



Metal–organic Frameworks for Hydrogen Storage: Theoretical Prospective

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Abstract

The adsorption of H₂ in dehydrated and hydrated Materials of Institute Lavoisier (MIL-101) was investigated theoretically. The effect of terminal water molecules on adsorption as one of the more vital MIL-n trivalent chromium-based porous carboxylates in metal-organic frameworks application in the renewable energy field was also theoretically studied. The MIL-101 structures were optimized for geometry and energy minimization was performed. The calculations were carried out using density functional theory approach with B3LYP functional and mixed basis set of Lanl2DZ and 6-31G(d, p) for Cr and light atoms (C, H, O, F), respectively, as implemented in the Gaussian 09 program package. The spin and atomic charges distribution on the Cr metal atoms, adsorbate, and water molecules are calculated using natural bond orbital (NBO). The density of states (DOS) for the clusters was obtained using Gaussian smearing of Kohn–Sham orbital energies. The natural bond orbital (NBO) for molecular orbital analysis and atomic charge calculations were utilized. For the dehydrated MIL-101, more adsorbate molecules were found near the exposed Cr₂ sites than the fluorine saturated Cr₁ sites. Furthermore, terminal water molecules in the hydrated MIL-101 made more interaction sites and enhanced adsorption.

Keywords: Metal-organic frameworks; Mil 101; Hydrogen Storage; DFT; Adsorption energy.

1. Introduction

In view of increasing demand worldwide, the development, handling, and processing of energy have become a priority. Nonetheless, this must be sustainable and consistent with the climate. To achieve reliable and cost-competent alternative energy sources, these fundamental issues must be addressed correctly and prepared for market readiness by 2030 [1]. Over the past three decades, there has been a sustained research activity in hydrogen gas storage [1,2].

Typical gas storage methods require extremely high pressure, leading to high safety issues in large storage tanks and relatively high energy consumption at the gas processing and development stage [3-5]. Both of these limitations are major obstacles to production and call for materials that can store large amounts of gas under standard conditions in safe environments [5-7].

So, a group of porous cooperation polymers, consisting of metal ions connected to one another by organic bridges, described as Metal-Organic Frameworks (MOFs) are explored due to their extremely high surface areas (up to 10,000 m²/g),

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porosity (up to 90 percent), and tunable pores with volumes (1–4 cm³/g), which are the most appealing characteristics [8–10]. They are considered as an alternative tool for gas storage and purification, particularly for the reduction of environmental pollution and energy crises [10,11].

Materials of Institute Lavoisier Chromium, as MIL-101(Cr), has been investigated for different energy applications as one of the most vital prototypical metal-organic frameworks (MOFs) for its high stable humidity, good thermal efficiency, exceptionally large pore volumes and surfaces, and for its multiple unsaturated chromium sites [12]. MIL-101(Cr) has the empirical formula of [Cr₃(O)X(BDC)₃(H₂O)₂] (BDC = benzene-1,4-dicarboxylate, X = OH or F) with two types of internal cages with diameters of 29 and 34 Å, pore aperture window diameters of up to 16 Å, and Brunauer-Emmett-Teller (BET) surface area of 4000 m²/g [13]. Hydrated MIL-101(Cr) contains terminal water molecules that can be removed under a high vacuum and thus create possible Lewis acid sites linked to an octahedral trinuclear Cr(III)₃O building system [14] to the dehydrated MIL-101(Cr).

In the literature, MIL-101 (Cr) has been extensively investigated in an attempt to enhance its H₂ uptake that has been recently reported to be 6.2 wt.% at 77 K, 80 bar, and BET surface area of 4100 m²/g [14, 15].

In this work, we will estimate the hydrogen gas adsorption capability of the MIL-101 (Cr) in both hydrated and dehydrated structures and will explain the physical interaction between gas molecules and the MOF. Also, we will search for the most favorable adsorption sites of gases via computing the adsorption energy and then analyze electronic properties based on the van der Waals dispersion-corrected density functional theory calculations.

2. Experimental

In this study, geometry optimization and energy calculations were carried out by the hybrid generalized gradient approximation B3LYP method (Becke's three-parameter exchange functional and the correlation functional from Lee, Yang, and Parr) [16, 17]. Mixed basis set of Lanl2DZ [18] and 6-31G(d, p) [19] for Cr and light atoms (C, H, O, F), respectively, that utilizes the Los Alamos National Laboratory 2 double zeta core potential on the transition metal were included. Pople-type double zeta basis set with polarization functions on all other atoms with Gaussian 09 software package [16] was used. The dispersion corrections for the non-bonding van der Waals interactions were included using Grimme's DFT-D3 method [20] to avoid double-counting of electron correlation effects.

Adsorption energies (KJ/mol) were determined from the equation between the gas and MOF clusters as;

$$E_{\text{ads}} = E_{\text{MOF-gas}} - E_{\text{MOF}} - E_{\text{gas}} \quad (1)$$

where $E_{\text{MOF-gas}}$, E_{MOF} , and E_{gas} are the total energies of the optimized geometries of MOF cluster alone with the isolated adsorbed gas molecule, the MOF cluster, and the gas molecule, respectively.

The Natural Bond Orbital [21] were used for the distribution of spin and atomic charges on the Cr metal atoms, Adsorbate and Water molecules. The density of states [22] for the models was obtained using Gaussian smearing of Kohn–Sham orbital energies.

3. Results and Discussions

According to MIL-101(Cr) empirical formula discussed before [13], Cr₃O trimers and 1,4-benzenedicarboxylic acids are combining the MIL-101 by assembled shared corner super tetrahedron with 8.6 Å free aperture micropores where the four vertices and six edges are occupied by the trimer and organic linker, respectively, resulting in a three-dimensional MTN zeotypic structure with a very high volume of cells (~702000 Å³) [23].

Each Cr is linked to 4 carboxylate oxygen-based atoms, 1 μ₃O oxygen-based atom and 1 terminal site. A fluorine atom or a terminal water molecule might occupy the terminal site. As a result, three-terminal sites are available for each Cr₃O trimer, with fluorine to water ratio of 1:2. Upon dehydration, terminal waters can be extracted and exposed Lewis acid sites in MIL-101 are thereby given. We considered the structures involved fluorine terminal atom and overall charges of different investigated MIL 101 are zero also based on previous work [23].

Figure 1 displayed the optimized structures of MOF, gas and MOF-Gas with terminal fluorine and saturation of cleavage bonds of Cr₃O by methyl group. The optimized structures are symbolized by MIL101 (hydrated), MIL101 (dehydrated), H₂ gas, MIL1, MIL2, MIL3, MIL4 for MOF (MIL-101 (Cr)) in both hydrated and dehydrated then hydrogen gas then MOF-Gas structures in hydrated and dehydrated forms, respectively, and four positions of entering hydrogen: Pos1 (Cr₂-F), Pos2 (Cr₁-O-H₂) then Pos3 (Cr₂-F), Pos4 (Cr₁-O-H₂).

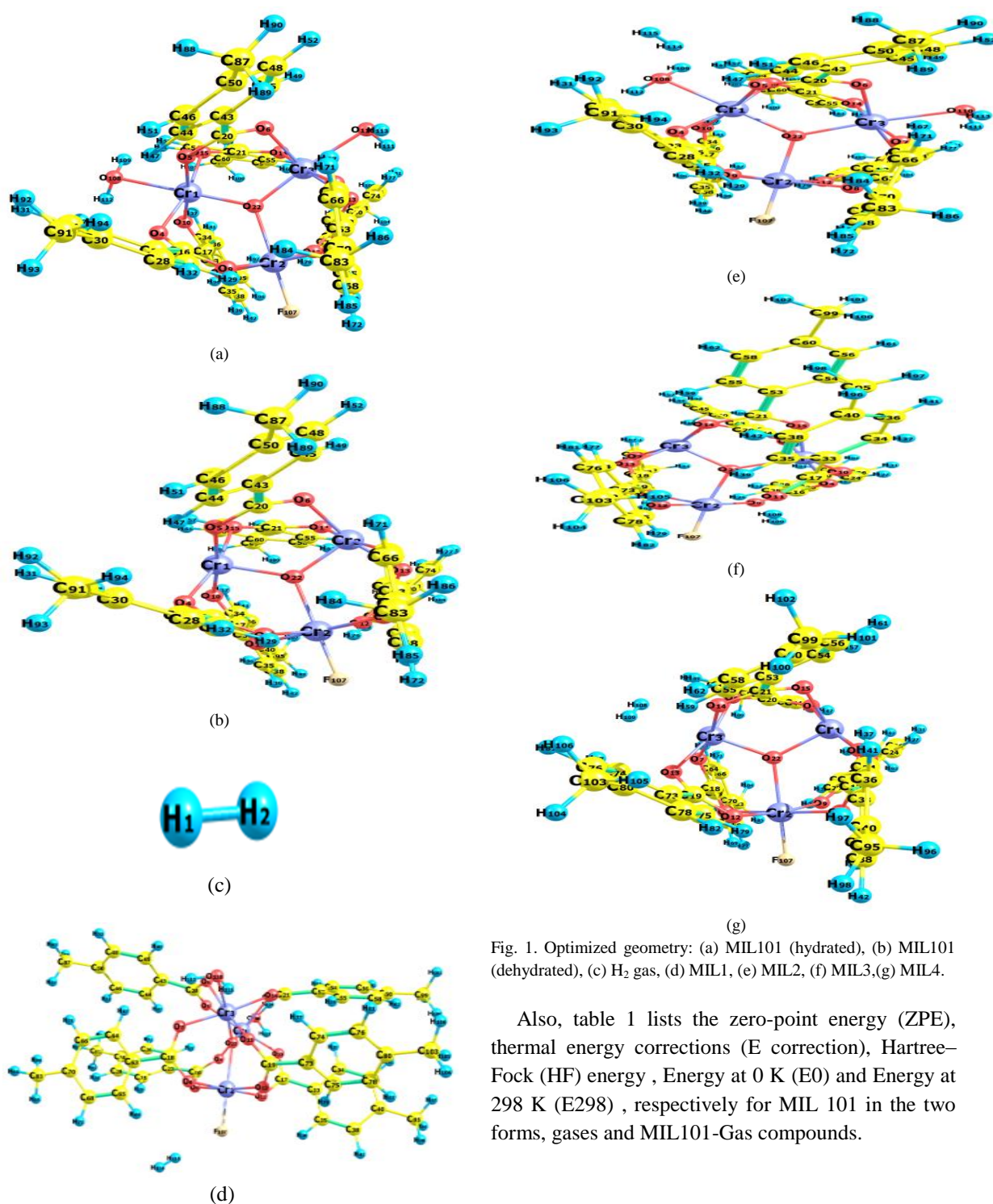


Fig. 1. Optimized geometry: (a) MIL101 (hydrated), (b) MIL101 (dehydrated), (c) H₂ gas, (d) MIL1, (e) MIL2, (f) MIL3, (g) MIL4.

Also, table 1 lists the zero-point energy (ZPE), thermal energy corrections (E correction), Hartree-Fock (HF) energy, Energy at 0 K (E0) and Energy at 298 K (E298), respectively for MIL 101 in the two forms, gases and MIL101-Gas compounds.

Table 1. Total energies of MOFs, Gases and MOF-Gas species in atomic units.

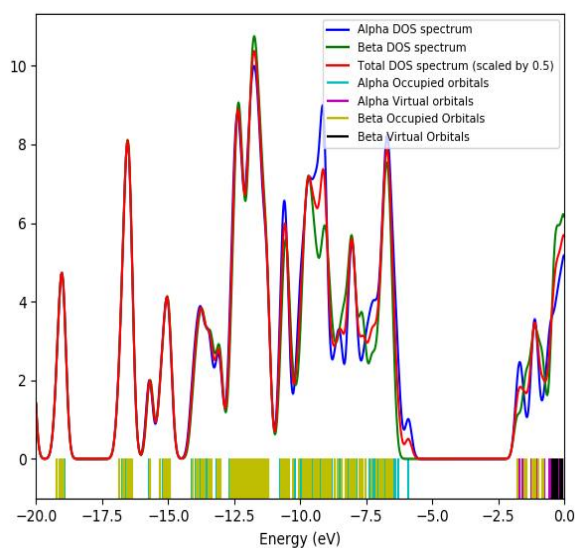
Species	ZPE	E correction	HF	E 0	E 298
MIL101 (Hydrated)	0.861	0.928	-3344.88	-3343.95	-3343.95
MIL101(Dehydrated)	0.810	0.873	-3344.80	-3191.08	-3343.93
H ₂ gas	0.010	0.012	-1.178	-1.16	-1.16
MIL 1	0.875	0.945	-3346.06	-3345.19	-3345.12
MIL 2	0.874	0.945	-3346.06	-3345.19	-3345.11
MIL 3	0.824	0.889	-3193.14	-3192.31	-3192.25
MIL 4	0.822	0.888	-3193.13	-3192.31	-3192.25

In table 2, energies of band gap in electron volt and calculated adsorption energies in KJ/Mol were listed. It was noticed that, the band gaps (E_g) for the dehydrated species of MOF and MOF-GAS are 3.66 and 3.54 eV, respectively, which are more stable than the hydrated ones (4.12 and 4.16 eV). On the other hand, the adsorption energies are -0.74, 2.215, -17.17 and -11.42 KJ/mol for MIL 1, MIL 2, MIL 3, and MIL 4, respectively. These values stated that hydrated forms have relatively better adsorption behavior than the dehydrated forms.

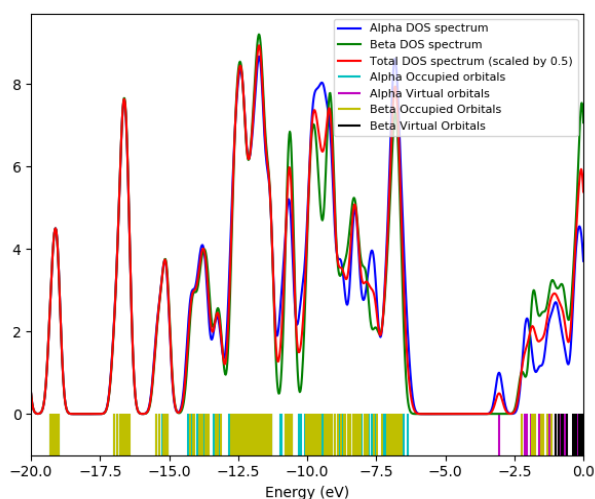
Table 2. Energies of adsorption and band gap energies for MOFs and MOF-Gas species.

Species	E_g (eV)	E_{ads} (KJ/mol)
MIL101 (Hydrated)	4.12	-
MIL101(Dehydrated)	3.55	-
MIL 1	4.16	-0.74
MIL 2	4.12	2.215
MIL 3	3.66	-17.17
MIL 4	3.55	-11.42

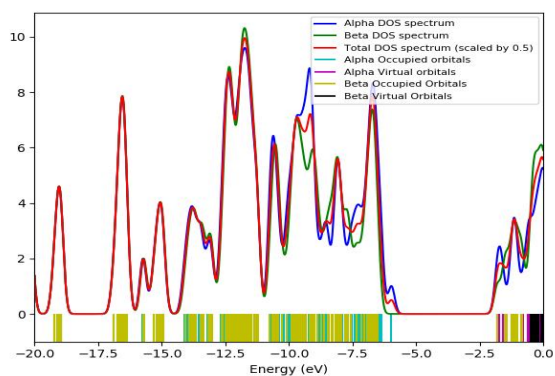
To rationalize the observed changes in the band region, the density of states (DOS) of hydrated form are higher than dehydrated forms. As shown in Figure 2, the DOS of MIL 101 forms (a, b) are characteristic of increased band gap of 3.55 eV for the dehydrated form to 3.66 eV of MOF-gas compounds. Also, the band gap was slightly increased, and a mid-gap state appeared at around 4.12 to 4.16 eV for hydrated MOF and hydrated MOF-GAS compounds, respectively. So, it appears that the Fermi level was mostly dominated by the contribution from the chromium atoms (near valence band). DOS of H_2 gas doesn't affect the band gap due to its buried orbitals.



(a)



(b)



(c)

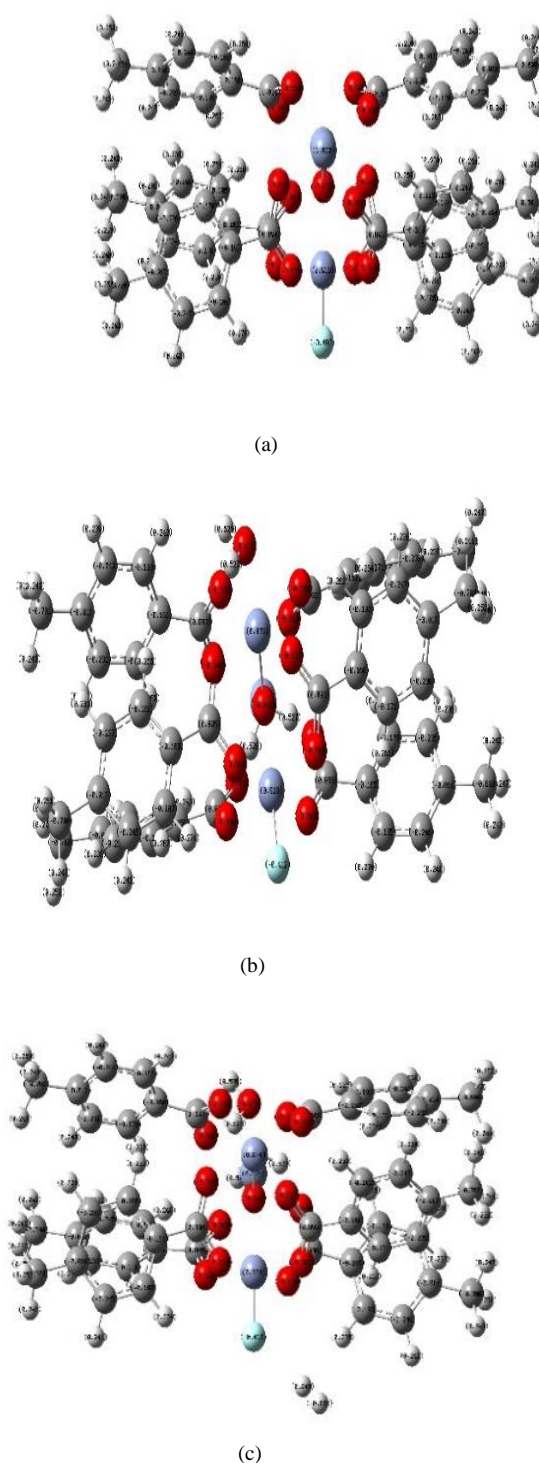
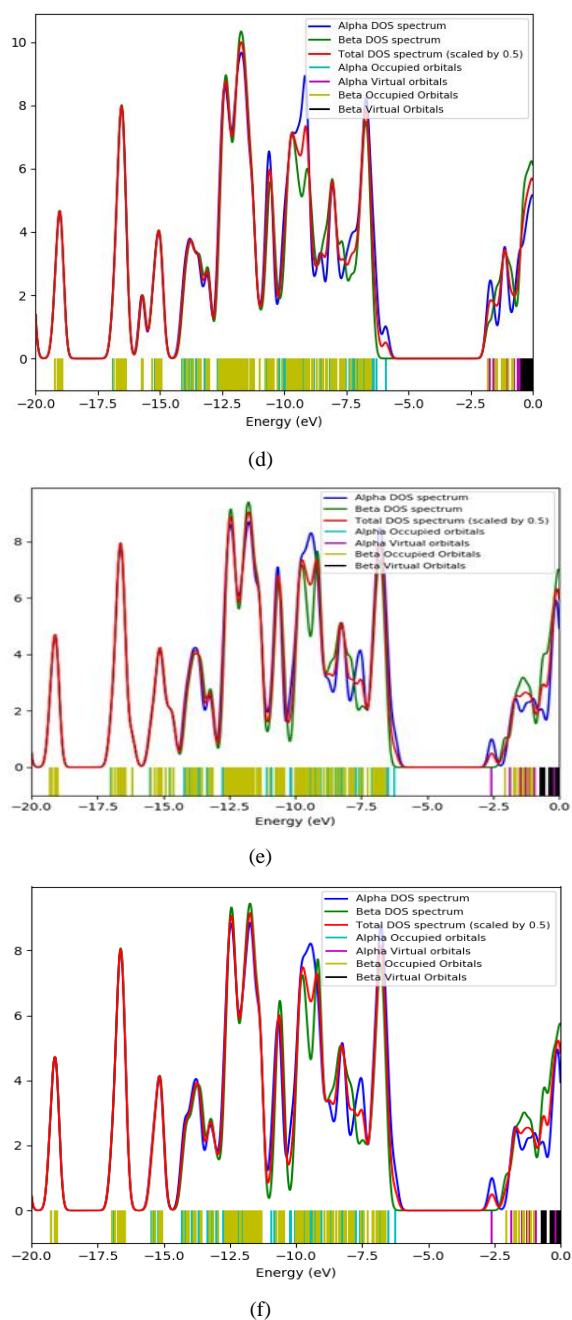


Fig. 2. Total density of states spectrum: (a) MIL101 (hydrated), (b) MIL101 (dehydrated), (c) MIL 1, (d) MIL 2, (e) MIL 3, (f) MIL 4.

According to figure 3, the total atomic charges Cr are noticed higher than oxygen and fluorine. For the dehydrated MIL-101, more adsorbate molecules were found near the exposed Cr2 sites than the fluorine saturated Cr1 sites. Furthermore, terminal water molecules in the hydrated MIL-101 vastly made interaction sites and enhanced adsorption.

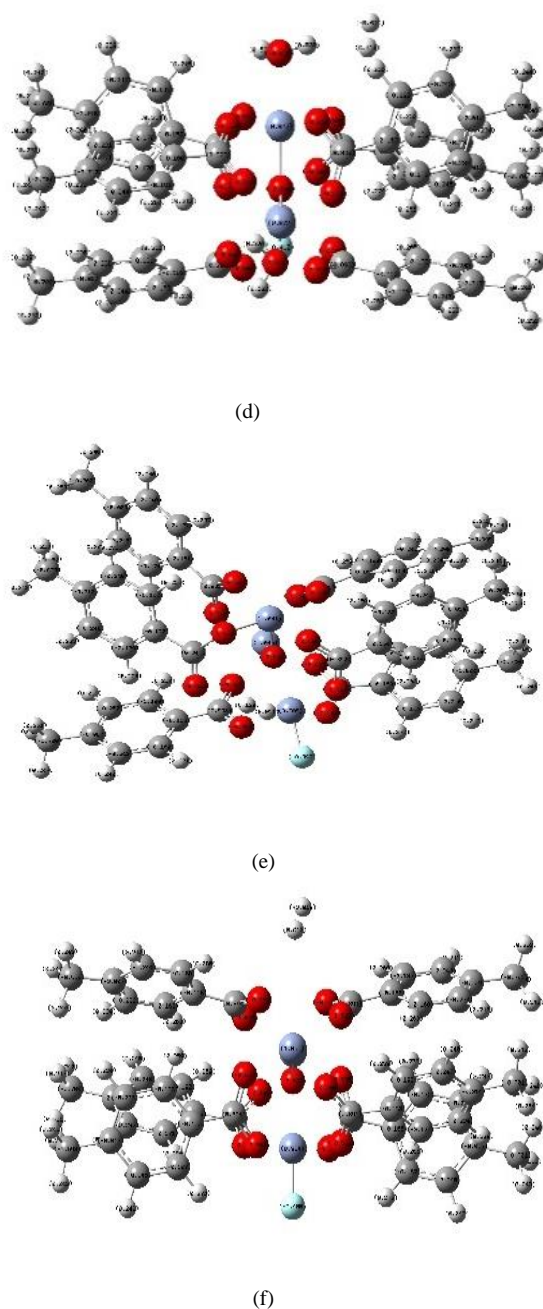


Fig 3. NBO: (a) MIL101 (dehydrated), (b) MIL101 (hydrated), (c) MIL 1, (d) MIL2. (e) MIL 3, (f) MIL4.

4. Conclusions

In this paper, Adsorption energies of H_2 in both hydrated and dehydrated MIL 101 (Cr) with density functional theory where we showed the higher selectivity of hydrated form of MIL 101 than the dehydrated form. Furthermore, less stability of the hydrated form was noticed than the dehydrated one at 298 K and 1 bar.

The present findings indicated that molecular modelling is an important tool for elucidating several parameters to fulfil the experimental findings. This is in good agreement with those obtained previously [24-40].

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7. Arabic abstract

الدراسة النظرية لامتماص الهيدروجين علي الجاف والرطب لمادة معهد لافوازييه (ميل-101). وقد تطرقت الدراسة النظرية أيضا لتأثير جزيئات الماء الطرفية على الامتماص لوحد من اكثر مركبات الميل الضرورية والمحتوي علي كروم و مجموعات الكربوكسيلات المسامية لما لها من أهمية في مجال الطاقة المتجددة. لقد قمنا بالبحث عن افضل شكل فراغي للمركب بدلالة الطاقة باستخدام نظرية الكثافة الدالية **B3LYP** ومجموعة قواعد مخلوطة من مجموعة **Lanl2DZ** علي ذرة الكروم و مجموعة **6-31G(d,p)** على كل من ذرات الكربون والهيدروجين والاكسجين والفلور كما هي مطبقة في حزمة برامج الجاوسيان 09. إن العزم المغناطيسي والشحنات قد تم حسابها على ذرات الكروم والجزيء الممتص وجزيئات الماء باستخدام طريقة حساب المدار الرابطة الطبيعي. إن كثافة المستويات لعناقيد المركبات الخاضعة للدراسة تم الحصول عليها بواسطة غطاء بشكل دوال الجاوسيان لمدارات كون شام. لقد تم استخدام مدار الرابطة الطبيعي لتحليل المدارات الجزيئية والشحنات الذرية. وأضحت الدراسة وجود جزيئات ممتصة اكثر لمركب الميل الجاف بالقرب من موقع ذرة الكروم المكشوفة مقارنة بموقع ذرة الكروم المشبعة بالفلور. وعلاوة علي ذلك، فإن جزيئات الماء الطرفية في جزيء الميل الرطب خلقت مواقع تفاعل أكثر وعززت من الامتماص.