

RAHUL VERMA

Computational Materials Scientist

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EDUCATION

Ph.D. in Theoretical and Computational Chemistry

Indian Institute of Technology Kanpur, India

2016 – Present

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

Research Associate Project

2015–2016

IIT Kanpur, India

- Ab-initio theoretical studies of molecular cluster aggregates
- Investigation of the weak interactions
- Fragmentation based Molecular Tailoring Approach (MTA)
- Complete Basis Set (CBS) limit for estimating binding energies

Gaussian

MTA

MESP

CBS

Ph.D Projects

2016–Present

IIT Kanpur, India

- Thesis Title: Modelling Catalytic Reactions over Zeolites (expected Submission in May 2023)
- Modelling reactions over zeolites using hybrid QM/MM technique
- Density Functional Theory based molecular dynamics simulations
- 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.
- Free energy computation using ab initio thermodynamics, metadynamics, umbrella sampling, and temperature accelerated sliced sampling (TASS) techniques
- Investigated catalytic reaction in metal loaded zeolites
- CO₂ activation and transformation

CPMD

DFT

QM/MM

TASS

GULP

AIMD

Ab-initio thermodynamics

Nudge Elastic Band

Intrinsic Reaction Coordinate

CP2K

Quantum Espresso

TASS

Umbrella Sampling

Metadynamics

TAMD/d-AFED

SKILLS

Programming Languages and Scripting

FORTRAN

Python

MPI

OpenMP

Git

Bash/Shell

Makefile

CMake

Vim

LaTeX

Matplotlib

numpy

scipy

PBS

Slurm

Visualisation and Analysis

VMD

GaussView

Avogadro

Jmol

XCrySDen

Molden

Gnuplot

Gimp

Computer Simulation

ORCA

NWChem

Material Studio

GULP

AMBER

PLUMED

Additional

- Linux Server Administration
- Package for reweighting enhance sampling simulation

ACHIEVEMENT

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

PUBLICATIONS

- 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