عنوان مقاله:

On the study of CO/H2 potential interactions with HKUST-1 MOFs using ab initio calculations

محل انتشار:

بیستمین کنگره شیمی ایران (سال: 1397)

تعداد صفحات اصل مقاله: 1

نویسندگان:

Fatemeh Sadat Banijamali - *School of Chemistry, College of Science, University of Tehran, Tehran, Iran*

Ali Maghari - *School of Chemistry, College of Science, University of Tehran, Tehran, Iran*

خلاصه مقاله:

DFT calculations are employed to study the metal–dihydrogen and metal-carbon monoxide interactions in order to CO/H2 gas separation, making use of a non-periodic model system (M2 paddle wheel with M=Cu), which is representative for many copper-containing MOFs [1,2]. All-electron DFT calculations were carried out with the Orca 3.0.3 program package. A geometry optimization of the isolated Cu2(bmc)4 paddle wheel (bmc = benzene-monocarboxylate) with three different orientations of the hydrogen molecule and one orientation for carbon monoxide molecule were considered: (a) side-on orientation I, H–H bond oriented along one O–Cu–O axis; (b) side-on orientation II, H–H bond bisecting the right angle between the O–Cu–O axes; (c) end-on orientation for H2 and CO. Single point calculations were employed to obtain a potential energy surface for H2 and CO with Cu atoms; all geometries were finally optimized. The resulting binding energies as a function of the distance were calculated and .the results show that the separation of the binary gas mixture of H2/CO is possible

کلمات کلیدی: