SULFUR HEXAFLUORIDE ADSORPTION PREDICTION IN MOBIL CATALYTIC MATERIALS (MCM) BY MOLECULAR SIMULATIONS

Aurelio Olivet, Carmelo Herdes, Jordi Faraudo and Lourdes F. Vega

Institut de Ciència de Materials de Barcelona (ICMAB-CSIC) Campus de la Universitat Autònoma de Barcelona, 08193 Bellaterra, Spain
aolivet@icmab.es

Classical molecular simulations, especially Grand Canonical Monte Carlo simulations and Molecular Dynamics, are becoming standard tools for the textural characterization of adsorbent and catalytic materials, as well as for predicting the capacity and selectivity of given adsorbents for specific applications. Although of general use, these tools become of great importance for porous materials for which classical macroscopic methods fail, due to the proximity of the adsorbing walls (commensurate with the size of the adsorbate) and/or the strong interaction exerted by them, all of them occurring at the nanoscale. Our group has been working on the application of these techniques to several systems. We will present here the case of a nanoporous material used for SF_6 storage applying these techniques. The study deals with several topics including two force fields for the fluid and the study of several microscopic properties.

The main results to be presented and discussed here deal with: 1) the influence of the molecule flexibility of SF_6 into the adsorption behaviour in MCM41 (AM5) by comparing a rigid [1] and a flexible model [2] of the fluid under the same simulated conditions (see Figure 1). 2) the prediction of the maximum loading for SF_6 on MCM41 (AM5), assuming the validity of the Pore Size Distribution of the adsorbent material obtained in a previous work [3]. The adsorption capacities of other silica based materials for the storage of SF_6 and/or other gases can be straightforward performed using the same methodology.

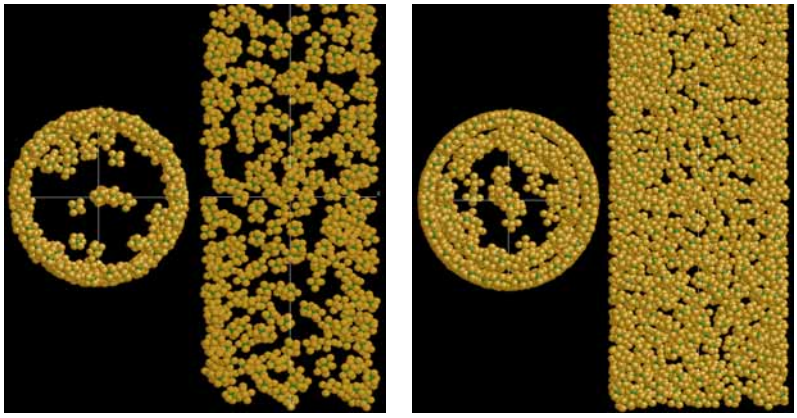

Figure 1. SF6 adsorption on a cylindrical pore of diameter 5nm at 296 K. Left figure: rigid model, Right figure: flexible model

References:

[1] A. Olivet, D. Duque, L.F. Vega, J. Chem. Phys. **123** (2005) 194508.
[2] A. Olivet, L.F. Vega, J. Chem. Phys. (submitted 2006).
[3] C. Herdes, M.A. Santos, F. Medina, L.F. Vega, Langmuir **21** (2005) 8733-8742