23a Adsorption of Water in Zeolites as Studied by Molecular Simulations

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Understanding the behavior of water confined in porous materials is a key issue in many applications such as ion exchange, molecular sieving and catalysis. In this paper we investigate the ability of standard semi-empirical interaction potentials of water to capture the essential experimental features of water adsorption in different zeolitic materials. It is found that the most popular effective water potentials (such as SPC or TIP4P) are doing a relatively good job in reproducing the equilibrium adsorption properties in aluminosilicate zeolites such as faujasite NaY and NaX, as well as in hydrophobic silicalite-1. In the second part of the work, we investigate in more details the adsorption mechanism of water in sodium faujasite, using Grand Canonical Monte Carlo (GCMC) simulations and the Replica-Exchange algorithm to accelerate the convergence of the MC simulations. Our aim is to understand the effect of the cation content (Si:Al ratio) on water adsorption. We found that a small amount of adsorbed water may, in some cases, drastically modify the nonframework cation distributions. This, in turn, has an noticeable effect on the co-adsorption of another molecular fluid (such as benzene or xylene). We were able to predict and understand at the molecular level why traces amount of water can modify the adsorption selectivity of a binary mixture of hydrocarbons in faujasite.