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RESEARCH PAPERS

圆柱孔的势能模型

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摘要 An analytical potential for cylindrical pores has been derived by introducing a variational method into the integration for the calculation of the interaction energy between the wall molecules and a test molecule, all of which are represented by Lennard-Jones potential. The model proposed gives good fito the results from the cylindrical surface model and the pseudoatom model. To test the potential proposed rigorously, we have carried out grand canonical ensemble Monte Carlo(GCMC) simulation of nitrogen in the MCM-41 pore at 77 K, and
compared the simulated adsorption isotherm with the experimental data reported in the literature. The simulated isotherm from our model is in almost qualitative agreement with experiment. Consequently, the model proposed provides an explicit and accurate description of cylindrical pores represented by the Lennard-Jones potential. Moreover, the model can be easily applied to a variety of cylindrical pores, ranging from cylindrical surface to finite thickness walls, in both theoretical studies and computer simulations.

关键词 圆柱孔 势能模型 MCM-41 GCMC 模拟 等温线 圆柱面 多孔介质 中孔介质 氮 活性碳 吸附

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A Potential Model for Cylindrical Pores

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Abstract An analytical potential for cylindrical pores has been derived by introducing a variational method into the integration for the calculation of the interaction energy between the wall molecules and a test molecule, all of which are represented by Lennard-Jones potential. The model proposed gives good fito the results from the cylindrical surface model and the pseudoatom model. To test the potential proposed rigorously, we have carried out grand canonical ensemble Monte Carlo(GCMC) simulation of nitrogen in the MCM-41 pore at 77 K, and compared the simulated adsorption isotherm with the experimental data reported in the literature. The simulated isotherm from our model is in almost qualitative agreement with experiment. Consequently, the model proposed provides an explicit and accurate description of cylindrical pores represented by the Lennard-Jones potential. Moreover, the model can be easily applied to a variety of cylindrical pores, ranging from cylindrical surface to finite thickness walls, in both theoretical studies and computer simulations.

Key words

potential model; cylindrical pores; GCMC MCM-41

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