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超临界甲烷在氯化锆层柱纳米材料中吸附的分子模拟

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摘要 用巨正则MonteCarlo(GCMC)方法模拟了甲烷在氯化锆层柱材料中的吸附。模拟中，
氯化锆层柱材料模型化为柱子均匀分布在层板间的层柱孔，非极性分子甲烷采用Lennard-Jones分子模型，
层板墙采用Steele的10-4-3模型，流体分子与柱子的相互作用采用点-点(sitetosite)
的方法计算。在高度理想化模型的基础上，引入交互作用参数kfw,
建立了有效势能模型。通过实验数据确定交互作用参数kfw，
从而使该模型能有效地表征流体与层板墙的相互作用。根据77K温度下氮气的实验吸附数据，
确定了流体和层板墙间的交互相作用参数。然后用这个有效的参数kfw=0.65
模拟了三个超临界温度下氯化锆层柱材料中甲烷的吸附情形，得到了它位的吸附等温线，
局部密度分布以有流体分子在层柱微孔中的瞬时构象，
并分析了温度对材料吸附性能的影响。结果表明GCMC方法是预测材料吸附性能的一种强有力的工具。

关键词 甲烷 超临界状态 氯化锆 纳米相材料 吸附 蒙特卡罗模拟

分类号 0647

Molecular simulation of adsorption of supercritical methane in pillared zirconium chloride

Cao Dapeng,Wang Wenchuan

Abstract Adsorption of supercritical methane confined in pillared zirconium chloride was simulated by suing grand canonical Monte Carlo (GCMC) method. In our simulation, a pillared zirconium chloride was modeled as a layered pillared pore with the uniform distribution of pillars. Steele's 10-4-3 potential was used for representing the interaction between Lennard-Jone methane molecule and a layered solid wall, and the sitesite interaction was also used for calculating the interaction between methane and pillares in the GCMC simulation. An effective model was developed by introducing the cross interaction parameter kfw to the ideal layered pillared model. Based on the experimental results with nitrogen at 77K, the cross interaction parameter between fluid molecule and a layered wall was determined from the simulation results that agreed well with the experimental ones. The effective parameter, kfw=0.65, was used to simulate adsorption of supercritical methane at various temperatures. The adsorption isotherms and the local density profiles of methane in pillared zirconium chloride were obtained, which indicated that the GCMC method was s useful tool for investigation of adsorption character of material.

Key words METHANE SUPER-CRITICAL STATE ZIRCONIUM CHLORIDE NANOPHASE MATERIALS ADSORPTION MONTECARLO SIMULATIONS

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