roemelt at Humboldt-Universität zu Berlin, focusing on multireference electronic structure theory and molecular magnetism in bio-inspired transition metal systems.

2014-19 **INSPIRE Scholarship**

Ministry of Science and Technology, Government of India — Delhi, India

- National scholarship for pursuing science education, awarded to top 1% of students based on 12th-grade academic performance.

Talks

May 2025 **Implementation of Spin-Orbit Coupling and calculation of molecular g-tensors with QD-NEVPT2 using Selected CI references**

Freie Universität Berlin — Berlin, Germany

Conferences and Workshops

Aug 2025 **7th Quantum Bio-Inorganic Chemistry Conference (QBIC VII)**

Humboldt-Universität zu Berlin — Berlin, Germany

Sep 2023 **Python Computing 4 Chemists (and others)**

RWTH Aachen University — Online

Publications

In Preparation E. F. Beyer, T. Dargel, L. Gerndt, A. Khedkar, T. Kull, J. Noetzel, A. Sergel, **G. Singh**, S. Wittek, P. Woite, *et al*, "HUMMR: A quantum chemistry program for strongly correlated molecular systems", *Manuscript in preparation*, In Preparation.

G. Singh, and M. Roemelt, "Spin-orbit coupling with quasidegenerate N-electron valence state perturbation theory using selected CI references for molecular g-tensor calculations", *Manuscript in preparation*, In Preparation.

2024 D. D. Malik, W. Ryu, Y. Kim, **G. Singh**, J. Kim, M. Sankaralingam, Y. Lee, M. S. Seo, M. Sundararajan, D. Ocampo, *et al*, "Identification, Characterization, and Electronic Structures of Interconvertible Cobalt–Oxygen TAML Intermediates", *Journal of the American Chemical Society 146(20):13817-13835*, 2024, doi: *10.1021/jacs.3c14346*.

2021 **G. Singh**, S. Gamboa, M. Orio, D. A. Pantazis, and M. Roemelt, "Magnetic exchange coupling in Cu dimers studied with modern multireference methods and broken-symmetry coupled cluster theory", *Theoretical Chemistry Accounts 140(10)*, 2021, doi: *10.1007/s00214-021-02830-0*.

S. Pylaeva, P. Marx, **G. Singh**, T. D. Kühne, M. Roemelt, and H. Elgabarty, "Organic Mixed-Valence Compounds and the Overhauser Effect in Insulating Solids", *The Journal of Physical Chemistry A 125(3):867-874*, 2021, doi: *10.1021/acs.jpca.0c11296*.