

# 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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[🌐 guritheochem](https://guritheochem)  
[🌐 7\\_TJlgAAAAJ](https://7_TJlgAAAAJ)

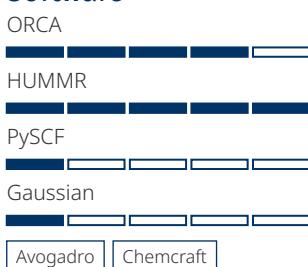
## Personal

Nationality: Indian  
Year of birth: 1996

## Languages



## Modelling & Scientific Software



## Programming Skills



## Version Control & Dev Tools



## 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  $[M^1(III)(\mu - O)_2M^2(III)]$ .

- Investigated electronic structure, energetics, and spectral properties of  $[L^1Ni(\mu - O)_2 CuL^2]^{2+}$  molecule using density functional theory.
- Explored the nucleophilicity of the  $[L^1M^1(\mu - O)_2M^2L^2]^{n+}$  system ( $M = Fe, Ni, Co$ , and  $Cu$ ) towards cyclohexanecarbaldehyde.

## PROJECTS

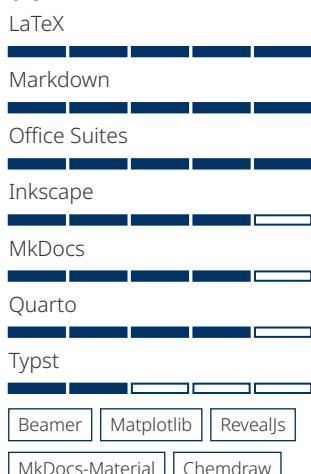
### 2020-25 HUMMR Program

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



## 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.