Amit Chaudhari

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About Me

I am a PhD researcher in computational chemistry at Cardiff University, where I integrate discriminative and generative AI with quantum mechanical modelling, to develop cost-effective and transferable workflows for materials modelling. I am part of an interdisciplinary collaboration between computational and experimental researchers in industry (Johnson Matthey and bp, through the bp-ICAM) and academia (University of Manchester), aiming to advance the fundamental understanding of complex catalytic materials for clean and sustainable energy production.

Education

PhD, Computational Chemistry, Cardiff University — Oct 2021 – Oct 2025

- Group of Dr Andrew Logsdail: integrating AI and quantum chemistry for atomistic materials modelling, including machine learned DFT+U projectors, interatomic potentials and meta-GGA functionals

MSc, Molecular Modelling: Distinction, University College London — Sept 2020 – Sept 2021

- Group of Sir Richard Catlow: simulating small molecule activation on supported nanocluster catalysts using DFT+U and geometric/electronic descriptors

MEng, Chemical Engineering: 2.1, University of Birmingham — Sept 2016 – June 2020

- Group of Professor Gary Leeke: designing nanoparticle catalyst preparation methods using supercritical fluids, guided by empirical solubility models and validated using electrochemical characterisation

Skills and Experience

Quantum Chemistry

- Density functional theory (GGA, meta-GGA, hybrid-DFT, DFT+U), with/without dispersion corrections and spin polarisation: **VASP**, **FHI-aims**, **PySCF**
- Testing deorbitalisation strategies for meta-GGA DFT in FHI-aims through source-level modifications: **Fortran90**
- High performance computing using CPU and GPU nodes on the UK (ARCHER2) and Welsh (Hawk, Isambard) national supercomputers: **Linux**
- Structure generation and structural fingerprints: **ASE**, **Pymatgen**, **DScribe**

Deep Learning

- Fine-tuning and inferencing foundation model machine learned interatomic potentials: **MACE**
- Constructing neural network meta-GGA exchange-correlation functionals: **PyTorch**, **Pylibxc**
- Generative approaches for inverse catalyst design *e.g.*, latent diffusion models: **PyTorch**, **PyTorch-Geometric**

Workflows for High-Dimensional Optimisation

- Symbolic regression and support vector machines: **SISSO**, **PySR**, **gplearn**, **Scikit-learn**
- Dimensionality reduction e.g., PCA, K-means clustering: **Scikit-learn**
- Bayesian optimisation, Monte Carlo sampling and LLMs: **GPyOpt**, **SuSMoST**, **GPT-4o**, **Mathstral-7B**

Publications

Machine learning generalised DFT+U projectors in a numerical atom-centred orbital framework

Amit Chaudhari, Kushagra Agrawal, Andrew Logsdail: https://doi.org/10.26434/chemrxiv-2025-332z0

Polymorph-induced reducibility and electron trapping energetics of Nb and W dopants in TiO_2

Amit Chaudhari, Andrew Logsdail, Andrea Folli: https://doi.org/10.26434/chemrxiv-2025-k90kd-v3

Ongoing Projects

- Multiscale modelling (Monte Carlo sampling and machine learned interatomic potentials) and experimental investigation of catalyst poisoning for green H_2 production
- Constructing deorbitalised meta-GGA exchange-correlation functionals using deep learning
- Integrating explainable and generative AI approaches for inverse catalyst design

Selected Oral Presentations

Machine learning generalised DFT+U projectors in a numerical atom-centred orbital framework: Psi-k and NCCR MARVEL Workshop on the Determination of Hubbard Parameters — Sept 2025 (Upcoming)

AI for scalable quantum chemical simulations – from DFT+U to orbital-free meta-GGAs: BIOVIA (Dassault Systèmes) — Aug 2025 (Upcoming)

Machine learning algorithms for simulating realistic catalytic reaction environments: Johnson Matthey and bp — Jan 2025

Machine learning the DFT+U projectors to model polarons in energy materials: FHI-aims UK Developers' and Users' Meeting and the Materials Chemistry Consortium Conference — May/July 2024

Combining DFT, global optimisation and machine learning to understand metal oxide support effects in catalysis: Johnson Matthey — 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 — Jan 2024

Sustainable Catalysis for Clean Growth- Advanced Methods Overview: bp International Centre for Advanced Materials Annual Conference — Oct 2023

Selected Poster Presentations

Towards a transferable kinetic energy density functional using symbolic regression and large language models: CECAM Machine Learning for Materials Discovery workshop — May 2025

Machine learning generalised DFT+U projectors to model polarons in catalyst and battery materials: Thomas Young Centre 7th Energy Materials workshop — July 2024

***Ab initio* adsorption phase diagrams using DFT-parameterised Monte Carlo methods**: STFC CCP5 Annual General Meeting — Sept 2023

Supervision and 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

Updated 12/07/2025