Binding energy of H$_2$ to MOF-5: A Model Study

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Using models simulating the environment of two distinct adsorption sites of H$_2$ in metal-organic framework-5 (MOF-5), binding energies of H$_2$ to MOF-5 were evaluated at the MP2 and CCSD(T) level. For organic linker section modeled as dilithium 1,4-benzenedicarboxylate (C$_6$H$_4$(COO)$_2$Li$_2$), the MP2 and CCSD(T) basis set limit binding energies are estimated to be 5.1 and 4.4 kJ/mol, respectively. For metal oxide cluster section modeled as Zn$_2$O(CO$_2$)$_6$, while the MP2 basis set limit binding energy estimate amounts to 5.4 kJ/mol, CCSD(T) correction to the MP2 results is shown to be insignificant with basis sets of small size. Substitution of benzene ring with pyrazine ring in the model for the organic linker section in MOF-5 is shown to decrease the H$_2$ binding energy noticeably at both the MP2 and CCSD(T) level, in contrast to the previous study based on DFT calculation results which manifested substantial increase of H$_2$ binding energies upon substitution of benzene ring with pyrazine ring in the similar model.

**Key Words:** MOF-5, Hydrogen adsorption, H$_2$, Binding energy

**Introduction**

Since its first synthesis by Yaghi and coworkers,$^1$ metal-organic framework MOF-5 has drawn a great deal of interests from academic and industrial communities due to its extraordinary storage capacity of hydrogen, becoming one of major candidates for future fuel carrier material. As a result, there have been numerous theoretical and experimental studies to understand the interactions between hydrogen molecules and MOF-5 and improve the storage capacity of IRMOF (isoreticular metal organic framework) class of molecules, especially in high temperature conditions.$^2$-27 For MOF-5, it has been known from previous studies$^8$-12,24$^b$ that there are two distinct hydrogen adsorption sites, metal (zinc) oxide cluster section and organic BDC (1,4-benzene dicarboxylate) linker section. albeit there are several different adsorption sites in metal (zinc) oxide cluster section (see Fig. 1). Since the interactions between hydrogen molecules and relevant adsorption sites in MOF-5 are mainly weak dispersion interactions, an accurate determination of H$_2$ binding energy to MOF-5 is a formidable task considering the size of the molecular system involved. Consequently, previous theoretical studies of hydrogen adsorption in MOF-5 often employed DFT (density functional theory) methods$^1,2,15,22,24$ or MP2 (second order Møller-Plesset perturbation theory) method.$^{4,6,11,26}$ However, even the use of MP2 method would not be sufficient to describe the weak dispersion interaction and high level correlation method would be required to accurately determine the binding energy of H$_2$ to relevant adsorption sites in MOF-5.

In a series of papers,$^4,6$ Ganz and coworkers performed a computational study of H$_2$ adsorption on MOF-5 and similar IRMOF molecules. Based on models representing the major adsorption sites cut from the entire MOF-5 framework, they found that the H$_2$ binding energy of the zinc oxide cluster section in MOF-5 could be stronger than the organic linker section by about 1.5 kJ/mol at the MP2 level. More recently, Sillar et al.$^{26}$ using more sophisticated models for H$_2$ adsorption sites in MOF-5, reported that the difference between the binding energies of metal oxide cluster section and organic linker section could be larger, being about 2.9 kJ/mol at the MP2 level. The major difference between the former and latter models is that the latter models by Sillar et al. employed end groups which simulates the actual enviroment of MOF-5 more closely in their models for H$_2$ adsorption sites in MOF-5. However, considering weak nature of interactions between a hydrogen molecule and MOF-5, it would be necessary to employ a more sophisticated electron correlation method beyond MP2 method to determine the H$_2$ binding energy to MOF-5 accurately. Accurate determination of H$_2$ binding energies to relevant sites in MOF-5 is important to understand the thermo-chemical properties and isotherm behavior of H$_2$ adsorption on MOF-5. Employment of high level electron correlation method with appropriate basis set is also important to correctly evaluate the effect of substituting the metal atoms

![Figure 1. Metal oxide cluster (Zn$_2$O(CO$_2$)$_6$) and organic linker (C$_6$H$_4$) sections in MOF-5. Metal oxide cluster sections are linked by organic linker in three dimensions to form an entire framework of MOF-5.](http://dx.doi.org/10.5012/bkcs.2011.32.12.4199)
or linker molecule to improve the $H_2$ adsorption capacity of MOF-5. As an example, it will be shown from our high level electron correlation study results that substitution of benzene ring by pyrazine in the organic linker section of MOF-5 appears to decrease the binding energy of $H_2$ to the linker section of metal-organic framework, in contrast to the results from previous DFT study on similar systems with different metals. The aim of this paper is to account the results from previous DFT study on similar systems with the linker section of metal-organic framework, in contrast to the metal-organic framework environment of organic linker section in MOF-5 but of smaller size. It has been suggested that the ratio ($\beta$) between the MP2 correlation binding energy contribution and CCSD(T) correlation contribution beyond the MP2 level ($\Delta C(T)$) converges rather fast with basis set, enabling the prediction of this ratio value at the basis set limit from the results with limited basis sets. Therefore, if it could be assumed that these ratios for reference (smaller) model system and MOF-5 local adsorption site environment are similar for $H_2$ interaction, one would be able to predict the accurate $H_2$ binding energies to MOF-5 local environment using the ratio $\beta$ obtained for smaller model system than actual MOF-5 system interacting with a hydrogen molecule. The $H_2$ binding energy to MOF-5 is obtained according to the following equation.

$$\Delta E_{CCSD(T)}^{\text{TOT}}(\infty) = \Delta E_{MP2}^{\text{TOT}}(\infty) + \beta_{\text{ref}} \Delta E_{MP2}^{\text{CORR}}(\infty)$$

where $\infty$ represents the basis set limit and $\beta_{\text{ref}}$ implies that $\beta$ value for smaller reference system is to be used in the equation. For $H_2$ binding to organic linker section in MOF-5, $H_2$-benzene system and $H_2$-BDCLi$_2$ (dilithium 1,4-benzenedicarboxylate) were chosen as the reference model (where $\beta$ is calculated) and actual model system representing the environment of organic linker section in MOF-5. (where $\Delta E_{MP2}^{\text{TOT}}(\infty)$ and $\Delta E_{MP2}^{\text{CORR}}(\infty)$ are calculated) were chosen, respectively. The $H_2$-BDCLi$_2$ system was also adopted as a model for $H_2$ interaction with the organic linker section in MOF-5 in ref. 4.

For $H_2$ binding to zinc oxide cluster section in MOF-5, however, it was difficult to choose a simpler reference model system. Therefore, in this case, only MP2 basis set limit binding energy for $H_2$-Zn$_6$(CO$_3$H)$_6$, which was also a chosen model for $H_2$ interaction with metal oxide cluster section in MOF-5 in ref. 4 and 26, was estimated and CCSD(T) correlation effect beyond the MP2 level was evaluated using the results with the 6-31G and 6-31G* basis set. $\Delta E_{MP2}^{\text{CORR}}(\infty)$ for $H_2$-BDCLi$_2$ and $H_2$-Zn$_6$(CO$_3$H)$_6$ were estimated from extrapolation of the results with aug-cc-pVXZ (X=D,T) or aug-cc-pVXZ basis sets which contained diffuse functions on selected atoms in addition to the cc-pVXZ basis sets.

Only valence electrons were correlated in the correlation calculations. All binding energies were computed with the counterpoise correction using Gaussian program package.

**Results and Discussion**

In Table 1 the ratio for $H_2$-benzene system is presented along with the corresponding results for $H_2$-BDCLi$_2$ system as well as $H_2$ binding energy estimates at the MP2 level for two systems. The geometry of $H_2$ was optimized at the MP2/6-31++G* level with the fixed BDCLi$_2$ geometry which was obtained from the optimization at the MP2/6-31G* level. In Figure 2 a schematic view of the optimized BDCLi$_2$-$H_2$ system is presented. $H_2$ is almost perpendicular to the benzene plane with the distance of about 2.9 Å between the ring center and the H atom closer to the benzene ring. Therefore, for $H_2$-benzene interaction, the hydrogen molecule was placed perpendicular to benzene ring with a distance of 2.9 Å between the ring center and the H atom closer to the benzene ring. Therefore, for $H_2$-benzene interaction, the hydrogen molecule was placed perpendicular to benzene ring with a distance of 2.9 Å between the ring center and the H atom closer to the benzene ring.
benzene ring. For the benzene-H$_2$ system, the basis set limit MP2 binding energy was obtained from separate extrapolations of Hartree-Fock and correlation contributions with the aug-cc-pVDZ and aug-cc-pVTZ basis sets (which were similar to the aug-cc-pVXZ basis set but did not contain diffuse functions for O and Li atoms in the system) by $X^{-3.4}$ and $(X+1)^{-3}$ ($X=D(2),T(3)$) formulas, respectively.

Similarly, the MP2 basis set limit binding energy for the BDCLi$_2$-H$_2$ system was obtained from extrapolations of HF and correlation contributions with the aug-cc-pVDZ and aug-cc-pVTZ basis sets (see the text). From the binding energy results in eq. (3), it is clear that employment of higher level electron correlation method beyond the HF and even the MP2 level along with proper basis sets is important for correct description of the interaction between a hydrogen molecule and BDCLi$_2$ (as well as benzene) as the HF and MP2 level binding energies are not close to the corresponding CCSD(T) level binding energies. Considering the major contribution to the interaction energies at the HF level would be electrostatic, the negative binding energy at the HF limit well manifests the failure of the electrostatic description of such molecular systems.

Although CCSD(T) calculations for BDCLi$_2$-H$_2$ system could be performed only with the aug-cc-pVDZ basis set and aug-cc-pVQZ basis set, the agreement of $\beta$ values for both basis sets appears to suggest that $\beta$ value of $-0.11$ with these basis sets is close to the converged value for BDCLi$_2$-H$_2$ system. Since the converged $\beta$ value for benzene-H$_2$ system also appears to be close to $-0.11$, $\beta$ value at the basis set limit for H$_2$-benzene system could be used to derive the CCSD(T) basis set limit binding energy of the BDCLi$_2$-H$_2$ system according to eq. (3). If one adopts $\beta$ value of $-0.11$ for the estimation of the BDCLi$_2$-H$_2$ basis set limit binding energy at the CCSD(T) level, application of eq. (3) yields 4.41 kJ/mol of the basis set limit CCSD(T) binding energy for the H$_2$-BDCLi$_2$ system. Alternatively, one may add the AC(T) value of $-0.63$ kJ/mol with the aug-cc-pVDZ basis set to the MP2 basis set limit result of 5.10 kJ/mol, which yields 4.47 kJ/mol for the CCSD(T) basis set limit binding energy for the BDCLi$_2$-H$_2$ interaction. Since AC(T) appears to increase with basis set (in magnitude), this value could be considered as the upper limit and we conclude that the binding energy of a hydrogen molecule to the BDCLi$_2$ would be very close to 4.4 kJ/mol, and, accordingly, hydrogen binding energy to organic linker section in MOF-5 would be close to 4.4 kJ/mol, considering the recent finding that the interaction of H$_2$ with relevant adsorption site is dominated by the local environment around the adsorption site in MOF-5.\(^{20}\)

It was suggested from DFT study\(^{15}\) that presence of nitrogen in the benzene ring would substantially increase the binding energy of H$_2$ to organic linker section. To investigate the effect of presence of the nitrogen atom in the benzene ring, pyrazine was introduced in BDCLi$_2$, thus forming PDCLi$_2$ (dilithium 1,4-pyrazinedicarboxylate, C$_2$N$_2$H$_2$(CO$_2$)$_2$Li$_2$) for interaction with H$_2$. As in the H$_2$-BDCLi$_2$ system, H$_2$ geometry in H$_2$-PDCLi$_2$ system was optimized at the MP2/6-31+G* level with the fixed PDCLi$_2$ geometry which corresponded to the MP2/6-31G* optimized geometry. The binding energy of H$_2$ to PDCLi$_2$ was calculated at the MP2 and CCSD(T) level with the aug-cc-pVDZ basis set, which yielded 3.19 and 2.67 kJ/mol, respectively. These results are smaller than the corresponding H$_2$ binding energies to BDCLi$_2$, by 0.63 and 1.12 kJ/mol, respectively (see Table 1), suggesting presence of nitrogen would decrease H$_2$ binding to the organic linker section in MOF-5. It is interesting to note that the difference between the H$_2$ binding energies to BDCLi$_2$ and PDCLi$_2$ is more prominent at the CCSD(T) level. Although previous DFT study explored different metals M other than Li in PDCM\(^{20}\), it appears from our high level correlation results that presence of nitrogen would not enhance H$_2$ binding to the organic linker section in MOF-5.

In Table 2 binding energies of H$_2$ to Zn$_3$O(HCO$_3$)$_2$ at the MP2 level are presented, which represents a model for metal oxide cluster section in MOF-5. The binding energy was

### Table 1. Total and correlation (in parentheses) binding energies (in kJ/mol) of H$_2$ to benzene and BDCLi$_2$

<table>
<thead>
<tr>
<th>Basis set</th>
<th>HF</th>
<th>MP2</th>
<th>CCSD(T)</th>
<th>β$^a$</th>
<th>HF</th>
<th>MP2</th>
<th>CCSD(T)</th>
<th>β$^a$</th>
</tr>
</thead>
<tbody>
<tr>
<td>6-31G*</td>
<td>-1.25</td>
<td>0.38(1.63)</td>
<td>-0.10(1.15)</td>
<td>-0.29</td>
<td>-1.52</td>
<td>0.62(2.14)</td>
<td>0.08(1.60)</td>
<td>-0.25</td>
</tr>
<tr>
<td>aug-cc-pVDZ</td>
<td>-0.82</td>
<td>4.01(4.83)</td>
<td>3.45(4.27)</td>
<td>-0.12</td>
<td>-1.05</td>
<td>4.42(5.47)</td>
<td>3.79(4.84)</td>
<td>-0.11(-0.11$^b$)</td>
</tr>
<tr>
<td>aug-cc-pVTZ</td>
<td>-0.91</td>
<td>4.45(5.36)</td>
<td>3.54(4.45)</td>
<td>-0.11</td>
<td>-1.17</td>
<td>4.79(5.96)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>CBS$^c$</td>
<td>-0.94$^d$</td>
<td>4.81(5.75)$^f$</td>
<td>4.18$^g$</td>
<td>-1.21$^f$</td>
<td>5.10(6.31)$^f$</td>
<td>4.41$^g$</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

$^a$ is the ratio between ΔC(T) and Δ$L_{MP2}$ defined in eq. (2). $^b$Value in parentheses corresponds to β value with aug'-cc-pVDZ basis set (see the text). $^c$For H$_2$-BDCLi$_2$, diffuse functions for Li and oxygen were not included in the calculations. $^d$Basis set limit estimates. $^e$Basis set limit was not obtained from extrapolation of aug'-cc-pVDZ and aug'-cc-pVTZ results (see the text). $^f$Basis set limit was obtained according to eq. 3 (see the text).

![Figure 2. A schematic view of an adsorbed H$_2$ on BDCLi$_2$ (dilithium 1,4-benzenedicarboxylate). Two lithium atoms are placed at each side of the molecule.](image-url)
from the experimental value by more than 4 compared to the experimental results for pure MOF-5 with Table 3 bond lengths and angles for the model systems are corresponding HF and correlation contributions with the aug binding energies were estimated by extrapolating the correlation contributions to the binding energy. Basis set limit estimates. Basis set limit was obtained from extrapolation of the aug-cc-pVDZ and aug-cc-pVTZ results by (X=D(2),T(3)) (see the text). Basis set limit was obtained from extrapolation of the aug-cc-pVDZ and aug-cc-pVTZ results by (X+1) \(X=2\) (for DZ, 3 for TZ) (see the text) computed at the MP2/6-31G\(^*\) optimized geometry of H\(_2\)-Zn\(_{n}\)O(HCO\(_2\))\(_{5}\) system, which is depicted in Figure 3. In Table 3 bond lengths and angles for the model systems are compared to the experimental results for pure MOF-5 with the corresponding bond lengths and angles shown in Figure 4. Although the angle between O(10)-C(1)-O(10) is different from the experimental value by more than 4° (4.6°) in case of BDC Li\(_2\) where Li replaced the metal cluster section in MOF-5, other geometrical parameter values for the model systems appear to be in good agreement with the experimental values, exhibiting the similarity of the model systems to the local environments of the MOF-5. The basis set limit Hartree-Fock and MP2 correlation contributions to the binding energies were estimated by extrapolating the corresponding HF and correlation contributions with the aug-cc-pVDZ and aug-cc-pVTZ basis sets by \(X=2\) and \((X+1)^{13}\) formulas (\(X=2\) for DZ, 3 for TZ), respectively. The aug-cc-pVXZ basis sets contain extra diffusion functions for Zn and O atoms in addition to the cc-pVXZ basis sets (\(X=2\) for DZ, 3 for TZ). As in the case of H\(_2\)-BDC Li\(_2\) interaction, the negative binding energies at the HF level well manifest the importance of employing high level correlation method along with proper basis set for this system.

Comparison of the MP2 results in Table 1 and Table 2 shows that H\(_2\) appears to bind more strongly to zinc oxide cluster section than organic linker section in MOF-5 as expected. Since direct calculations at the CCSD(T) level with large basis sets are computationally too demanding for this complex, CCSD(T) correction to the MP2 level result was made only with the 6-31G and 6-31G\(^*\) basis set, which showed only \(-0.1\) kJ/mol change (increase for 6-31G and decrease for 6-31G\(^*\)) of MP2 binding energy at the CCSD(T) level. Recently Sillar \textit{et al.} also reported 0.06 kJ/mol increase of H\(_2\) binding energy to Zn\(_{n}\)O(CO\(_2\))\(_{5}\) from the MP2 to the CCSD(T) level with the cc-pVDZ basis set.\(^{26}\) They also reported that substitution of end hydrogen in Zn\(_{n}\)O(CO\(_2\)H\(_{5}\)) with phenyl (-C\(_6\)H\(_{5}\), Ph) ring increased the H\(_2\) binding energy by about 2 kJ/mol at the MP2 level. This would give the MP2 basis set limit binding energy estimate of more than 7 kJ/mol for H\(_2\)-Zn\(_{n}\)O(CO\(_2\)Ph\(_{5}\)) interaction. Thus, the H\(_2\) binding energy difference between the linker and metal oxide cluster section in MOF-5 appears to be more than 2 kJ/mol at the MP2 level. With regard to accurate evaluation of H\(_2\) binding energy to the metal oxide cluster section in MOF-5, although it cannot be precluded that a large basis set calculation close to the basis set limit at the CCSD(T) level could decrease the corresponding MP2 level H\(_2\) binding energy to Zn\(_{n}\)O(CO\(_2\)H\(_{5}\)) (or Zn\(_{n}\)O(CO\(_2\)Ph\(_{5}\)))

**Table 2.** Binding energies (in kJ/mol) of H\(_2\) to Zn\(_{n}\)O(HCO\(_2\))\(_{5}\) at the HF, MP2 and CCSD(T) level

<table>
<thead>
<tr>
<th>Basis set</th>
<th>HF</th>
<th>MP2</th>
<th>CCSD(T)</th>
</tr>
</thead>
<tbody>
<tr>
<td>6-31G</td>
<td>-2.96</td>
<td>-1.09</td>
<td>-0.96</td>
</tr>
<tr>
<td>6-31G*</td>
<td>-3.10</td>
<td>-0.33</td>
<td>-0.44</td>
</tr>
<tr>
<td>aug-cc-pVDZ*</td>
<td>-2.47</td>
<td>3.42(5.89)*</td>
<td>4.59(7.03)*</td>
</tr>
<tr>
<td>aug-cc-pVTZ*</td>
<td>-2.44</td>
<td>5.43(7.86)*</td>
<td></td>
</tr>
<tr>
<td>CBS estimate*</td>
<td>-2.43*</td>
<td>4.54*</td>
<td></td>
</tr>
</tbody>
</table>

\(^{a}\)cc-pVXZ basis set added by extra diffuse functions for Zn and O atoms from the aug-cc-pVXZ basis sets (\(X=2\),T). \(^{b}\)Values in parentheses represent the correlation contributions to the binding energy. \(^{c}\)Basis set limit estimates. \(^{d}\)Basis set limit was obtained from extrapolation of the aug-cc-pVDZ and aug-cc-pVTZ results by \(X=2\) (DZ, 3 for TZ) (see the text). \(^{e}\)Basis set limit was obtained from extrapolation of the aug-cc-pVDZ and aug-cc-pVTZ results by \((X+1)^{13}\) (X=D(2),T(3)) (see the text).

**Table 3.** Bond length and angle values for model systems

<table>
<thead>
<tr>
<th>Bond lengths (Å)</th>
<th>Bond angles (°)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Zn(23)-O(11)(^{a})</td>
<td>Zn(23)-O(16)(^{a})</td>
</tr>
<tr>
<td>1.96 Å</td>
<td>1.95 Å</td>
</tr>
<tr>
<td>1.27 Å</td>
<td>1.28 Å</td>
</tr>
<tr>
<td>1.49 Å</td>
<td>1.41 Å</td>
</tr>
<tr>
<td>1.40 Å</td>
<td>1.09 Å</td>
</tr>
<tr>
<td>107.3°</td>
<td>111.7°</td>
</tr>
<tr>
<td>107.0°</td>
<td>129.5°</td>
</tr>
<tr>
<td>128.0°</td>
<td>121.8°</td>
</tr>
<tr>
<td>119.1°</td>
<td>116.8°</td>
</tr>
</tbody>
</table>

\(^{a}\)The numbers in parentheses represent the numbers for the corresponding atoms in Fig. 4. \(^{b}\)Ref. 2.

Figure 3. A schematic view of an adsorbed H\(_2\) on Zn\(_{n}\)O-(CO\(_2\)H\(_{5}\)). ZnO core is represented by a tetrahedron at the center of the molecule.

Figure 4. Part of the metal core and BDC linker section in MOF-5. Atoms are represented by numbers. carbon: 1-10, oxygen: 11-19, Zn: 20-23, hydrogen: 24-27.
In this paper, using models representing the H2 adsorption sites in MOF-5 and employing high level ab initio CCSD(T) method, we focused on accurate evaluation of H2 binding energy to two distinct adsorption sites, organic linker section and metal oxide cluster section, in MOF-5. For organic linker section which was modeled as 1,4-benzene dicarboxylate lithium (Li-O2(C6H4(CO2)Li)), H2 basis set limit binding energy estimate at the CCSD(T) level amounts to about 4.4 kJ/mol. For metal oxide cluster section which was modeled as ZnO(CO2)H6, while the MP2 basis set limit binding energy of H2 was estimated to be 5.4 kJ/mol from basis set extrapolation, CCSD(T) calculations with relatively small basis sets such as 6-31G or 6-31G* showed negligible change from the corresponding MP2 binding energies of H2. If this tendency of negligible difference between the MP2 and CCSD(T) binding energies also holds true for large basis set calculations, the binding energy of H2 to metal oxide cluster section in MOF-5 could be expected to be close to 5.4 kJ/mol. However, if one adopts ZnO(CO2)H6 as a model for metal oxide cluster section in MOF-5 (which would be more similar to the actual environment in MOF-5 than ZnO(CO2)H6), H2 binding energy to metal oxide cluster section in MOF-5 could be more than 7 kJ/mol as the substitution of hydrogen with phenyl group in ZnO(CO2)H6 was shown to increase the H2 binding energy by about 2 kJ/mol at the MP2 level. Therefore, it appears that the metal oxide cluster section could bind the H2 molecule more strongly than the organic linker section by about 3 kJ/mol as long as the CCSD(T) binding energy of H2 near the basis set limit for metal oxide cluster section does not decrease the corresponding MP2 results significantly. Although accurate estimate of large basis set effect at the CCSD(T) level on H2 adsorption affinity to metal oxide cluster section in MOF-5 cannot be made at the present time, increase of basis set in similar but smaller H2-ZnO(CO2)H5OH system than H2-ZnO(CO2)H6 system appears to increase the binding energy of H2 at the CCSD(T) level, suggesting that the difference in binding energies of H2 to metal oxide cluster and organic linker section in MOF-5 could be larger than 3 kJ/mol. This result also appears to be in accord with the previous neutron powder diffraction study which found the metal oxide cluster as the primary adsorption site while organic linker only plays a secondary role for the hydrogen adsorption in MOF-5.8

We also found that presence of nitrogen in the benzene ring would decrease the H2 binding energy to the organic linker section in MOF-5, which is in contrast to the previous prediction based on DFT calculations. This finding, along with the accurate estimate to the H2 binding affinity to the organic linker section and metal oxide cluster section in MOF-5 using ab initio methods, illustrates the danger in relying on results based on DFT methods in cases where weak dispersion attraction is a dominant interaction force and illuminates the utility of the methodology employed in this study in such cases.

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References