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氮气在**MCM－41**分子筛中的吸附：实验和分子模拟

曹达鹏,陈建峰,沈志刚,张现仁,汪文川

北京化工大学化学工程学院.北京(100029);北京化工大学教育部超重力工程 研究中心.北京(100029)

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摘要 用美国Micromeritics公司生产的ASAP2010物理吸附仪测定了低温（77 K） N_2在MCM-41分子筛中的吸附等温线，获得了表征MCM-41特征的BET比表面、BJH孔 容和平均孔径。同时用巨正则Monte Carlo（GCMC）模拟方法考究了N_2在MCM-41中 的吸附，得到了N_2在MCM-41中的模拟吸附等温线，分析了流体在MCM-41分子筛中 的微观结构。GCMC模拟中MCM-41介孔材料模型化为圆柱孔，N_2模型化为Lennard- Jones（LJ）球。N_2和MCM-41介孔墙壁间的相互作用采用Tjatjopoulos-Feke- Mann（TFM）势能模型进行表征。通过使模拟和实验结果有一个好的吻合，确定了 一组有效的MCM-41分子筛的势能参数（σ_(ww) = 0.265 nm，∈_(ww)/k = 190 K ）。这为以后其他吸附质在MCM-41中吸附的预测奠定了基础、提供了依据。

关键词 分子筛 吸附 蒙特卡罗法 微观结构

分类号 0641

Adsorption of Nitrogen in MCM-41: Experiment and Molecular Simulation

Cao Dapeng,Chen Jianfeng,Shen Zhigang,Zhang Xianren,Wang Wenchuan

College of Chemical Engineering, Beijing University of Chemical Technology.Beijing(100029);Research Center of the Ministry of Education for High gravity Engineering and Technology, Beijing University of Chemical Technology.Beijing (100029)

Abstract Adsorption isotherm of nitrogen in MCM-41 at temperature T = 77 K was measured by using the ASAP 2010 volumetric adsorption analyzer produced by Micromeritics Instrument Corp.. The BET specific surface was obtained. Based on the BJH analysis method, which is a suitable method for analyzing adsorption of fluid in meso-porous materials, the BJH adsorption cumulative pore volume and average pore diameter were also solved. The grant canonical Monte Carlo (GCMC) simulation was also carried out to investigate the adsorption of nitrogen in MCM-41 at T = 77 K. In our GCMC simulation, the MCM-41 material was modeled as cylindrical pore, and nitrogen was considered as the Lennard-Jones spherical molecule. The Tjatjopoulos-Feke-Mann (TFM) potential was used for representing the interaction between nitrogen molecules and cylindrical pore walls. In the simulation, the diameter size was taken from the result measured. Simulated adsorption isotherm of nitrogen in MCM-41 was obtained, and the micro-structure of the fluid in MCM-41 was also analyzed, which is good guidance to understand the mechanism of adsorption. Note that a set of parameters representing MCM-41 was determined by making the experiment isotherm and simulation isotherm in a good agreement, which is a basis for predicting the adsorption of other adsorbate in MCM-41.

Key words MOLECULAR SIEVE ADSORPTION MONTE CARLO METHOD MICRO-STRUCTURE

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通讯作者