Ameeya Bhusan SAHOO

Doctoral Researcher – Homepage
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Education

2025 - Present **Doctor of Philosophy in Physical and Engineering Sciences (Condensed Matter Physics)**
University of Bordeaux, France
Thesis: Hybridizing Massively Parallel DFT Calculations with Quantum Algorithms Toward Efficient Material Properties Prediction

2020 - 2022 **Master of Science in Chemistry (Theoretical and Computational Chemistry)**
Central University of Punjab, Bathinda, India
CGPA: 7.22/10.00

2016 - 2019 **Bachelor of Science in Chemistry (Honours)**
Utkal University, Odisha, India
CGPA: 7.49/10.00

Work Experience

CSIR-National Chemical Laboratory Pune, INDIA
Project Associate I *July 2022 - Sept 2024*

Project: High Entropy Alloys for hydrogen storage application operable at Room Temperature (HEART)

Skills

- **Quantum Algorithms**: Variational Quantum Eigensolver (VQE), Quantum Phase Estimation (QPE)
- **Simulation Packages**: BigDFT, VASP, ORCA, Quantum Espresso, Gaussian, LAMMPS
- **Scientific Data Analysis and Visualization**: VESTA, phonopy, VMD, GNUPLOT, MatPlotlib
- **Scientific Programming**: Python, FORTRAN, shell-scripting, LaTeX for scientific writing
- **Operating Systems**: Linux, Windows
- **Machine Learning**: TensorFlow, PyTorch

Research Experience

•University of Bordeaux, France *April 2025 - Present*
Doctoral Researcher

– Hybrid classical–quantum workflow combining massively parallel DFT (BigDFT) with quantum algorithms.
– Construction and analysis of sparse Hamiltonians for quantum simulation (VQE/QPE) with locality and cost metrics.

•CSIR-National Chemical Laboratory, India *July 2022 - Sept 2024*
Project Associate I

– Structure prediction of Mg- and Ti-based hydrogen-storage alloys using evolutionary algorithms (USPEX).
– Electronic structure, phonons (DFPT), and hydrogen diffusion using VASP, phonopy, and ab-initio MD.
– Publication: Wilson N., Verma A. D., Maharana P. R., **Sahoo A. B.**, & Joshi K. (2024). HyStor: an experimental database of hydrogen storage properties for various metal alloy classes. *International Journal of Hydrogen Energy*, *90*, 460–469. DOI.

•Central University of Punjab, India *Aug 2021 - June 2022*
Master's Thesis

– Generated CCSD/def2-TZVPP potential energy surface for H_2 recombination on pyrene using ORCA.