DPhil studentship in Computational Chemistry

Title: ***Machine Learning Interatomic Potentials for Metal-Ligand Interactions***

Supervisor: Professor Fernanda Duarte

Start date: 1st October 2026

Applications are invited for a fully-funded **DPhil** studentship in *Machine Learning Interatomic Potentials for Metal-Ligand Interactions* available from October 2026, to work under the supervision of **Professor Fernanda Duarte** in the Department of Chemistry at the University of Oxford.

The studentship will cover course fees at a Home rate and provide a stipend of no less than the standard UK Research Council rate (currently set at £20,780 p.a.) for 4 years. Please note the eligibility criteria set out by the UKRI at: https://www.ukri.org/what-we-do/developing-people-and-skills/esrc/funding-for-postgraduate-training-and-development/eligibility-for-studentship-funding/

The successful candidate will join the Duarte group in the Department of Chemistry to develop innovative strategies for generating Machine Learning Interatomic Potentials (MLIPs) that accurately capture the dynamic nature of metal-ligand interactions. These models will enable predictive simulations of structural, thermodynamic, and kinetic properties in complex systems relevant to catalysis, supramolecular chemistry, and biology. The candidate will benefit from close collaboration with experimentalists, training in a range of computational techniques, as well as being part of a supportive, diverse, and international research team. The Duarte group focuses on the development and application of computational approaches to model chemical processes across multiple size and time scales. The team has pioneered methodologies for exploring chemical reactivity, including tools such as *autodE* and *mlp-train*, which form the foundation of this project. More information can be found on the group website.

Candidates with a first-class or strong upper second-class undergraduate degree in Chemistry or a related subject are encouraged to apply. The candidate is expected to have a strong commitment to research and should have demonstrated the ability to independently learn new skills. The successful applicant will be based in the Physical and Theoretical Chemistry Laboratory (PTCL), Oxford.

Candidates should submit a formal application for DPhil in Chemistry via the Oxford online application system:

https://www.ox.ac.uk/admissions/graduate/application-guide

https://www.ox.ac.uk/admissions/graduate/courses/dphil-chemistry

Please quote **FD/Chem/2026** under ‘Departmental Studentship Applications’.

Application deadline: **12.00 noon UK time on 30 of January 2026.**

Queries relating to the application and admission process should be directed to: graduate.admissions@chem.ox.ac.uk; tel.: +44 (0) 1865 272569.

The Department of Chemistry holds the Athena SWAN Silver Award and the Duarte group is dedicated to promoting diversity, equality and inclusion.