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Rahul Verma

Computational Materials Scientist

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Research Experience

Postdoctoral Research – North Carolina State University *Raleigh, NC, USA | 2024 – Present*

- Developing machine learning potentials to extend the length and time scales accessible to first-principles simulation with *ab initio* accuracy.
- Peptide interactions at solid–liquid interfaces using *ab initio* and classical molecular dynamics.
- Free energy computation and enhanced sampling methods to characterize interfacial adsorption and reaction thermodynamics.
- Developed an automated workflow toolkit (SPARC) for constructing reactive ML potential models.
- **Tools:** VASP, CP2K, DeepMD-kit, MACE, PLUMED.

Doctoral Research – Indian Institute of Technology Kanpur *Kanpur, India | 2016 – 2023*

- Thesis: *Modelling of Catalytic Reactions over Zeolites*. Investigated catalytic transformations in metal-loaded zeolites, including CO_2 activation and conversion.
- Density functional theory calculations on bulk, surface, and heterogeneous solid systems, and hybrid quantum mechanics/molecular mechanics (QM/MM) simulations of extended catalytic environments.
- Reaction pathways using transition state search, intrinsic reaction coordinate (IRC), and nudged elastic band (NEB) methods.
- Free energy computation using enhanced sampling methods, metadynamics, umbrella sampling, and temperature accelerated sliced sampling (TASS); developed reweighting package for reconstructing free energy from enhanced MD trajectories.
- **Tools:** VASP, CP2K, CPMD, Gaussian, PLUMED, GULP.

Research Associate – Indian Institute of Technology Kanpur *Kanpur, India | 2015 – 2016*

- Electronic structure studies and fragmentation based approaches to molecular clusters to understand packing patterns in molecular crystals.

Education

Indian Institute of Technology Kanpur *2016 – 2023*

Ph.D. in Theoretical and Computational Chemistry – Advisor: Prof. Nisanth N. Nair *Kanpur, India*

Chhatrapati Shahu Ji Maharaj University *2011 – 2013*

Master of Science in Chemistry *Kanpur, India*

Chhatrapati Shahu Ji Maharaj University *2008 – 2011*

Bachelor of Science *Kanpur, India*

Software and Open-Source Contributions

SPARC – A Workflow for Constructing Machine Learning Potentials

- End-to-end workflow that automates dataset generation, active learning, and training, of machine learning potentials, to reduce the training data required for production quality models .

Reweighing–TASS – Reweighting of Enhanced Sampling Simulations

- Modular Fortran program to reconstruct free energy surface from temperature accelerated sliced sampling (TASS) trajectories generated with CPMD or PLUMED, using WHAM reweighting or the mean force (PMF) method.

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Technical Skills

Languages	FORTRAN, Python, MPI, Bash/Shell, Makefile, CMake
Operating Systems	Familiar with Windows and Linux internals
Simulation	VASP, Quantum Espresso, CP2K, CPMD, Gaussian, ORCA, Materials Studio, GULP, LAMMPS, AMBER, GROMACS, PLUMED
Machine Learning	DeepMD-kit, NequIP, MACE
Visualization	VMD, GaussView, Avogadro, Jmol, XCrySDen, Gnuplot, Matplotlib
Scientific Python	ASE, NumPy, SciPy, Pandas, PyTorch, TensorFlow
HPC and Tooling	PBS, Slurm, LSF, Git

Awards and Fellowships

Senior Research Fellow, Council of Scientific and Industrial Research *2018 – 2021*

Junior Research Fellow, Council of Scientific and Industrial Research *2016 – 2018*

All India Rank 42, joint CSIR–UGC NET examination (Chemical Sciences) *2014*

Publications

8. **Verma, R.**, Joshi, N., and Pfaendtner, J. (**2026**), 'SPARC: An Automated Workflow Toolkit for Accelerated Active Learning of Reactive Machine Learning Interatomic Potentials', *J. Open Source Softw.*, 11(121) 9468.
7. **Verma, R.** and Sahoo, S. K. (**2025**), 'Recent Advances and Challenges in Modeling Catalytic Reactions in Zeolites', *ChemistrySelect*, 10(41) e01858.
6. **Verma, R.** and Nair, N. N. (**2022**), 'Proton-Exchange Reaction in Acidic Zeolites: Mechanism and Free Energetics', *J. Phys. Chem. C*, 126(45) pp. 19169–19177.
5. Kang, C., **Verma, R.**, Sonpal, A., Shoji, A., Chipot, C., and Pfaendtner, J. (**2026**), 'A Force-Kernel Reformulation of the Extended-System Adaptive Biasing Force for Free-Energy Calculations', *J. Chem. Theory Comput.*, 22(14) pp. 7313–7325.
4. Kumar, A., Jindal, M., Rawat, S., Sahoo, A., **Verma, R.**, Chandra, D., Kumar, S., Thallada, B., and Yang, B. (**2022**), 'Anisole hydrodeoxygenation over Ni–Co bimetallic catalyst: a combination of experimental, kinetic and DFT study', *RSC Adv.*, 12(47) pp. 30236–30247.
3. Qayoom, I., **Verma, R.**, Murugan, P. A., Raina, D. B., Teotia, A. K., Matheshwaran, S., Nair, N. N., Tägil, M., Lidgren, L., and Kumar, A. (**2020**), 'A biphasic nanohydroxyapatite/calcium sulphate carrier containing Rifampicin and Isoniazid for local delivery gives sustained and effective antibiotic release and prevents biofilm formation', *Sci. Rep.*, 10, 14128.
2. Singh, G., **Verma, R.**, Wagle, S., and Gadre, S. R. (**2017**), 'Explicit hydration of ammonium ion by correlated methods employing molecular tailoring approach', *Mol. Phys.*, 115(21–22) pp. 2708–2720.
1. Singh, G., **Verma, R.**, and Gadre, S. R. (**2015**), 'Understanding Packing Patterns in Crystals by Analysis of Small Aggregates: A Case Study of CS_2', *J. Phys. Chem. A*, 119(52) pp. 13055–13063.