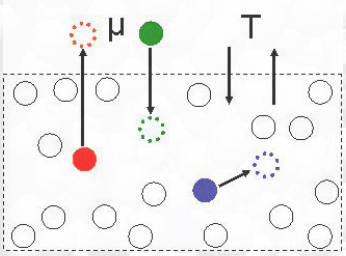
MOLECULAR THERMODYNAMICS 5

Delivery period:
Semester 2 (Jan to Mar) --- Tues & Thurs am
Two 50-minute lectures --- 10 weeks
Three 2-hour computing workshops

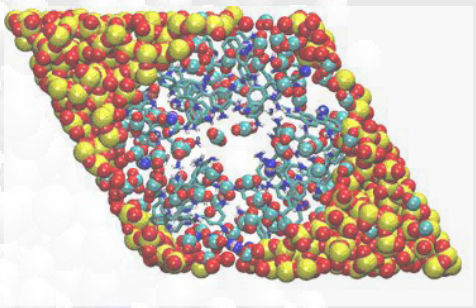
Course organiser:
Dr Lev Sarkisov, Dr Tina Dueren
Email: lev.sarkisov@ed.ac.uk, tina.duren@ed.ac.uk

COURSE DESCRIPTION

This course provides an introduction to molecular thermodynamics and molecular simulation methods. It addresses the fundamental principles of thermodynamics derived on the basis of intermolecular interactions, and it provides hands-on experience of molecular simulation methods through computing workshops.



Schematic of GCMC simulation

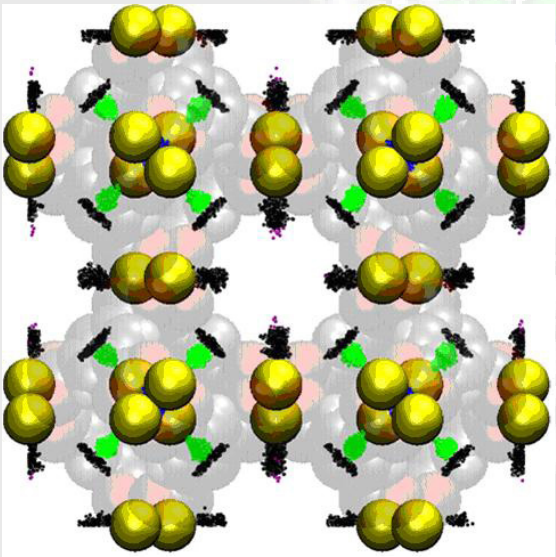


CO_2 adsorbed in functionalised MCM-41

MAIN TOPICS

1. Introduction to molecular thermodynamics
2. Heat/work/energy from molecular perspectives
3. Entropy/Thermodynamic forces
4. Free energy and Maxwell relations for mixtures from molecular principles
5. Molecular thermodynamics of simple liquids and gases / Intermolecular forces
6. Introduction to molecular simulations: Molecular Dynamics & Monte Carlo methods
7. Molecular thermodynamics of adsorption and binding
8. Molecular simulation of adsorption
9. Molecular simulation of carbon capture processes
10. Molecular thermodynamics of vapour liquid equilibria and mixtures

Workshop 1: Molecular dynamics of bulk liquids
Workshop 2: Simulation of lipid bilayers
Workshop 3: Simulation of adsorption separation for carbon capture



Adsorption sites in CuBTC from molecular simulation

LEARNING OUTCOMES

Learning outcomes:

1. Understand the principles of molecular thermodynamics; relations between microscopic interactions and macroscopic, bulk properties.

2. Formulate chemical engineering problems in a form in which they are amenable to solution by molecular thermodynamics methods.

3. Appreciate the capabilities of different simulation methods and understand the underlying concepts of Monte Carlo and molecular dynamics simulation methods, including relevant statistical mechanical theory.

4. Apply molecular simulation methods to chemical engineering problems using appropriate software.