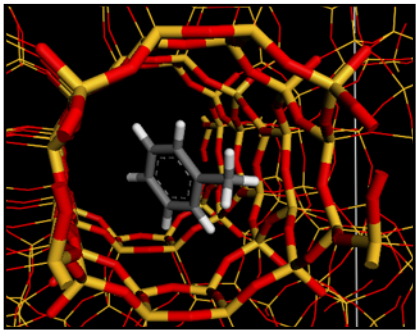
CASE STUDY

ADSORPTION MECHANISM OF CARBON DIOXIDE IN ZEOLITES



Improving the capture and storage of "green houses gases" such as CO2 is a complex activity. Researchers at the Royal Institution in England used Materials Studio to study the role of microporous zeolite in this phenomenon.

Industry sectors

- Pharmaceutical
- Chemicals
- Environmental Chemistry

Organizations

- Université de Provence
- Université Montpellier
- Royal Institution of Great Britain

Product

- Sorption

Scientists at the Universite de Provence, Universite Montpellier and the Royal Institution of Great Britain have used the Sorption module of Accelrys Inc. to study CO_2 adsorption in faujasites in a joint experimental and simulation study[1].

They obtained adsorption isotherms and enthalpies of adsorption in very good agreement with experiment. A proposed mechanism for the CO_2 adsorption was validated by the trends observed for the enthalpies of adsorption.

INTRODUCTION

Environmentally friendly and economically favorable separation, capture, and storage of gases represent very important technological challenges. This is particularly the case for carbon dioxide: the excessive emission of this known green-house gas is leading to global warming[2]. The systems currently used for carbon dioxide removal and sequestration have several disadvantages, such as the need for additional processing and corrosion controls[3].

Among the potential adsorbent nanoporous candidates, zeolites are very promising[4] due to their environmentally friendly character and their strong affinity for carbon dioxide. These materials also offer attractive choices as sorbents because they have a number of parameters that are easily tuned in the laboratory: pore size, Si/Al ratio, and choice of extra-framework cation. Zeolite membranes in combination with noble metals can also be used as catalysts[5] for reforming carbon dioxide into fuels[6].

RESULTS

In this study a force field was derived from ab initio calculations[7] to represent the interactions between carbon dioxide and zeolite framework. This allowed accurate reproduction of the experimental data in three different faujasite forms, DaY, NaY, and NaLSX using the Sorption program. (see Fig.1.)

Both the simulated adsorption isotherms and the enthalpies of adsorption (not shown in Fig. 1) were in very good agreement with the recent experimental data obtained from microcalometry measurements. This established modeling as a predictive tool for the evaluation of the performance of different types of zeolites materials with respect to CO_2, which is of great environmental and economical importance.

In addition to macroscopic data like the adsorption isotherm, molecular modeling also provides a detailed atomistic view of processes in the zeolite. This made it possible for the scientists to propose a mechanism for CO_2 adsorption in each of the different faujasites that is consistent with the evolution of the enthalpy of adsorption as a function of CO_2 coverage.

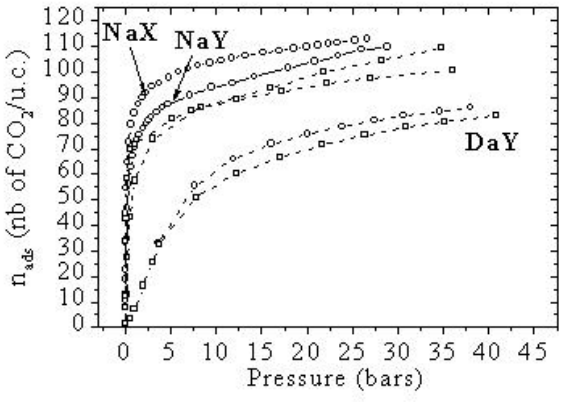


Figure 1. *Absorption isotherms for carbon dioxide adsorption on DAY, NaY, and NaLSX at 300 K: squares represent the simulation results, open circles the experimental measurements.*

This work demonstrated that this modeling approach is an effective predictive tool for evaluating the performance of different types of zeolite materials with respect to CO_2. Modeling can thus be used to determine the specific characteristics of the adsorbent that will provide the best CO_2 storage.

Dr Guillaume Maurin, Universite´Montpellier II, said, "Today and in the near future, the emerging approach will be to deploy modelling tools to aid the development of smart alternative industrial processes. To be successful, those performing modelling need to be able to bounce their ideas and results off unique experiments that can be carried out under similar conditions to those found on the industrial scale. The scientific originality of our research is to develop within different EU projects (RTN INDENS & STREP DeSANNS) modeling tool which, starting from problems related to energy and environmental areas, is able to design a given corresponding zeolite or MOF materials. The prediction of the adsorption properties of these systems via Grand Canonical Monte Carlo simulations is crucial for designing new promising materials which could be produced on a large scale for industrial applications in adsorption technology."

To learn more about Materials Studio by Accelrys, go to **accelrys.com/materials-studio**

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