Applications are invited for a PhD studentship starting in September 2025 to be supervised by Prof. Adrian Mulholland and cosupervised by Prof. Neil Allan (Centre for Computational Chemistry, School of Chemistry, University of Bristol).

**Interactive virtual reality for simulation, data visualization and virtual collaboration**

This project will involve the development, application and testing of interactive virtual reality methods for chemical applications, including in catalysis, linking to developments in AI, and developing human computer interaction, including user prompts, for practical virtual reality applications in chemistry. Interactive VR allows users to visualize complex data. manipulate systems intuitively, and to collaborate virtually, working together in the same virtual environment, even when physically distant. We have developed tools for interactive molecular dynamics simulation in virtual reality (iMD-VR), in which users (and groups of users) can manipulate and drive MD simulations, in applications ranging from catalysis to molecular design and chemical education (see references below). In iMD-VR, users drive changes (such as ligand binding or motion of promoters in zeolite catalysts) in molecular systems. VR offers an accessible way to interact with the molecular world and accelerate simulations “on the fly” using human intuition. We have shown that users complete molecular modelling tasks more rapidly and accurately with iMD-VR than with traditional mouse and screen approaches. It provides a method to accelerate discovery processes, allowing rare events to be analysed on otherwise inaccessible timescales. It also allows for teamworking in virtual environments. Altogether, this is changing the way science is carried out. iMD-VR provides a prototype and exemplar for the developing field of interactive simulation, which we will extend in this project. We will extend and apply this open source software framework, and test other VR programs and approaches, in this project for interactive simulation, modelling, data analysis and virtual collaboration in VR. This will include development of interaction methods user tests. Targets include promoters, biocatalysts and other catalysts, and processes in bioenergy, sustainable feedstocks and processes, and renewable fuels. We will add features to the user interface for molecular editing and visualization, enable connections with a wide range of simulation codes of interest in materials, bio and catalyst modelling. We also develop interfaces with other visualization and simulation packages. In this project, we will test and add bespoke features for visualization, user interaction, simulation playback, analysis and recording; develop tools for interactive molecular editing and design and apply machine learning and AI methods, combining human and machine intelligence. We will develop, features and test user friendliness and effective human computer interaction, using AI tools and methods, for visualisation, interaction, analysis and virtual collaboration.

**References**

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**Candidate Requirements**

Applicants must have obtained, or be about to obtain, a First or Upper Second Class UK degree, or the equivalent qualifications gained outside the UK, in Chemistry, Computer Science or in a related discipline.

**How to Apply**

Please make an online application for this project at: <https://www.bristol.ac.uk/study/postgraduate/apply/>

**Funding**

A full studentship will cover UK tuition fees, a training support fee and a stipend (£23,280 for 25/26, to increase each year) for 3.5 years.