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Abstract of the doctoral thesis “Modelling of Adsorptive Properties of Hybrid Porous Materials”

The present dissertation constitutes a contribution to current understanding of the microscopic mechanism of gases adsorption in two types of nanoporous materials: model carbon slit pores and in flexible metal-organic frameworks (MOFs). The applied methodology includes both: molecular simulations (using the Grand Canonical Monte Carlo method) and experimental measurements (using the inverse gas chromatography). For hydrogen adsorbed in carbon nanopores we show that the simulated amount of gas stored in pores is independent on the adopted representation (united atom or all atom) of hydrogen molecule, down to T = 77 K and up to gas pressure of 400 bar. For simple gases (CO_2, CH_4, C_6H_6) adsorption in flexible MOFs a simple methodology of identification of transition states during lattice deformation induced by adsorption is proposed and implemented. A numerical screening of a large database of existing and hypothetical Metal-Organic Framework structures was performed, to identify the MOFs with highest selective CO_2 adsorption from humid CO_2/CH_4 mixture, and to explain the origin of high CO_2 adsorption in selected MOFs in presence of water.