# RAHUL VERMA


**Computational Materials Scientist**

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## EDUCATION

### Postdoctoral Researcher
**North Carolina State University**

NC, USA | 2024–present

### Ph.D. in Theoretical and Computational Chemistry
**Indian Institute of Technology Kanpur, India**

2016 – 2023 | Kanpur, India

### Research Associate
**Indian Institute of Technology Kanpur**

2015 – 2016 | Kanpur, India

### Master of Science in Chemistry
**Chhatrapati Sahu Ji Maharaj University**

2011 – 2013 | Kanpur, India

### Bachelor of Science
**Chhatrapati Sahu Ji Maharaj University**

2008 – 2011 | Kanpur, India

## SCIENTIFIC RESEARCH EXPERIENCE

### Postdoctoral Research

2024–current | NC State University, USA

- Machine learning interatomic potentials
- Bio-molecular interactions at the solid-liquid interface
- *ab-initio and classical* molecular dynamics simulation
- Free energy and enhance sampling methods

VASP | CP2K | DeepMD-kit | MACE

### Ph.D Projects

2016–2023 | IIT Kanpur, India

- Thesis Title: **Modelling of Catalytic Reactions over Zeolites**
- Density Functional Theory (DFT) calculation for bulk, surface, and heterogeneous solid systems, hybrid quantum mechanics/molecular mechanics (QM/MM) method.
- Optimization of the pathways in a chemical reaction using the transition state (TS) calculation, intrinsic reaction coordinate (IRC) method, and nudged elastic band (NEB) method.
- Molecular dynamics simulation (classical, *ab-inito*, and ML Potentials).
- Free energy computation using, metadynamics, umbrella sampling, and temperature accelerated sliced sampling (TASS) techniques
- Investigated catalytic reaction in metal loaded zeolites
- $CO_2$ activation and transformation

VASP | CP2K | CPMD | Gaussian | PLUMED | GULP

## REFERENCES


**Prof. Jim Pfaendtner**

@ Department of Chemical and Biomolecular Engineering, NC State University, USA

wjpfaend@ncsu.edu

**Prof. Nisanth N. Nair**

@ Department of Chemistry, IIT Kanpur, Kanpur

nnair@iitk.ac.in


## SKILLS

### Programming Languages and Scripting

FORTRAN | Python | MPI | Git | Bash/Shell | Makefile | CMake | Vim | LaTeX | Matplotlib | numpy | scipy | PBS | Slurm | LSF

### Visualisation and Analysis

VMD | GaussView | Avogadro | Jmol | XCrySDen | Molden | Gnuplot | Gimp

### Computer Simulation

VASP | Quantum Espresso | Gaussian | ORCA | Material Studio | LAMMPS | Gromacs | AMBER | PLUMED | DeepMD-kit | NequIP | MACE

## SOFTWARES

- **Automated workflow for developing machine learning interatomic potentials** (SPARC)
- **Package for reweighting enhance sampling simulations** (Reweighing-TASS)

## ACHIEVEMENT

- AIR-42 in joint CSIR-UGC exam, 2014 (Chemical Science)
- Junior Research Fellow (2016–2018)
- Senior Research Fellow (2018–2021)

## PUBLICATIONS


- *J. Open Source Softw.*, **2026**, 11, 121, 9468.
- *ChemistrySelect*, **2025**, 10, 41, e01858.
- *J. Phys. Chem. C.*, **2022**, 126, 45 19169–19177.
- *RSC Adv.*, **2022**, 12, 30236–30247.
- *Sci. Rep.*, **2020**, 10, 14128.
- *Mol. Phys.*, **2017**, 115:21-22, 2708–2720.
- *J. Phys. Chem. A*, **2015**, 119, 52, 13055–13063.