عنوان مقاله:

Monte Carlo simulation of methane and n-butane adsorption on silicalite-1

محل انتشار:

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خلاصه مقاله:

Adsorption of methane and n-butane in silicalite-1 has been studied by using Configurational-bias Monte Carlo simulations of linear alkane molecules in the grand-canonical ensemble. The molecular interactions between gas molecules and molecules in the wall of silicalite-1 cage have been considered as consisting of three parts; part 1: dispersion interactions which were described by Lennard-Jones 6-12 potential, part 2: torsion interactions which were described by the cosine potential and part 3: bond-bending potential which were described by the harmonic bend potential model. The grand canonical ensemble was utilized in the simulation and the parameters of each potential function were evaluated. The size of each cage of silicalite-1 on adsorption was examined and the results be compared with experimental and analyticaltheoretical models. It was seen that the results were in good agreement .with both theoretical and experimental results

کلمات کلیدی:

Adsorption; Monte Carlo; Silicalite-1; Methane; n-Butane; Potential model

لینک ثابت مقاله در پایگاه سیویلیکا: