

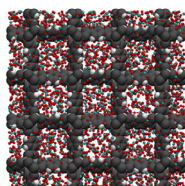
2-DAY WORKSHOP

Molecular Simulation of Carbon Capture and Storage in Novel Porous Materials

Wednesday 25th & Thursday 26th April, 2012

Location:

Institute for Materials and Processes,
The University of Edinburgh, UK



Workshop organiser:

Dr Lev Sarkisov
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Cost:

Adsorption Research Industrial Consortium (ARIC) members: **FREE!***

Non-ARIC members: **£500 for 2 days**, including lunch and dinner.

* (for up to 2 representatives from each ARIC company)

This workshop is being offered as part of the Innovative Gas Separations for Carbon Capture (IGSCC) project (www.eng.ed.ac.uk/carboncapture/igsc.html), and will be of significant benefit to anyone interested in learning more about the simulation of adsorption phenomena in porous materials with a particular emphasis on carbon capture. The role of molecular simulation in the development and optimization of adsorption separation processes has become increasingly important for the following reasons:

- Molecular simulations provide fundamental insights into adsorption phenomena that may guide the design of new materials with tailored functionalities.
- Molecular simulations offer an efficient alternative to tedious and time-consuming experiments, e.g. for multi-component adsorption and adsorption at high pressures.
- With 1000s of new materials synthesized every year, computer simulations can be used as a quick and efficient screening tool to identify the most promising candidates.

AIMS of Workshop For Days 1 & 2:

AM: Learn about the fundamentals of statistical mechanics, molecular simulation and adsorption.

PM: Run your own computer simulations of adsorption in the laboratory, using specific case studies covering:

- Adsorption of CO₂ in a metal-organic framework.
- Adsorption from a multi-component mixture, corresponding to a typical flue gas composition.
- Calculation of the self-diffusion coefficients for adsorbed species.

By the end of the workshop, you will be able to set up your own simulations of adsorption in porous materials and interpret the results.

If you would like to participate in the workshop or have any queries, please email: Lev.Sarkisov@ed.ac.uk.

A detailed programme of the workshop, including the timetable and logistics will be distributed to interested parties in February 2012.