Ashwini Verma

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About

I am a Ph.D. candidate specializing in machine learning driven design and synthesis of material and process optimization. My research interests encompass the application of machine learning, active learning, deep learning, probabilistic optimization, reinforcement learning, and large language models in the field of material science. I am truly committed to ethical research practices and aim to develop solutions that enhance environmental sustainability and positively impact society.

Work Experience

Senior Research Fellow, CSIR-NCL, India **Dec 2023 - Present**

- Developed and implemented five ML models to screen millions of metal compositions, identifying potential candidates for solid-state hydrogen storage.

Junior Research Fellow, CSIR-NCL, India **Jan 2022 - Nov 2023**

- Completed grad school courses. Developed expertise in data preprocessing, analysis, and feature engineering, while curating material databases.

Ph.D. Intern, Indian Institute of Technology, Patna, India **Sep 2022 - Dec 2022**

- Synthesis and characterization of Mg-based compositions predicted by ML models, confirming a 90% match with experimental results, demonstrating the robustness of ML-driven material discovery.

Project Assistant-I, CSIR-NCL, India **Sep 2021 - Aug 2022**

- Developed a faster method for predicting the structure and energy of metal clusters by combining density functional theory, deep learning, and reinforcement learning.

Education

Ph.D degree, Physical Science
CSIR-National Chemical Laboratory, (CSIR-NCL India) *Jan 2022- Present*

Masters in Physics **CGPA 8.86/10**
Rashtrasant Tukadoji Maharaj Nagpur University, India *July 2017- May 2019*

Post Graduation Diploma in Industrial Robotics **CGPA 9.9/10**
Oberoi Center of Excellence, Nagpur University, India *July 2016- May 2017*

Bachelors in Physics, Mathematics and Computer Science **CGPA 8.3/10**
Government Institute of Science, Nagpur, India *July 2013- May 2016*

Patents

2023 K Joshi and **A Verma**, System to predict PCT curve for metal alloys used for solid-state hydrogen storage. Provisional Patent No. 202311064135

2022 K Joshi and **A Verma**, System and method for identification of materials for hydrogen storage. Provisional Patent No. 202211028454

Publications

Published

2024 **A Verma** and K Joshi, MH-PCTpro: A Machine learning model for rapid prediction of Pressure - Composition - Temperature (PCT) isotherms, ChemRxiv., DOI:https://doi.org/10.26434/chemrxiv-2024-g33f9

2024 **A Verma**, N Wilson and K Joshi, Solid state hydrogen storage: Decoding the path through machine learning, International Journal of Hydrogen Energy 50, 1518-1528

2024 N Wilson, **A Verma**, PR Maharana, AB Sahoo And K Joshi, HyStor: An Experimental Database of Hydrogen Storage Properties for Various Metal Alloy Classes, International Journal of Hydrogen Energy 90, 460-469

2023 R Modee, **A Verma**, K Joshi And U Priyakumar, MeGen - generation of gallium metal clusters using reinforcement learning, Machine Learning: Science and Technology 4 (2), 025032

2022 R Modee, S Agarwal, **A Verma**, K Joshi And U Priyakumar , DART: Deep Learning Enabled Topological Interaction Model for Energy Prediction of Metal Clusters and its Application in Identifying Unique Low Energy Isomers, Physical Chemistry Chemical Physics 23 (38), 21995-22003

In preparation

2025 **A Verma**, P Kumar, S Kumar and K Joshi, Synthesis and Characterization of Machine Learning-Predicted Mg-Based Composites for High-Capacity Hydrogen Storage. to be communicated

2025 **A Verma** and K Joshi, EQUIP: Machine Learning approach for Optimizing Metal Hydride Equilibrium Plateau Pressure. draft

Technical Skills

Programming Languages

- Proficiency in Python, Git, Github, Shall Script, C, C++, LATEX
- Understanding of high-performance computing and CPU/GPU parallel programming (MPI, OpenMPI, and MPI4Py)
- Advanced user of Linux and Windows

Machine Learning

- Extensive experience of building and validating machine learning and deep learning models for material property prediction and process optimization.
- Libraries & tools: Numpy, Scipy, Pandas, Dask, cuDF, NUMBA, Scikit-learn, RAPIDS, CuML
- Deep Learning Frameworks: Pytorch, Tensorflow, Keras

Density Functional Theory

- Experience with VASP for metal cluster structure optimization. Knowledge of surface modeling for heterogeneous catalysis studies.
- Familiarity with scientific packages like Quantum Espresso, Virtual NanoLab (VNL), Materials Project, Atomic Simulation Environment (ASE), Visual Molecular Dynamics (VMD) and others.

Molecular Dynamics

- Beginners level experience of using LAMMPS and DeepMD for building the machine learning potential for metal clusters.
- Basic understanding of molecular dynamics atomistic simulations, enhanced sampling techniques, and Markov state modeling

Experimental

- Lab-scale experiments for catalyst synthesis by ball milling method, characterization of catalyst, and measurement of hydrogen storage properties using Sieverts method.

Workshops & Training

2025 Emerging Topics in Molecular Dynamics Simulations, organized by the CSIR-National Chemical Laboratory, India

2024 School on Parallel Programming and Parallel Architecture for High Performance Computing organized by ICTP, Italy, in Kathmandu, Nepal

2024 PARAM Utkarsh - HPC Training Programme, organized by C-DAC Bangalore, India

2024 Computational Design of Electrocatalyst (CDE-2024), organized by the Department of Physics, SRM University, India

2023 AI-ML in Materials and Manufacturing, organized by COEP Technological University, India

2023 From Concept to Commercialization workshop organized by CSIR-National Chemical Laboratory, India

2022 Fundamentals of accelerated data science, organized by NVIDIA at GPU Technology Conference (GTC)

Conferences

Hackathon	2nd International Conference on Green Hydrogen (ICGH-2023) at Bharat Mandapam, New Delhi, organized by the Government of India. 2024
Oral	International conference on materials genome (ICMG-III) , hosted by the Department of Physics, SRM University. 2024
Oral	NCL-RF Foundation Day Celebration at CSIR-NCL, Pune, India. 2024
Poster	Industrial outreach Program International Partnership for Hydrogen and Fuel Cells Economy (IPHE) outreach program on hydrogen and fuel cell at IIT-Delhi, India. 2024
Poster	International conference on advances in renewable energy hosted by Harishchandr Research Institute, Prayagraj, India. 2023
Poster	Science Day celebration at CSIR-NCL, Pune, India. 2019
Participation	International Conference on Green Hydrogen (ICGH-2023) at New Delhi's Vigyan Bhawan, organized by the Government of India. 2023
Participation	International Conference on Materials Genome (ICMG-II), hosted by the Department of Physics, SRM University. 2022

Academic Achievements

2024 **First runner-up** in the Green Hydrogen Hackathon (GH2thon) organized by the Government of India at Bharat Mandapam, New Delhi, India.

2024 **First runner-up** in poster competition at International Partnership for Hydrogen and Fuel Cells Economy (IPHE) outreach program on hydrogen and fuel cell at IIT-Delhi, India

2023 **CSIR-NCL Krishnan Award** for best research publication in computational science with the highest impact factor in 2023, CSIR-NCL, Pune, India.

2023 **Best poster award** in National Science Day celebrations at CSIR-National Chemical Laboratory (NCL) (Feb-2023)

2022 Recipient of the **national-level INSPIRE fellowship** for pursuing Ph.D.

2020 **386th All India Rank** in Graduate Aptitude Test in Engineering (GATE).

2019 **Gold medalist (Dr. Meghnad Saha gold medal)** at master's degree. First Rank in University at M.Sc. Physics, RTM Nagpur University

References

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