

Molecular Dynamics Simulation Studies of *p*-Xylene in OH-free Si-MCM-41

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We report on modeling efforts and molecular dynamics computer simulations of the structure and self-diffusion of *p*-xylene in OH-free Si-MCM-41 as a function of loading. Both the guest molecules and Si-MCM-41 are modeled as flexible entities. With this newly developed intermolecular force field the average potential energy of *p*-xylene in the pore increases with increasing loading. The adsorption of *p*-xylene in MCM-41 is primarily associated with the van der Waals interactions of the model, whereas the contribution from electrostatic interactions is relatively small (about 2 kcal/mol), in accordance with other aromatic hydrocarbons adsorbed in zeolite catalysts. The calculated self-diffusion coefficients of *p*-xylene in Si-MCM-41 are well comparable with diffusion coefficients of pyridine in MCM-41 and of the same order of magnitude as in liquid *p*-xylene. Increasing the loading results in non-negligible mutual *p*-xylene interaction, thus leading to a decrease of the self-diffusion coefficient.

Key words: Molecular Dynamics; Adsorption; Diffusion; *p*-Xylene; Si-MCM-41.