Amit Chaudhari

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

Education and Research Experience

PhD Computational Chemistry	Cardiff University Group of Dr Andrew Logsdail	Oct. 2021- March 2025
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 using machine learned interatomic potentials • Leveraging symbolic regression, deep learning, large language models and latent diffusion models for catalyst modelling and inverse design		
MSc Molecular Modelling Distinction	University College London Group of Sir Richard Catlow	Sept. 2020- Sept. 2021
Understanding small molecule activation on supported single atom/nanocluster catalysts using quantum mechanical modelling (DFT+*U*) and geometric/electronic descriptors.		
MEng Chemical Engineering 2:1	University of Birmingham Group of Professor Gary Leeke	Sept. 2016- June 2020
Designing nanoparticle catalyst preparation methods using supercritical fluid deposition and antisolvent precipitation, guided by empirical solubility models and validated using electrochemical characterisation.		

Skills and Experience

Quantum Mechanical Simulations

- Density functional theory (GGA, meta-GGA, hybrid-DFT and DFT+*U*), with/without dispersion corrections and spin polarisation: **VASP**, **FHI-aims**
- Constructing kinetic energy density functionals for "*deorbitalised"* meta-GGA DFT in **FHI-aims (Fortran90)**
- High performance computing using CPU and GPU nodes on the UK (ARCHER2) and Welsh (Hawk, Isambard) national supercomputers (**LINUX**)

Data-Driven Methods

- Deep neural networks and latent diffusion models: **PyTorch**
- Large language models: **GPT-4o**, **Mathstral-7B *via* Hugging Face Transformers**
- Symbolic regression and classification: **SISSO++**
- Support vector machines and principal component analysis: **Scikit-learn**
- Bayesian optimisation and Monte Carlo sampling: **GPyOpt**, **SuSMoST**
- Machine learned interatomic potentials (fine-tuning and inference of pre-trained foundation models): **MACE**
- Structural fingerprints and materials modelling (geometry optimisation and molecular dynamics): **ASE**, **DScribe**, **Pymatgen**, **PyTorch-Geometric**

Oral Presentations

1. **Machine learning algorithms for simulating realistic catalytic reaction environments**: *Johnson Matthey and bp, Cardiff, January 2025*
2. **Machine learning the DFT+*U* projectors to model polarons in energy materials**: *Materials Chemistry Consortium Conference (Novel Algorithms for Materials Modelling), July 2024, Daresbury; FHI-aims UK Developers' and Users' Meeting, May 2024, Warwick*
3. **Combining DFT, global optimisation and machine learning to understand metal oxide support effects in catalysis**: *Johnson Matthey Computational Modelling Group, Reading, May 2024*
4. **Designing catalysts for Net-Zero 2050 using first-principles computational modelling**: *Cardiff Chemistry Conference, May 2024*
5. **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*
6. **Sustainable Catalysis for Clean Growth- Advanced Methods Overview**: *bp International Centre for Advanced Materials Annual Conference, Manchester, October 2023*
7. **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*

Poster Presentations

1. **Advancing *ab initio* materials modelling using symbolic regression and large language models***: CECAM Machine Learning for Materials Discovery (ML4MD) workshop, May 2025, Finland*
2. **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*
3. ***Ab initio* adsorption phase diagrams using DFT parameterised Monte Carlo methods**: *STFC CCP5 Annual General Meeting, September 2023, Warwick*

Funding Awards

- 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