

Supplementary Information

Ab Initio Study of Hydrogen Adsorption in COF-10

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Validation of the k-points

The number of k points along each direction should be approximately inversely proportional to the corresponding length of the cell, so that the densities of k points along each direction are close. In this study, the simulation box consists of a 2×2×1 supercell of COF-10. Higher k point densities bring better computation accuracy but at the same time higher cost. Before the 1×1×6 Gamma centered k-point mesh was selected, a convergence test was conducted, and the results are shown in Table S1. As shown in Table S1, higher k point densities result in lower energies. However, for fork point densities higher than the 1×1×6 k-point mesh, the decreases in energy are insignificant. The 1×1×6 k-point mesh was selected based on the balance between accuracy and cost.

Table S1. The convergence test of k point densities

k points	Energies of COF-10 / eV
1×1×1	-882.0453
2×2×2	-912.0568
3×3×3	-913.2914
4×4×4	-913.3611
5×5×5	-913.3655
6×6×6	-913.3676
1×1×6	-913.3672
2×2×6	-913.3674
3×3×6	-913.3671
4×4×6	-913.3675
5×5×6	-913.3678

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Densities of hydrogen at 77 K

Table S2. Densities of hydrogen at 77 K

Pressure / bar	Density / (mol L ⁻¹)	Pressure / bar	Density / (mol L ⁻¹)	Pressure / bar	Density / (mol L ⁻¹)	Pressure / bar	Density / (mol L ⁻¹)
0.048684	0.007811	0.546053	0.085986	3.66	0.5656	32.9	5.373
0.062237	0.009373	0.589474	0.092246	5.54	0.86672	36.6	5.9554
0.072237	0.010935	0.642105	0.10007	6.67	1.0578	39.8	6.5368
0.080658	0.012497	0.696053	0.10946	7.92	1.2496	44	7.1986
0.092368	0.01406	0.751316	0.11729	9.29	1.4741	48.6	7.9381
0.104211	0.015622	0.801316	0.12512	10.5	1.6673	53.4	8.751
0.114211	0.017185	0.855263	0.13295	12	1.9096	60.1	9.7902
0.124342	0.018747	0.909211	0.14078	13.3	2.1529	66.5	10.651
0.169737	0.026561	0.967105	0.15175	16.7	2.642	72.8	11.791
0.226316	0.035939	1.015789	0.15802	17.4	2.8058	79.5	12.746
0.267105	0.042192	1.072368	0.16742	19.5	3.1342	86.4	13.736
0.330263	0.051573	1.15	0.17213	22.9	3.7117		
0.376316	0.059392	1.91	0.2977	26.5	4.2918		
0.436842	0.068777	2.78	0.43935	29.5	4.7904		

Cluster geometries of C

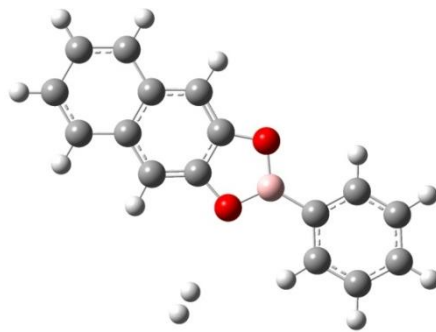


Figure S1. Cluster geometry of C cut from the optimized unit cell structures of H₂ adsorption in COF-10 (A1).

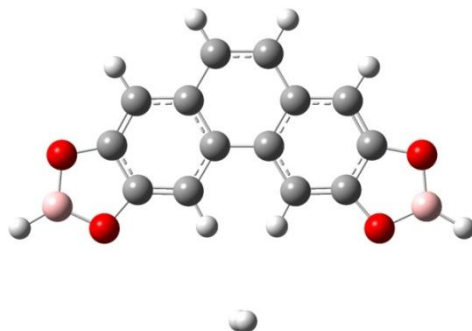


Figure S2. Cluster geometry of C cut from the optimized unit cell structures of H₂ adsorption in COF-10 (A2).

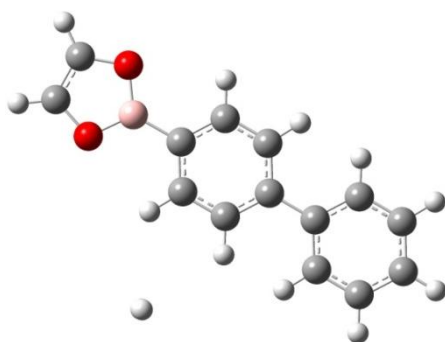


Figure S3. Cluster geometry of *C* cut from the optimized unit cell structures of H₂ adsorption in COF-10 (A3).

Cluster geometries of *C'*

The smaller model *C'* is adopted for CCSD(T) calculations. *C'* is still too large for CCSD(T) calculations and has to be divided into two parts.^{1,2} All dangling bonds are saturated with hydrogen atoms. The adsorption energy of *C'* is the sum of the divided parts.

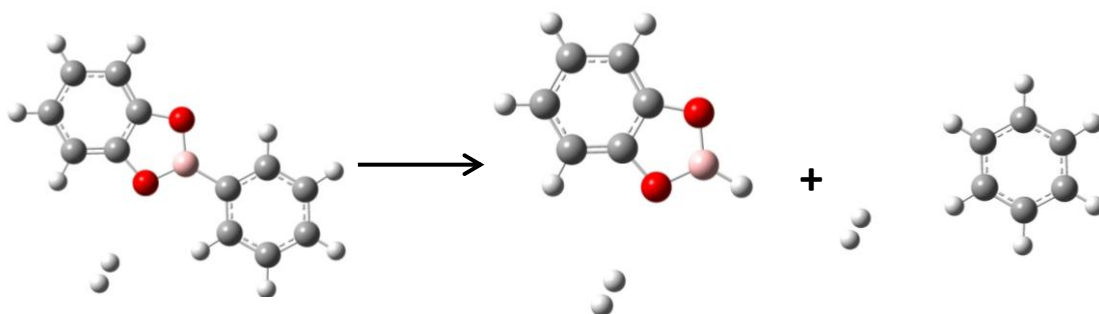


Figure S4. Cluster *C'* of A1 is divided into two smaller parts.

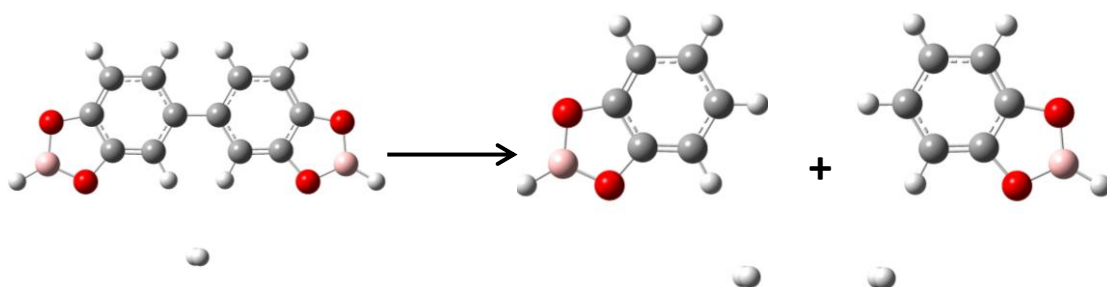


Figure S5. Cluster *C'* of A2 is divided into two smaller parts.

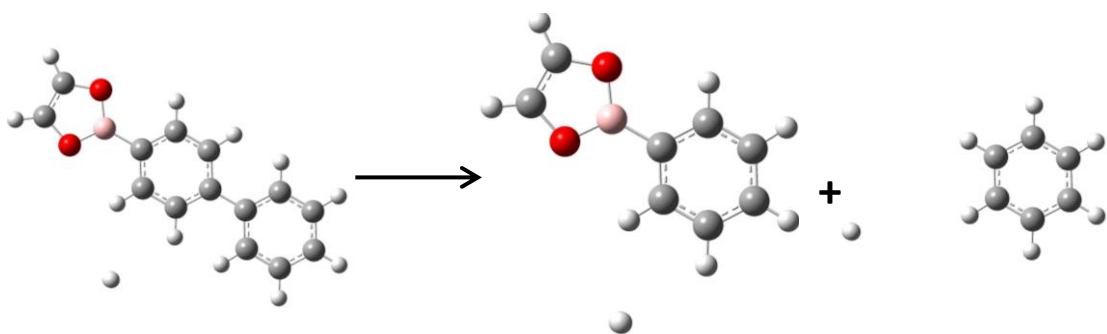


Figure S6. Cluster *C'* of A3 is divided into two smaller parts.

Cartesian coordinates of the optimized adsorption configurations extracted from the CONTCAR files

Compound name

A1:

O 0.8186722492164079 0.3793893249281006 0.4989655901983611
O 0.6224494294501450 0.4403857132614229 0.4999259040461864
O 0.5613357390439132 0.1829817413361865 0.4985059938910204
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O 0.3796197544839798 0.5616446152139712 0.5131736669838529
O 0.4392791087148247 0.8187788789500728 0.4974176067871554
O 0.6219575393065025 0.1828511721365029 0.4980235565848282
O 0.5616727487618224 0.3797345383291574 0.4973671556854719
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A2:

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