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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, doi.org/10.26434/chemrxiv-2025-332z0-v2

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.org/10.26434/chemrxiv-2025-fgv2

Polymorph-Induced Reducibility and Electron Trapping Energetics of Nb and W Dopants in TiO₂
Chaudhari A, Logsdail A, Folli A. *J. Phys. Chem. C*, 2025, 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**, **DScrive**, **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+<i>U</i> 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+<i>U</i> 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+<i>U</i> 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 TiO₂ polymorphs using DFT+<i>U</i> 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+<i>U</i> 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 15/10/2025