Influence of lattice dynamics on structural transformations and adsorption in hybrid nanoporous materials

Wpływ dynamiki sieci na transformacje strukturalne oraz adsorpcję w hybrydowych materiałach nanoporowatych

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Abstract

In this dissertation several aspects of structural transformations in metal-organic frameworks are addressed. The computational methodology used here is based on atomistic simulations with extensive application of Density Functional Theory and Grand Canonical Monte Carlo methods. Both dynamic (phonon analysis) and thermodynamic (thermodynamic potentials) approaches have been applied. Lattice dynamics calculations of low frequency phonons used as indicators of the potential structural transformations are performed. Several rigid and flexible metal-organic frameworks have been investigated to determine correlations between lattice vibrations and adsorption-induced deformations. Thermodynamic osmotic potential has been used to compute deformation-dependent energy profiles as the functions of temperature and presence of guest molecules in the pores. The proposed methodology allows for accurate description of the structural properties of metal-organic frameworks and, simultaneously, of the adsorption process. The proposed methodology does not require any experimental input. Therefore, it is applied to predict and interpret the relevant experimental results.