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Understanding the mechanism of hydrogen adsorption into metal organic frameworks

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Abstract

Hydrogen adsorption mechanism into MOF-5, a porous metal-organic framework (MOF) has been studied by density functional theory calculation. The selected functionals for the prediction of interaction energies between hydrogen and potential adsorption sites of MOF-5 were utilized after the evaluation with the various functionals for interaction energy of $H_2\cdots C_6H_6$ model system. The adsorption energy of hydrogen molecule into MOF-5 was investigated with the consideration of the favorable adsorption sites and the orientations. We also calculated the second favorable adsorption sites by geometry optimization using every combination of two first adsorbed hydrogen molecules. Based on the calculation of the first and the second adsorption sites and energies, it has been suggested that the hydrogen adsorption into MOF-5 follows a cooperative mechanism in which the metal sites initiate the propagation of the hydrogen adsorption on the whole frameworks. In addition, the interaction mode between the simple benzene ring with hydrogen is significantly changed when the benzene ring has been incorporated into the framework of MOF-5.

Keywords: Metal-organic frameworks; MOFs; Hydrogen adsorption; Density functional theory

1. Introduction

Microporous metal-organic frameworks (MOFs) are crystalline compounds formed through the self-assembly of metal-ions or metal-clusters and various bridging organic ligands [1]. Yaghi et al. claimed that a series of isoreticular MOFs (IRMOFs) having zinc oxo acetate clusters and aromatic organic linkers could uptake hydrogen significantly at both low and room temperature [2]. They showed also that Zn ions were the primary adsorption sites and organic linkers also could contribute to the additional hydrogen adsorption, which was supported by inelastic neutron scattering experiments. Since then various MOFs have been investigated and their design strategies have been suggested toward promising hydrogen storage materials to meet the economic capabilities in the DOE standards [3]. However, the key structural features of MOFs to enhance adsorption amount of hydrogen are not found until now except that the presence of the aromatic rings of the organic linkers is seemingly favorable [4–11]. Consequently, the understanding of the mechanism of hydrogen adsorption into MOFs including interactions between adsorbed hydrogen molecules is highly required.

Previous theoretical works have been directed at investigating adsorption energy of hydrogen into the host frameworks. For example, Okamoto et al. found the non-repulsive intermolecular distance between two hydrogen molecules and showed the way of adsorption energy estimation using the vertical orientation of hydrogen molecule on graphene plane based on the Møller-Plesset (MP2) methodology [12]. But in this work the binding energy for hydrogen adsorption was overestimated as it was not calibrated by basis set superposition error (BSSE) correction. Later, Hübner et al. considered the BSSE correction for the adsorption energy of hydrogen on benzene with the calibrated value of −0.93 kcal/mol [13]. Furthermore they investigated the influence of the functional groups of benzene ring on hydrogen adsorption by setting up a

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model system of lithium terephthalates. However, this approach to mimic the environment of MOFs seems to be insufficient to investigate fully the geometric and electronic perturbation of MOFs for hydrogen adsorption. Recently, Ceder et al. reported elegant results on the hydrogen adsorption into MOFs by density functional theory (DFT) calculation [14]. They investigated adsorption sites of hydrogen on MOF-5 and found the stability of adsorption depends on the adsorption sites, but did not consider the functional dependency and the interaction between adsorbed hydrogen molecules.

The inelastic neutron scattering (INS) method has been used to characterize the adsorption of inert gases [15] or hydrogen [16] on MOFs. For the considered adsorbates, the observed adsorption sites were similar to each other, and the relative binding strength was measured.

We carried out DFT calculations on the system consisting of hydrogen molecules and benzene or MOF-5 as the adsorbents. The functional dependency and the interaction between adsorbed hydrogen molecules were also considered in our calculation. The main aims of this study are as follows. (1) The screening of the appropriate functionals and their validation to study the adsorption of hydrogen into MOF-5. (2) Characterization of hydrogen binding sites in MOF-5. (3) Comparison of hydrogen adsorption on benzene with that on MOF-5. (4) Understanding hydrogen adsorption mechanism into MOFs including interaction between adsorbed hydrogen molecules.

2. Methods

Our calculation of hydrogen adsorption into MOFs was focused on MOF-5, one of the most widely studied MOFs with relatively simple structures. In order to investigate the hydrogen adsorption into MOF-5 using DFT calculation, we considered three computational aspects carefully. First, the adequate functionals should be selected to represent the interaction between the adsorbate and adsorbent properly. Second, the model structure mimicking the real adsorption system should be constructed effectively and adequately. Finally, the pair of the first and the second hydrogen molecules adsorbed should be allocated and optimized systematically on the MOF-5 framework surface.

All of the theoretical calculations were performed by DMol^3 program in the MS Modeling 3.1^{TM} package [17], which is the quantum mechanical code using density functional theory (DFT). The double numeric polarization basis set [18] was used and any pseudopotential representation for the special treatment of core electrons was not used in our calculations.

2.1. Choice of adequate functional for hydrogen

To determine the adequate functionals and to validate their reliability, eight kinds of generalized gradient approximation (GGA) level density functionals (BP, BOP, BLYP, PBE, RPBE, VWN-BP, PW91 and HCTH [19–26]) were examined by calculating the interaction energy between hydrogen and benzene molecules. After comparison of our results with the data from MP2 level calculation on the interaction of hydrogen with benzene [27], the three functionals (HCTH, PW91 and PBE) were chosen and utilized for the investigation on the adsorption of hydrogen molecules into MOF-5.

2.2. Model buildup for hydrogen adsorption

The unit cell of MOF-5 (Fig. 1A) contains eight $Zn_4O(BDC)_3$ (BDC = benzenedicarboxylate) formula units which is too large for the calculation of every possible configuration of the first and second adsorbed hydrogen pairs. To save computation time we constructed the simplified cluster model (Fig. 1B), which is a side of the crystal structure of MOF-5 with 10 BDCs replaced by acetate groups, $(CH_3COO)_5Zn_4O(BDC)Zn_4O(CH_3COO)_5$. Our approach to construct the model is similar with the previous work [28], but our model could present a seamless representation including metal center and organic linker for tracing all of the possible adsorption positions using single model structure. All possible adsorption sites in our model were classified as metal site, carboxylato site and ring site as shown in Fig. 1B.

2.3. Assessment of first adsorption energy for hydrogen

The initial configuration was constructed using one randomly oriented hydrogen molecule. The number of the initial structure was more than 10 independent hydrogen-MOF-5 complexes per each site (metal site, carboxylato site and ring site). Local density approximation (LDA) level functional was adopted for the initial optimization of geometry to reduce the computational cost. When the duplicated configurations and the unstable binding ones were found, they were excluded for further calculation. These processes resulted in 14 distinct and stable structures that were regarded

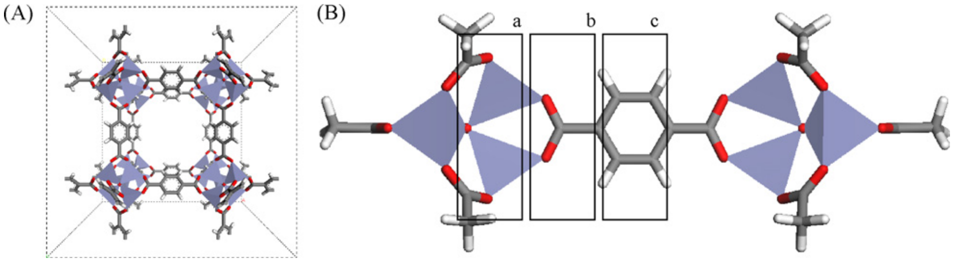

Fig. 1. The structures for MOF-5. (A) The unit cell of MOF-5 which consists of metal-clusters and organic linkers is represented as eight Zn_4OL_3 (L = organic linker) formula units. (B) Adsorption positions are classified into three positions: (a) metal site, (b) carboxylato site and (c) ring site.

as the final configurations, and fully optimized using GGA level using three functionals (HCTH, PW91 and PBE) to determine the interaction energy.

2.4. Assessment of two hydrogen adsorption

The model complexes, MOF-5 and every combination of the first adsorbed two hydrogen molecules were chosen as the initial structures for the investigation of second adsorption processes. It was also considered that the second hydrogen can be adsorbed on the same or opposite direction with respect to the benzene plane. For example, when a hydrogen molecule is already above the benzene ring site, the second can approach to the carboxylato site from the upper or below the benzene ring site. The number of complexes was reduced to 105 after excluding redundant or unreasonable pairs by considering both the symmetry of the model complexes and a hydrogen–hydrogen non-repulsive distance, 3.4 Å [12].

3. Results and discussions

3.1. The screening and validation of functionals for hydrogen adsorption

Using previously mentioned eight functionals the respective potential energy surface of the $H_2\cdots C_6H_6$ complex was monitored for various orientations of hydrogen, and the resulting potential curves are represented in Fig. 2B. We could classify the functionals into two classes from the viewpoint of the energetics (Fig. 2B). RPBE, HCTH, PW91 and PBE functionals had a shallow but clear energy minimum and were found to be adequate for the study of hydrogen adsorption, while BP, BOP, BLYP, and VWN-BP functionals showed just repulsive or very weak interaction energy between hydrogen molecule and benzene, which deviates seriously from the previous results based on MP2 level calculations [12,13,27]. The equilibrium distances between the center of hydrogen molecule and the center of benzene for hydrogen's vertical approach as depicted in Fig. 2A were 3.54 Å (HCTH), 3.32 Å (PW91), and 3.34 Å (PBE), respectively. These values reasonably coincided with the previous MP2 studies [12,13,27]. In case of RPBE functional, the potential energy surface seemed to be reasonable, but the equilibrium distance, 3.88 Å, was too large. Finally, the three DFT functionals, HCTH, PW91 and PBE were regarded adequate with quantitative precision for the investigation of weak interaction between hydrogen and benzene or benzene-like adsorbent. This screening result is thought to be reasonable because the previous works using the PBE and PW91 functionals turned out to be appropriate in estimating the weak interaction energy by DFT calculation [29,30].

We also investigated the changes in the interaction energy according to the direction of *attack* and the orientation of the hydrogen molecule (Table 1). All the functionals showed the same trend that the interaction energy increases in the order of side, edge, and face approaches to the benzene ring. Among the various directions of *attack* and orientations of the hydrogen molecule studied, the vertical *attack* was most favorable. Again, these results of DFT calculation are well agreed with the previous MP2 level study [13].

3.2. The 1st hydrogen adsorption sites and their binding energy

After the LDA level optimization of initial configurations of the MOF-5 model structure with a single hydrogen molecule, we obtained the final geometries and their binding energies using three functionals (HCTH, PW91 and PBE) at GGA level

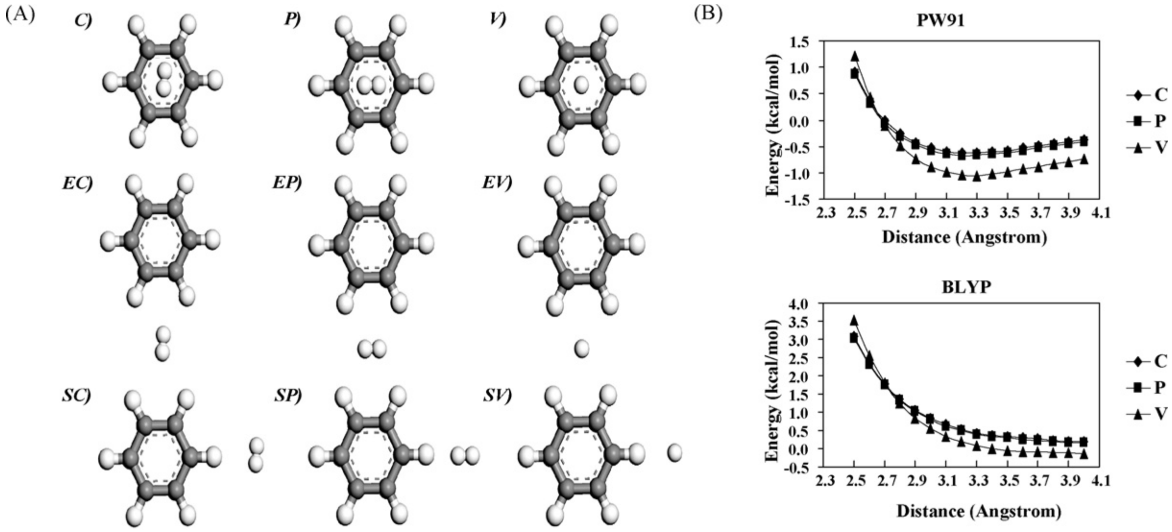

Fig. 2. Classified adsorption sites and potential energy surface scanning for various $H_2\cdots C_6H_6$ models. (A) The adsorption sites and orientations of hydrogen on benzene were classified as follows: C) cross attack on benzene, P) parallel attack on benzene, V) vertical attack on benzene, EC) cross attack at the edge of benzene, EP) parallel attack at the edge of benzene, EV) vertical attack at the edge of benzene, SC) cross attack at hydrogen side of benzene edge, SP) parallel attack at hydrogen side of benzene edge, SV) vertical attack at hydrogen side of benzene edge. (B) Potential energy surface scanning of hydrogen on benzene ring for PW91 and BLYP functional, representative results for each case of adequate and inadequate series of functionals.

Table 1
The hydrogen binding energies on benzene according to the functionals

Orientation[a]	HCTH (kcal/mol)	PW91 (kcal/mol)	PBE (kcal/mol)
Benzene_C	−0.70	−0.59	−0.37
Benzene_P	−0.70	−0.60	−0.37
Benzene_V	−0.95	−0.90	−0.68
Benzene_EC	−0.79	−0.50	−0.30
Benzene_EP	−0.79	−0.48	−0.28
Benzene_EV	−0.89	−0.61	−0.40
Benzene_SC	−0.57	−0.34	−0.17
Benzene_SP	−0.48	−0.29	−0.13
Benzene_SV	−0.60	−0.43	−0.28

[a] The orientation was represented in Fig. 2A.

Table 2
The first adsorption energy as a function of adsorption site in modeled MOF-5

Adsorption Site[a]		E_1 (kcal/mol)		
Position	Orientation	HCTH	PW91	PBE
Metal site	P	−1.08	−1.02	−0.67
	V	−0.72	−0.76	−0.48
	SC	−0.60	−0.80	−0.31
	SP	−0.64	−0.69	−0.37
	SV	−0.70	−0.73	−0.36
Carboxylato site	C	−0.45	−0.69	−0.37
	O	−0.84	−1.00	−0.66
	P	−0.27	−0.59	−0.31
Ring site	C	−0.19	−0.59	−0.15
	P	−0.60	−0.40	−0.29
	V	−0.27	−0.37	−0.35
	EC	−0.21	−0.38	−0.34
	EP	−0.35	−0.53	−0.30
	EV	−0.33	−0.55	−0.41

[a] Adsorption sites were named by the position in MOF-5 and orientation of hydrogen molecules as shown in Fig. 3.

(Fig. 3). We found that the adsorption at metal sites was generally stronger than at carboxylato or ring sites regardless of functional types (Table 2).

It is remarkable that the adsorption on the edge of the benzene in MOF-5 was significantly stronger than the adsorption on the edge of isolated benzene; though it is generally expected that vertical *attack* onto an isolated benzene molecule is more favorable than vertical *attack* at the edge, the approach of hydrogen molecule to the edge of the benzene in MOF-5 is more favorable (Table 1). This difference might be due to the change of electronic environment from isolated benzene to benzene in MOF-5, more specifically phenylene of the terephthalate. Ceder et al. warned problems of using models with only organic-linkers to predict the power of hydrogen storage because the change in charge distribution caused by Zn_4O cluster might be critical to the adsorption capabilities of organic linkers. To avoid this problem, we included two Zn_4O clusters in our model and obtained fairly different results from Ceder's organic-linker-only model [14]. We believe that the charge redistribution caused by Zn_4O cluster was fully considered during the study of hydrogen adsorption using our model. Because our cluster model was constructed using the side of IRMOF, one of the adsorption sites near the metal cluster named III in Ceder et al.'s was missed. We found, however, another asymmetric adsorption position, carboxylato *O*, residing between the Zn_4O cluster and organic linker [14]. This theoretical prediction of adsorption position close to the organic linker can be supported by the recent cryogenic X-ray experiments on MOF-5 using Ar or N_2 as probe gases [15]. Both our prediction and the X-ray analyses indicate that the edge site can be one of the favorable adsorption sites and substitution of the terephthalate linkers with other aromatic groups may be a useful way to increase hydrogen adsorption.

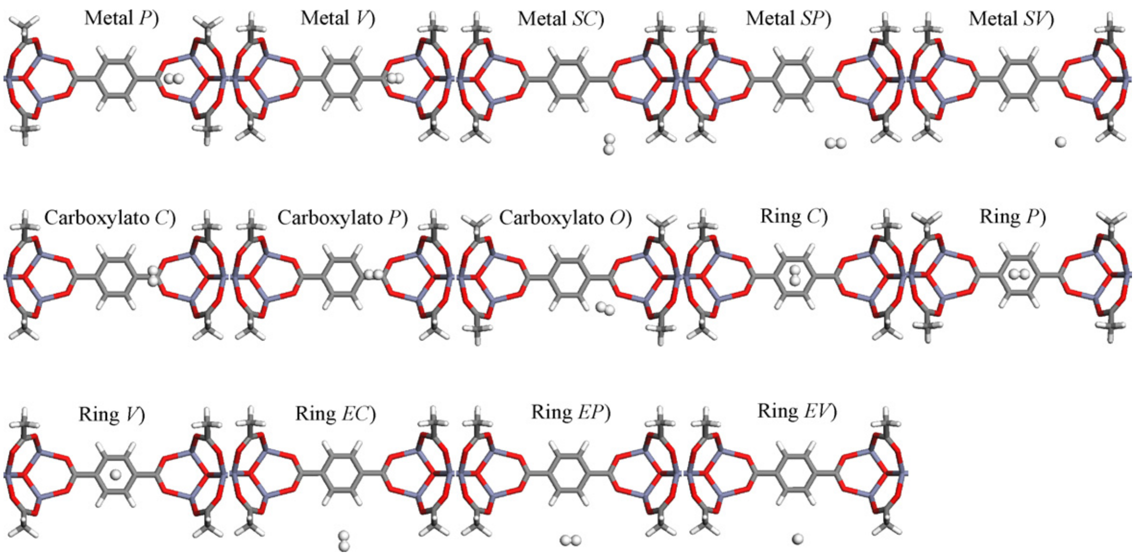

Fig. 3. First hydrogen adsorption sites on MOF-5. Notation is the combination of the position in Figs. 1B and 2A except O), "O)" means parallel attack to the framework geometry but oblique orientation.

Table 3
The binding energies and its pairing energies of two hydrogen molecules into MOF-5[a]

Position1	Position 2	Number of pairing[b]	HCTH(kcal/mol)		PW91(kcal/mol)		PBE(kcal/mol)	
			E_{12}	E_{pairing}	E_{12}	E_{pairing}	E_{12}	E_{pairing}
Metal	Metal	15	−2.64	−0.57	−2.07	−0.26	−1.18	−0.39
			−2.01	−0.51	−1.68	−0.08	−0.96	−0.08
			−1.70	−0.38	−1.45	0.02	−0.77	0.11
Metal	Carboxylato	15	−2.61	−1.44	−1.99	−0.23	−1.26	−0.25
			−2.01	−0.74	−1.63	−0.06	−0.92	−0.04
			−1.38	−0.42	−1.33	0.03	−0.70	0.07
Metal	Ring	36	−2.04	−1.13	−1.83	−0.45	−1.13	−0.26
			−1.58	−0.48	−1.43	−0.14	−0.80	−0.04
			−1.23	−0.01	−1.18	−0.01	−0.54	0.11
Carboxylato	Carboxylato	6	−2.68	−1.96	−2.10	−0.10	−1.30	−0.10
			−2.08	−1.04	−1.57	−0.05	−0.90	−0.01
			−1.04	−0.50	−1.18	0.00	−0.61	0.03
Carboxylato	Ring	18	−1.87	−1.21	−1.73	−0.36	−1.10	−0.10
			−1.38	−0.53	−1.34	−0.11	−0.78	−0.03
			−0.89	−0.02	−1.00	−0.02	−0.48	0.04
Ring	Ring	15	−1.48	−0.53	−1.37	−0.62	−0.88	−0.35
			−1.05	−0.37	−1.15	−0.22	−0.69	−0.04
			−0.73	0.47	−0.95	−0.02	−0.52	0.08

[a] The positive values in pairing energy mean destabilization while the negative values mean stabilization. The energies in each combination are narrated by order of minimum, average, and maximum values.

[b] The coupling of hydrogen is constructed by inter-horizontal and intra-horizontal configurations of MOF-5 cluster model as described in Fig. 4.

3.3. Two hydrogen adsorption energy and synergy effect

In order to investigate the cooperative adsorption process of two hydrogen molecules, we defined paring energy, E_{pairing} as:

$$E_{\text{pairing}} = E_{ij} - (E_i + E_j) \tag{1}$$

where E_i is the adsorption energy of a single hydrogen molecule on site i and E_{ij} is the adsorption energy of two hydrogen molecules on both sites i and j at the same time.

In this DFT study, we tried to find how the adsorbed hydrogen molecules interact with each other during the adsorption process. The goal of this study was to find any interaction energy difference between the individual hydrogen adsorption and the simultaneous adsorption of two hydrogen molecules. Furthermore we wanted to expand this process to the multi-hydrogen adsorption processes.

Most pairing energies calculated from Eq. (1) (Table 3) had large negative values, indicating that the adsorption of multiple hydrogen molecules is favorable as previously suggested by MP2 level study [31]. A negative value of E_{pairing} means that the simultaneous adsorption of two hydrogen molecules is more favorable than individual adsorption of two hydrogen molecules, that is, the first adsorbed hydrogen molecule helps the second hydrogen to be adsorbed more easily. We also found that this *synergy effect* depends on the adsorption position; pairs of hydrogen molecules with at least one molecule adsorbed on the metal site always have more negative pairing energies than the pairs with no molecule on the metal sites. Because the metal site had the largest adsorption energy in the first hydrogen adsorption process, the first hydrogen molecule adsorbed on the metal site might initiate the hydrogen adsorption across the whole frameworks.

In terms of functional dependency, HCTH functional was somewhat different from PW91 and PBE functionals. While HTCH gave the similar energy values of the first hydrogen adsorption all three functionals, HCTH functional overestimated the weak binding energy during the pairing energy

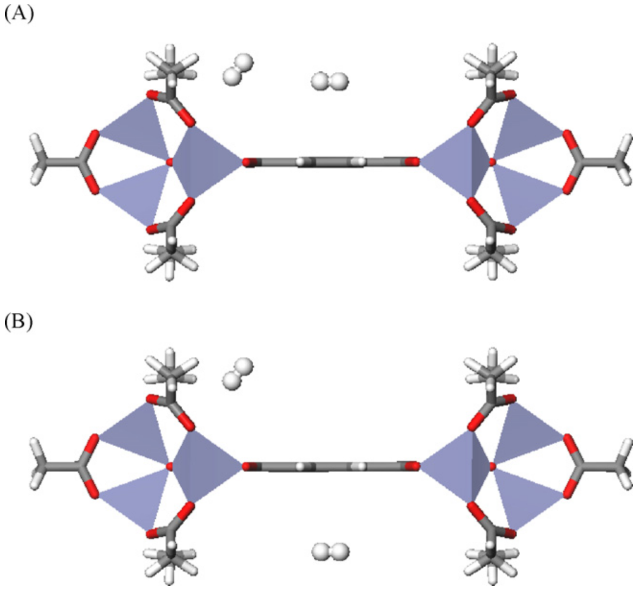

Fig. 4. Adsorption models with two hydrogen molecules on Metal V and Ring P sites (A) the intra-horizontal configuration, (B) the inter-horizontal configuration.

calculation. However, PW91 and PBE resulted in consistent data for both adsorption and pairing energy. Therefore, among the various functionals studied, PW91 and PBE are the most appropriate functionals for weakly binding systems.

We also investigated the strength of the *synergy effect* for the two specific cases, where two hydrogen molecules are in the intra- or inter-horizontal combination around *metal V* and *ring P* (Fig. 4). The pairing energy of the intra-horizontal combination was −0.35 kcal/mol in PW91 or −0.08 kcal/mol in PBE while the pairing energy of the inter-horizontal combination was −0.11 kcal/mol in PW91 or 0.05 kcal/mol in PBE. These results indicate that a pair of hydrogen molecules located within the non-repulsive distance prefers the intra-horizontal combination to the inter-horizontal combination, although the energy difference between the two configurations is not large. Similar trends were found for other intra- and inter-horizontal combinations (data not shown).

4. Conclusions

Through this modeling study on MOF-5, three important results have been obtained. First, the hydrogen adsorption occurs via a cooperative mechanism in which the adsorptions on metal sites initiate the propagation of the adsorption across the whole frameworks. Although it has not yet been determined whether the *synergy effect* is meaningful at finite temperature, the cooperative mechanism of inter-hydrogen interaction may affect the adsorption phenomena. On the basis of the *ab initio* molecular dynamics calculations, Ceder et al. suggested the possibility of hydrogen cloud formation at the center of MOF pores, which could be considered as one of the cooperative processes induced by the intermolecular interaction of hydrogen molecules [14]. Consequently, further studies about the dynamic nature of hydrogen using a MOF model with increased number of hydrogen molecules are required to investigate hydrogen adsorption phenomena of MOFs at finite temperature. Second, the interaction modes between the benzene ring and the hydrogen molecules change significantly when the benzene ring has been incorporated into the framework of MOFs. Finally, modification at the edge of the aromatic linkers is one of the possible ways to enhance the hydrogen adsorption capacity of MOFs and this attempt was verified by recent experimental and theoretical studies [13,31,32].

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