Amit Chaudhari

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Education

PhD, Computational Chemistry: Cardiff University, Johnson Matthey and bp Oct 2021 – Oct 2025

- **Thesis: Physics-informed machine learning for modelling defect-driven catalytic phenomena**
- Group of Dr Andrew Logsdail: applying and developing methods for DFT+U parameterisation, learning non-local density functionals and catalyst multiscale modelling
- Industrial secondment at Johnson Matthey Technology Centre for modelling industrial catalysts

MSc, Molecular Modelling: 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 (**distinction**)

MEng, Chemical Engineering: 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 (2:1)

First-Author Publications

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

Chaudhari A, Agrawal K, Logsdail A. *Digit. Discov.* (Invited Submission), 2025, DOI: 10.1039/D5DD00292C

Mixture-of-Experts Transformers for Faithfully Deorbitalized Meta-GGA Density Functionals

Chaudhari A, Logsdail A. *ChemRxiv Preprint*, 2025, DOI: 10.26434/chemrxiv-2025-mrgzj-v2

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, DOI: 10.1021/acs.jpcc.5c04364

***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, DOI: 10.26434/chemrxiv-2025-fgv2m

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

- Learning non-local exchange-correlation functionals using mixture-of-experts transformers: **PyTorch**, **Pylibxc**
- Fine-tuning and inferencing foundation model machine learned interatomic potentials: **MACE**

Workflows for Screening and Scientific Machine Learning

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

Ongoing Projects/ Contributions

- 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

Future Research Interests

- Accelerating electronic structure methods using modern AI/machine learning
- High-throughput simulations of defects in complex oxides using self-interaction-corrected DFT
- Training next-generation foundation models for the discovery of novel functional materials

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 26/11/2025