

## Physical & Theoretical Chemistry Studentship Projects

### Project Titles

- 1) Application of Molecular Modelling and VR Technologies to Fundamental Studies of Zeolite Catalysis
- 2) New Force Field Development to Improve Conformational Searches in Zeolites

### Supervisors:

Prof. Neil Allan (University of Bristol)

Prof. Adrian Mulholland (University of Bristol)

### The project:

Zeolites are vitally important materials used as catalysts and adsorbents in the processing of renewables, oil and gas. The origin of the unique behavior of zeolites, whether as selective adsorbents or as catalysts for particular transformations. These two projects will explore the use of molecular simulations (chiefly molecular dynamics and Monte Carlo) and related virtual reality techniques to model reactions in zeolites and the catalytic mechanisms involved. New forcefields will be derived and used to study zeolite reactivity and selectivity. Possibilities for bio-inspired additive and catalyst design will be explored by investigating possible analogies with natural enzymes. The four-year projects will involve substantial collaboration with the BP Group Research Departments in the UK and USA for their personal development and knowledge of the industry, and training in and use of Bristol University's High-Performance Computing facilities.

Further details are available from Profs Adrian Mulholland ([adrian.mulholland@bristol.ac.uk](mailto:adrian.mulholland@bristol.ac.uk)) and Neil Allan ([neil.allan@bristol.ac.uk](mailto:neil.allan@bristol.ac.uk)). Our research websites are <https://mulhollandgroup.wordpress.com/> and <http://www.chm.bris.ac.uk/pt/allan/Research/>

### Funding:

Successful applicants will receive a EPSRC Industrial CASE studentship that covers fees and access charges as well as providing a £15,009 tax free stipend p.a. +£2,000 p.a. top up.

### How to apply:

Please make an online application for this project at <http://www.bris.ac.uk/pg-howtoapply>. Please select Chemistry PhD on the Programme Choice page. You will be prompted to enter details of the studentship in the Funding and Research Details sections of the form.

### Deadline:

The deadline for applications is 19<sup>th</sup> May 2019. However, we reserve the right to withdraw the advert early in the event that suitable candidate is found.