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# Adsorption of small molecules in the intermediate structures of breathing MOF

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MIL-53 is a MOF porous structures which exhibits very pronounced flexibility. As a consequence, adsorption of CO2 causes its reversible structural transformation, induced by the host-guest interactions. Here, we present detailed molecular modeling study of adsorption of CO2 and CH4 in the intermediate structures of the MOF. We use 20 intermediate structures, between the open pore one and the closed pore form of MIL-53, to study adsorption during the "breathing"of the MOF 1. 18 intermediate structures were prepared using geometrical interpolation (Fig. 1) and they have been optimized using the DFT quantum calculations. Each structure is rigid and it represents an instantaneous non-equilibrium MOF configuration.

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RASPA code is used for molecular simulation [2]. Grand Canonical Monte Carlo and Molecular Dynamic methods are applied to calculate isotherms of adsorption and diffusion coefficients at various temperatures. The simulated adsorption in the intermediate structures show differences in adsorption mechanism of CO2 and CH4. The modeling of adsorption in the intermediate structures allows us to analyze the states which are not in equilibrium and are not accessible in conventional adsorption experiments. For better understanding of the interactions model applied during the process of adsorption, we compare our results with experimentally measured isotherms of adsorption.
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