Pulkit Joshi

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PROFILE

Theoretical and computational chemist specializing in **electronic structure methods, density functional theory, and quantum chemistry simulations**. Recognized for **independent research leadership** (beyond-RPA methods, embedding approaches), **collaborative projects** across international institutions, and **excellent communication skills** demonstrated through teaching, mentorship, publications, and numerous oral/poster presentations. Proficient in **FORTRAN**, **Python**, **HPC environments**, and widely used quantum chemistry software. A **reliable team member** with proven ability to train others, disseminate results effectively, and secure recognition through awards and invited talks.

RESEARCH INTERESTS

- Development of **advanced electronic structure methods** for **open-shell systems, metastable states, and negative ion resonances**, with direct applications to problems in **atmospheric and astrochemistry**.
- **Density functional embedding theory** and multiscale approaches for realistic materials modeling and condensed-phase chemistry.
- Theoretical frameworks for understanding **light–matter interactions**, including excitation processes and spectroscopy.
- Characterization of **noncovalent interactions, charge-transfer states, and long-range correlation effects**, bridging theory with experimentally measurable properties.
- Integration of **HPC simulations, method development, and collaborative science** to connect fundamental theory with real-world chemical phenomena.

EDUCATION AND TRAINING

PhD in Chemical Sciences (Theory and Computation) Aug 2018 – Dec 2024
Tata Institute of Fundamental Research (TIFR), Mumbai, India
Thesis: Fifth-rung density functionals for open-shell intermolecular interactions and negative ion resonances
Grade: 8.22/10.00

MSc in Chemistry (Physical Chemistry) Jul 2016 – May 2018
St. Stephen's College, University of Delhi, India
Thesis: Enhancement of light harvesting property of porphyrin-based MOFs using quantum dots
Grade: 77.90%

BSc (Hons) in Chemistry Jul 2013 – May 2016
St. Stephen's College, University of Delhi, India
Grade: 87.63%

SKILLS

Core Competencies: Density Functional Theory, Quantum Chemistry, Intermolecular Interactions, Metastable States, Negative Ion Resonances, Embedding Techniques, Ab Initio Molecular Dynamics
Programming & Tools: FORTRAN, Python, R, MATLAB, Git, Linux, Bash, LaTeX
Software Expertise: Turbomole, ORCA, CP2K, Psi4, CFOUR; Visualization with Avogadro, Gabedit, VMD, Molden
Strengths: Independent Research, Cross-disciplinary Collaboration, Problem-Solving, Team Leadership, Mentoring, Scientific Communication

RESEARCH EXPERIENCE

Postdoctoral Researcher Feb 2025 – Present
Computational Material Science Group, Friedrich-Schiller-University Jena, Germany

- Developing advanced **density functional embedding theory** coupled with periodic charge-dipole electrostatics for material science applications.
- Contributing both as an **independent researcher** and as part of an interdisciplinary team in collaborative projects.

Research Associate Sep 2024 – Dec 2024
Quantum Chemistry Group, TIFR, Mumbai, India

- Investigated negative ion resonance states in ammoniated benzene using nuclear charge extrapolation.
- Demonstrated strong problem-solving and independent project execution relevant to Birch reduction-type processes.

Graduate Research Scholar Jul 2019 – Sep 2024
Quantum Chemistry Group, TIFR, Mumbai, India

- Developed **beyond-RPA composite corrections**, improving accuracy of noncovalent interactions by over 50%.
- Created **complex-RPA nonlocal functionals** for negative ion resonances; achieved accuracy comparable to high-level wavefunction methods.
- Reduced computational cost by two orders of magnitude using analytic continuation approximation, enabling application to solvated systems.
- Validated experimental NMR/IR spectra of Oxo-Rhenium(V) complexes, directly supporting interdisciplinary collaboration in medicinal chemistry.

Earlier Research Projects 2015 – 2019

- **London dispersion in open-shell dimers** (TIFR, 2019) – Applied MBPT to weak binding interactions.
- **Molecular electronics** (TIFR, 2019) – Modeled charge transport in molecular rectifiers.
- **Big data applications in chemistry** (CSIR–IICT, Hyderabad, 2017) – Applied clustering to repurpose FDA-approved drugs.
- **Virus protein modeling** (St. Stephen's College, 2015–2016) – Built accurate homology models of Tomato Leaf Curl Bangalore Virus proteins.

PUBLICATIONS

*(† equal contribution; * corresponding author)*

2024

- Abhisek Ghosal†, **Pulkit Joshi**†, and Vamsee K. Voora*. *Taming Negative Ion Resonances Using Nonlocal Exchange-Correlation Functionals. J. Phys. Chem. Lett.*, 15(22), 5994–6001. (Cover Highlight)
- **Pulkit Joshi**, and Vamsee K. Voora*. *Generalized perturbative singles corrections to the random phase approximation method: Impact on noncovalent interaction energies of closed- and open-shell dimers. J. Chem. Phys.*, 160, 044104.

2023

- Shubhangi Das, **Pulkit Joshi**, and Malay Patra*. *Necrosis-Inducing High-Valent Oxo–Rhenium(V) Complexes with Potent Antitumor Activity: Synthesis, Aquation Chemistry, Cisplatin Cross-Resistance Profile, and Mechanism of Action. Inorg. Chem.*, 62(48), 19720–19733.

TEACHING EXPERIENCE

Teaching Assistant, Friedrich-Schiller-University Jena

- **Advanced Computational Material Science (2025)** – Designed and evaluated assignments; conducted independent seminars use of Material Studio software for structure optimization, molecular dynamics simulations.
- **Algorithms for Scientific Computing (2025)** – Designed and evaluated assignments; conducted independent seminars on Python for data visualization, machine learning techiques, and statistics.

Teaching Assistant, Tata Institute of Fundamental Research, Mumbai

- **Symmetry in Chemistry (2021)** – Designed and evaluated assignments; assisted in course delivery under Dr. Vamsee K. Voora.
- **Quantum Chemistry I (2019)** – Delivered lectures on vectors, matrices, variational methods, and perturbation theory; developed assignments under Prof. Jyotishman Dasgupta.

MENTORSHIP, SERVICE, AND OUTREACH

TIFR, Mumbai (2018 – 2023)

- Mentored junior members in **software installation, HPC usage, and quantum chemistry techniques**.
- Authored documentation for HPC cluster management, improving group efficiency.
- Organized lab visits for 30+ first-year students, encouraging early research exposure.
- Volunteered in *Frontiers of Science* outreach, guiding 50+ high-school students in interdisciplinary science demonstrations.

St. Stephen's College, Delhi (2014 – 2016)

- Scribed for visually impaired students during university examinations.
- Tutored introductory science and mathematics to underprivileged students.

CONFERENCES AND PRESENTATIONS

2025

- Collaborative Research Center Meeting, Dornburg, Germany – Oral Talk: *Fast computation of optical properties in hybrid nanostructures.*

2024

- International Conference on Molecular Electronic Structure, Pescara, Italy – Poster: *Role of exact exchange and dynamical long-range polarization effects in negative ion resonances.*
- Turbomole: Today and Tomorrow, Oxford, UK – Oral Talk: *Beyond-RPA corrections for open-shell intermolecular interactions.*
- TIFR Annual Chemistry Conference, Mumbai/Hyderabad, India – Oral Talk: *Complex nonlocal density functionals for negative ion resonances*; Poster: *Generalized perturbative singles corrections to RPA.*

2023

- Intermolecular Interactions and Properties of Gases, Liquids and Solids, Graz, Austria – Poster: *Generalized perturbative orbital relaxation corrections based on RPA.*
- 17th International Congress of Quantum Chemistry, Bratislava, Slovakia – Poster: *Generalized perturbative orbital relaxation corrections based on RPA.*

2022

- Spectroscopy and Dynamics of Molecules and Clusters, Malpe, India – Poster: *A generalized perturbative orbital relaxation correction based on RPA.*

2021

- ACS Fall Meeting (virtual) – Poster Presentation.
- TIFR Annual Chemistry Conference, Mumbai, India – Poster: *Weak interactions in open-shell systems using response theory.*

2019

- TIFR–Weizmann Interaction Meeting, Mumbai, India – Poster: *Role of long-range correlation effects on the fate of metastable states.*

2016

- National Seminar on Analytical Sciences in Sustainable Development, New Delhi, India – Poster: *Homology modelling of Replication Association Protein of Tomato Leaf Curl Bangalore virus.*

AWARDS AND HONOURS

- 2024 – International Travel Grant, CSIR (Govt. of India).
- 2024 – International Travel Grant, SERB (Govt. of India).
- 2018 – All India Rank 60 in CSIR-JRF(NET) among 36,000+ applicants.
- 2018 – Meritorious Award, Department of Chemistry, University of Delhi.
- 2017 – Summer Research Fellowship, Indian Academy of Sciences, INSA, NASI.
- 2016 – Best Poster Award, National Seminar, New Delhi.
- 2013 – INSPIRE Scholarship for Higher Education (Top 1%, Govt. of India).