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Diffusion and adsorption of N_2 and C_2H_6 in ZIF-8 MD and MC simulations

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Molecular Dynamics (MD) and Gibbs-Ensemble Monte-Carlo (GMC) simulations give insight into the adsorption and diffusion properties of N_2 and C_2H_6 molecules adsorbed in ZIF-8 [1]. The framework flexibility plays an important role in achieving correct transport properties [2]. Particularly, for N_2 a gate opening effect could be observed. The window sizes were determined by the orientation of the imidazolate linkers and a transition from a closed structure at low N_2 loading (approximately 0.5–18.4 N_2/cage), to an open one, at high loading (approximately 20–30 N_2/cage) was found (see Fig. 1). This is in agreement with [3]. The results of MD simulations and of experiments for N_2 and C_2H_6 are compared. The simulation results illustrate that the transition of the orientation of imidazolate linkers of the ZIF-8 framework for both, 4 and 6-membered rings were induced by N_2 guest molecules.

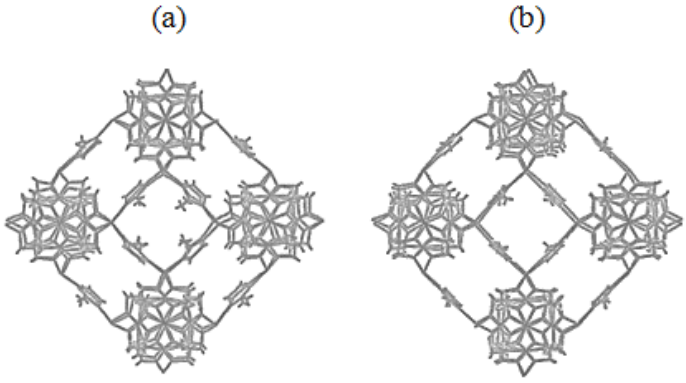

Figure 1: ZIF-8 window structures at (a) low loading and (b) high loading of N2 guest molecules.

References

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