# Amit Chaudhari

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## Education

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

- Group of Dr Andrew Logsdail: leveraging physics-informed machine learning to study intractable problems in electronic structure and materials modelling (heterogeneous catalysis)

**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

## First-Author Publications

**Machine Learning Generalised DFT+$U$ Projectors in a Numerical Atom-Centred Orbital Framework**

Chaudhari A, Agrawal K, Logsdail A. *ChemRxiv Preprint*, 2025, https://doi.org/10.26434/chemrxiv-2025-332z0

***Ab Initio* Insights into Support-Induced Sulfur Resistance of Ni-Based Reforming Catalysts**

Chaudhari A, Stishenko P, Hiregange A, Hawkins C, Sarwar M, Poulston S, Logsdail A. *ChemRxiv Preprint*, 2025, https://doi.org/10.26434/chemrxiv-2025-fgv2

**Polymorph-Induced Reducibility and Electron Trapping Energetics of Nb and W Dopants in $TiO_2$**

Chaudhari A, Logsdail A, Folli A. *J. Phys. Chem. C*, 2025, https://doi.org/10.1021/acs.jpcc.5c04364

## 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 implementations of 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 fingerprints: **ASE**, **Pymatgen**, **DScribe**, **PyTorch-Geometric**

**Deep Learning**

- Constructing transformer-based deorbitalized meta-GGA exchange-correlation functionals: **PyTorch**, **Pylibxc**
- Fine-tuning and inferencing foundation model machine learned interatomic potentials: **MACE**

**Workflows for Scientific Machine Learning**

- Symbolic regression and support vector machines: **SISSO**, **PySR**, **gplearn**, **Scikit-learn**
- Inferencing large language models for high-complexity symbolic regression and generative molecular modelling: **GPT-4o**, **ChemGPT**
- Dimensionality reduction *e.g.*, PCA, K-means clustering: **Scikit-learn**
- Bayesian optimisation and Monte Carlo sampling: **GPyOpt**, **SuSMoST**

## Ongoing Projects/ Contributions

- Learning deorbitalized meta-GGA exchange-correlation functionals using deep learning
- Simulating defects and polarons in semiconductor metal oxides using DFT+$U$
- Integrating explainable and generative AI algorithms for inverse homogeneous 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

**Physics-informed machine learning for modelling defect-driven catalytic phenomena**: Johnson Matthey and bp — Sept 2025

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

**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**: Collaborative Computational Project Number 5 Annual General Meeting — Sept 2023

## Supervision and Funding Awards

- Awarded the 1st Collaborative Computational Project Number 5 (CCP5) Postgraduate Industrial Secondment worth £2248.80, which facilitated computational and experimental collaboration with partners at Johnson Matthey Technology Centre, Sonning Common, UK (EPSRC grant number EP/V028537/1).
- Supervised research students as part of Nuffield and MChem projects

*Updated 10/10/2025*