73h Computational Study of Low Density Water Formation in Hydrophobic Nanopores of Silicalite by Means of Estimating Adsorption Isotherms with Different Water Models

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Recently there has been an interest on the competitive adsorption of organics from water with hydrophobic zeolites. Silicalite drew particular attention since it has a higher Si/Al ratio which creates a more hydrophobic structure compared to other hydrophobic zeolites. To estimate the adsorption behavior of organics from water in silicalite first it is important to understand the dynamics of pure water adsorption. Numerous investigators have used molecular simulation techniques to study the dynamics of water confined in nanopores of silicalite. Some of them found that water presented a low density, vapor like behavior within the pores. In this study we have performed Grand Canonical Monte Carlo and Molecular Dynamics simulations at 298.15 K with different water models to estimate the water adsorption isotherms and study the dynamics of water in silicalite. Water models used in this study can be classified under three groups. Liquid water models, a water model optimized to the vapor-liquid coexistence properties and an electric-field dependent model. All liquid water models failed to reproduce the experimental adsorption isotherms by significantly overestimating the number of water molecules adsorbed, on the other hand, two other models estimated the adsorption isotherms within an acceptable range. Liquid water models and the vapor-liquid coexistence model failed to reproduce the experimental self diffusion coefficient of water in silicalite whereas electric-field dependent model gave a very good match with the experimental and theoretical findings reported in literature. No hydrogen bond formation between water molecules was observed during our simulation with the electric-field dependent model. With the liquid water model and vapor-liquid coexistence model a number of hydrogen bonds were detected which was less in the case of vapor-liquid coexistence model.