Amit Chaudhari

Email ***chaudharia@cardiff.ac.uk***
Mobile ***+44 7907879653***
Webpage ***https://amitmc1.github.io/Materialsmodelling/***

Education

MEng Chemical Engineering	**MSc Molecular Modelling**	**PhD Computational Chemistry**
University of Birmingham	University College London	Cardiff University
Sept 2016- June 2020	Sept 2020- Sept 2021	October 2021-March 2025

PhD Summary: Integrating Machine Learning Algorithms in *Ab-Initio* Modelling

Designing/applying algorithms and workflows to improve DFT-based atomistic materials modelling (heterogeneous catalysis), in collaboration with **Johnson Matthey** and **bp**:

- Optimising *ab-initio* methods: DFT+*U* projectors and meta-GGA DFT functionals
- Multiscale modelling accelerated using machine learned interatomic potentials
- Leveraging symbolic regression, deep learning and large language models

Quantum Chemistry

• Planewave and all-electron density functional theory, with Hubbard (DFT+*U*) and dispersion (D3) corrections, with/without spin polarisation	VASP and FHI-aims
• Constructing kinetic energy density functionals for deorbitalising the exchange correlation energy in meta-GGA DFT	FHI-aims (Fortran90)
• High performance computing using CPU and GPU nodes on the UK (ARCHER2) and Welsh (Hawk, Isambard) national supercomputers	LINUX

Methods and Software Packages

• Structure generation, geometry optimisation and molecular dynamics	ASE/Pymatgen
• Finetuning foundation model machine learned interatomic potentials	MACE/ASE
• Deep neural networks	PyTorch
• Symbolic regression/classification using sparse regression and large language models (MistralAI's Mathstral-7B and OpenAI's GPT-4o)	SISSO++ and Hugging Face Transformers
• Support vector machines and principal component analysis	Scikit-learn
• Bayesian optimisation	GPyOpt
• Parallel tempering Monte Carlo	SuSMoST
• Computing structural fingerprints using many body tensor representations	DScribe

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Conference Talks

- **Machine learning the DFT+*U* projectors to model polarons in energy materials:** *FHI-aims UK Developers' and Users' Meeting, May 2024, Warwick; Materials Chemistry Consortium Conference (Novel Algorithms for Materials Modelling), July 2024, Daresbury*
- **Designing catalysts for Net-Zero 2050 using first-principles computational modelling:** *Cardiff Chemistry Conference, May 2024*
- **Accurate modelling of n-type doped TiO_2 polymorphs using DFT+*U* with occupation matrix control:** *Materials Chemistry Consortium Workshop on the Modelling Point Defects, January 2024, Lancaster*
- **A computational study of the adsorption and activation of H_2, CO and CO_2 on stoichiometric CeO_2(110) supported Cu_{1-3} nanoclusters:** *World Congress in Oxidation Catalysis, September 2022, Cardiff*

Presentations to Industry

- **Machine learning algorithms for simulating realistic catalytic reaction environments:** *Johnson Matthey and bp, Cardiff, January 2025*
- **Combining DFT, global optimisation and machine learning to understand metal oxide support effects in catalysis:** *Johnson Matthey Computational Modelling Group, Reading, May 2024*
- **Sustainable Catalysis for Clean Growth- Advanced Methods Overview:** *bp International Centre for Advanced Materials Annual Conference, Manchester, October 2023*

Poster Presentations

- **Advancing *ab*-initio materials modelling using symbolic regression and large language models***: CECAM Machine Learning for Materials Discovery (ML4MD) workshop, May 2025, Finland*
- **Machine learning generalised DFT+*U* projectors to model polarons in catalyst and battery materials:** *Thomas Young Centre 7th Energy Materials workshop: from data to discovery of new energy materials, July 2024, London*
- ***Ab-initio* adsorption phase diagrams using DFT parameterised Monte Carlo methods:** *STFC CCP5 Annual General Meeting, September 2023, Warwick*

Competitive Funding Awards and Supervision

- STFC CCP5 Postgraduate Industrial Secondment worth £2248.80 supporting placement at Johnson Matthey Technology Centre, Sonning Common, UK
- Supervised research students as part of Nuffield and MChem projects