

# 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

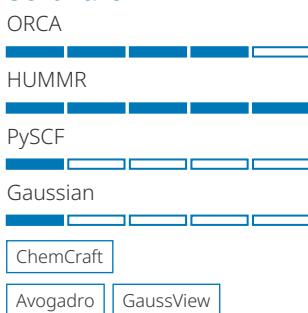
## Personal

Nationality: Indian  
Year of birth: 1996

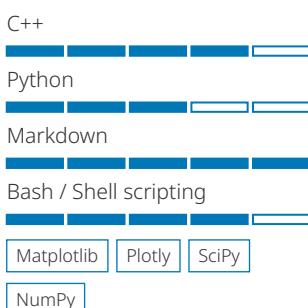
## Languages



## Modelling & Scientific Software



## Programming Skills



## EDUCATION

2020-now	<b>PhD in Chemistry</b>	BERLIN, GERMANY
	HUMBOLDT-UNIVERSITÄT ZU BERLIN	
2017-19	<b>MSc in Chemistry</b>	MUMBAI, INDIA
	INDIAN INSTITUTE OF TECHNOLOGY BOMBAY	
2014-17	<b>BSc (Hons.) in Chemistry</b>	DELHI, INDIA
	HANSRAJ COLLEGE, UNIVERSITY OF DELHI	

## RESEARCH EXPERIENCE

### PhD Thesis

2020-now	<b>Ab Initio Insights into Molecular Magnetism: A Multireference Study of Transition Metal Complexes</b>	BERLIN, GERMANY
	HUMBOLDT-UNIVERSITÄT ZU BERLIN	
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:		
<ul style="list-style-type: none"><li>• Studied magnetic exchange coupling of two copper dimers with methods such as CASSCF/DMRGSCF + NEVPT2, DDCI, and BS-LPNO-CCSD.</li><li>• Investigated the electronic structure of an ambiguous cobalt-oxo intermediate through a collaborative theoretical and experimental study.</li><li>• Developed a new methodology to calculate spin-orbit coupling and <i>g</i>-tensors by combining QD-NEVPT2 with selected CI references, and tested it on benchmark systems.</li></ul>		

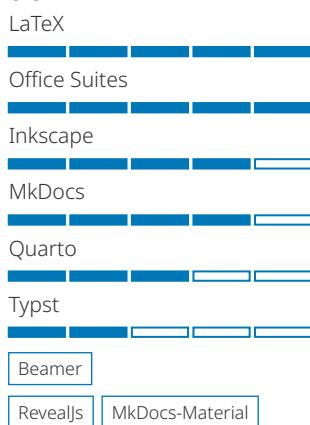
### Master's Thesis

2018-19	<b>A Theoretical Investigation of Hetero Binuclear Diamond-shaped-core Complexes</b>	MUMBAI, INDIA
	INDIAN INSTITUTE OF TECHNOLOGY BOMBAY	
Supervisor: Prof. G. Rajaraman		
This project was a theoretical study of hetero-binuclear inorganic molecules with a diamond-shaped core of $[M^1(III)(\mu - O)_2 M^2(III)]$ .		
<ul style="list-style-type: none"><li>• Investigated electronic structure, energetics, and spectral properties of <math>[L^1Ni(\mu - O)_2 CuL^2]^{2+}</math> molecule using density functional theory.</li><li>• Explored the nucleophilicity of the <math>[L^1M^1(\mu - O)_2 M^2L^2]^{n+}</math> system (<math>M = Fe, Ni, Co</math>, and <math>Cu</math>) towards cyclohexanecarbaldehyde.</li></ul>		

## PROJECTS

2020-25	<b>HUMMR Program</b>	BERLIN, GERMANY
	ROEMELT GROUP AT HUMBOLDT-UNIVERSITÄT ZU BERLIN	
<ul style="list-style-type: none"><li>• Worked as a developer on the HUMMR program, devoted to conducting accurate and efficient multireference electronic structure calculations.</li><li>• Implemented Angeli et. al.'s QD-NEVPT2 method in the program.</li><li>• Wrote the spin-orbit coupling module for calculation of spin-orbit coupling and <i>g</i>-tensors.</li></ul>		

## Design & Documentation



## Version Control & Dev Tools



## 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. Oriol, 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.