

Gurjot Singh

PHD CANDIDATE, COMPUTATIONAL CHEMISTRY

Interests

- Quantum Chemistry
- Computational Chemistry
- Electronic Structure Theory
- Ab Initio Methods
- Transition Metal Chemistry
- Molecular Magnetism

Contact and Links

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- 🏠 7_TJlgAAAAJ

Personal

Nationality: Indian
Year of birth: 1996

Languages

English

Hindi

Modelling & Scientific Software

ORCA

HUMMR

PySCF

Gaussian

ChemCraft

Avogadro

GaussView

Programming Skills

C++

Python

Markdown

Bash / Shell scripting

Matplotlib

Plotly

SciPy

NumPy

EDUCATION

2020-now **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-now **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 $[M^I(III)(\mu-O)_2M^II(III)]$.

- Investigated electronic structure, energetics, and spectral properties of $[L^I Ni(\mu-O)_2 Cu L^II]^2+$ molecule using density functional theory.
- Explored the nucleophilicity of the $[L^I M^I(\mu-O)_2 M^II L^II]^n+$ 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 & Documenta- tion

LaTeX

Office Suites

Inkscape

MkDocs

Quarto

Typst

Beamer

RevealJs

MkDocs-Material

Version Control & Dev Tools

Git

GitHub Actions

GitLab CI

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 **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.