2° Simposio sobre Adsorción Adsorbentes y sus Aplicaciones

MOLECULAR SIMULATION OF METHANE ADSORPTION IN MIL-101 USING MONTE CARLO METHODOLOGY

D. Gonçalves[(1)], P. Silvino[(1)], S. Lucena[(1)*]

[(1)] Grupo de Pesquisa em Separações por Adsorção, DEQ-UFC, Universidade Federal do Ceará, BRASIL.

*lucena@ufc.br

ABSTRACT

MIL-101 is a new class of Metal-Organic Framework (MOF) material with giant pores built by the connection of hybrid microporous supertetrahedra which further assemble with formation of two types of mesoporous cages. This particular framework gives high methane storage capacities. In this study, we investigated adsorption equilibrium properties of methane in MIL-101 (Cr) using the Monte Carlo methodology in the grand canonical ensemble (GCMC). The MIL-101 (Cr) framework was constructed from crystallographic data [1]. We tested general force fields. Adsorption isotherms were performed at room temperature using two methane models, united atom (UA) [2] and atom-atom (AA) [3]. NVT simulations using argon at 30 K and methane at 150 K were carried out to estimate adsorption sites. Potential maps of selected sections of the framework were performed to give the energy of each site. We found that adsorption energy varies from 4.4 to 0.3 kcal/mol being maximum at supertetrahedra. The theoretical methane storage (V/V) capacity of MIL-101 and the isosteric heat of adsorption also were predicted.

Keywords: MIL-101, Methane and Adsorption properties

References

[1] Férey, G.; Mellot-Draznieks, C.; Serre, C. Millange, F.; Dotour, J.; Surblé, S.; Margiolaki, I. *A chromium terephthalate-based solid with unusually large pore volumes and surface area*, Science, (2005), 2040-2042.
[2] Martin, M. Siepmann, J. *Transferable potentials for phase equilibria. 1. United-Atom description of n-alkanes*. The Journal of Physical Chemistry B, (1998), 2569-2577.
[3] Murad, S.; Gubbins, K. Molecular *dynamics simulation of methane using singularity-free algorithm*. Computer modeling of matter, (1978), 62-71.