Title: Computational investigation of adsorption of saturated and unsaturated hydrocarbons in CPO-27 Metal-Organic Framework

Abstract:

The adsorption of hydrocarbons on coordinatively unsaturated sites (cus) in CPO-27 Metal-Organic Framework (MOF) was investigated computationally. Different levels of density functional theory (DFT), including vdW-DF2, PBE, DFT-D2 functionals, were used and their performance was compared to a reference method DFT/CC and available experimental data. The adsorption properties of Cu and Mg containing CPO-27 for ethane, ethylene, propane and propylene separations were investigated and discussed.

Keywords: adsorption, metal-organic frameworks, density functional theory, coordinatively unsaturated sites, open metal sites