Introduction

CO₂ Capture and Storage (CCS) represents a serious strategy to reduce CO₂ emissions in the global challenge of mitigating global warming. CCS involves scrubbing vast amounts of CO₂ from energy producing combustion processes (coal burning) and permanently storing it. Currently, large scale CCS is not practical because an energy and cost effective technology to scrub CO₂ from combustion flue streams has not been developed.

Metal Organic Frameworks for CO₂ Capture

Metal Organic Frameworks (MOFs) are materials which have recently been shown to display exciting promise for CO₂ capture (Science 2008, 319, 939). MOFs are nanoporous solids, meaning they have pores and cavities at the scale of molecules. These pores give some MOFs huge internal surface areas and the ability to reversibly capture vast amounts of CO₂, some as much as 83L of gas per 1L of material.

MOFs could form the basis of a new energy efficient technology to scrub CO₂ from the combustion flue stream of coal burning power plants (which are the world’s biggest single source of CO₂).

The most serious limitation of MOFs for CO₂ capture is that they are poisoned by water, a major combustion product, and other common combustion products.

Methodology

Molecular simulation has been found to be predictive of binding site localisation within a Metal Organic Framework. The geometry of the rigid ZIF-8 structure as well as that of the small molecules must be optimized using high accuracy Density Functional Theory calculations.

In order to explore the potential energy surface of the system being studied, several Grand Canonical Monte Carlo (GCMC) simulations are run, using molecular mechanics and in house developed scripts.

The Grand Canonical (GC) part inserts and deletes guest molecules, which reaches equilibrates with a gas reservoir at a given pressure. The Monte Carlo (MC) part of the code involves random samplings of the system based on thermodynamics at regular time steps. At each step, the new configuration of guest molecules within the rigid ZIF can either be accepted or not depending on thermodynamic criteria. It should however be noted that a less energetically favourable configuration always has a finite probability of being accepted. The statistical sampling of molecule positions gives binding data based on probability distributions.

Results

The different isosurface and probability plots, which give a good idea of the possible binding sites within ZIF-8, depend strongly on the type of guest molecule being analyzed. This shows that binding is likely to differ depending on the guest molecule being adsorbed by the ZIF-8 Metal Organic Framework.

Future Work

This structural data could be used for comparison with experimental data in order to evaluate the accuracy of GCMC simulation for ZIF-8 analysis. Computational guest molecule uptake could also be compared to experimental guest molecule uptake.

References