Covalent Organic Frameworks for Extremely High Reversible CO_2 Uptake Capacity: A Theoretical Approach

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Figures

Fig. S1. Pore diameter of COF-10.

Fig. S2. (a)~(d) Atomic charges of four model molecules analyzed by NPA.

Fig. S3. Snapshot of CO_2 located between two COF layers.

Fig. S4. Binding sites and energies (E_b in kcal/mol) of COF-8, COF-10, and TP-COF.

Fig. S5. (a) The density distribution (red dots) of CO_2 in COF-5 at fixed loadings of 50, 100, 200, and 300 CO_2 molecules per 2x2x6 cell. **(b)** The density distribution (red dots) of CO_2 in COF-8, COF-10 and TP-COF at a fixed loading of 50 CO_2 molecules per 2x2x6 cell.

Tables

Table S1. Crystalline structure data of COFs.

Table S2. Crystalline structure data of new COFs

References

Fig. S1. Pore diameter of COF-10.

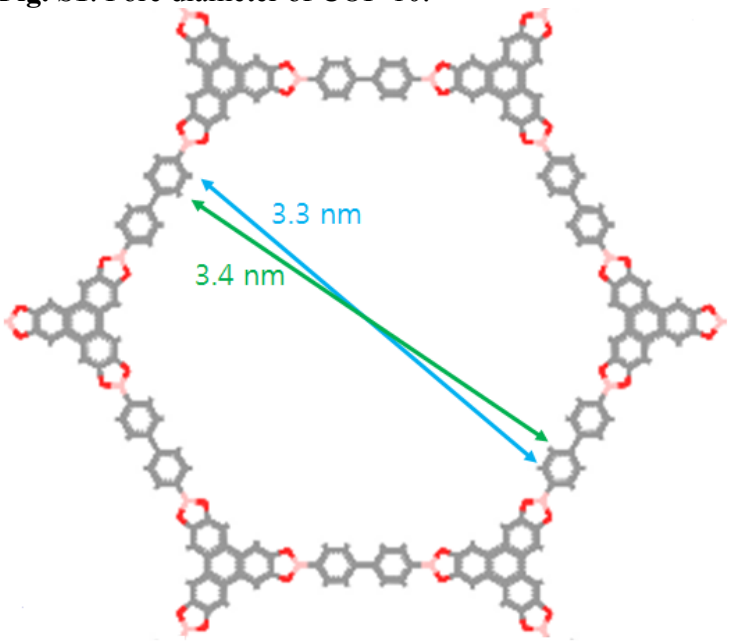

Fig. S2. (a) Natural atomic charges on COF-5.

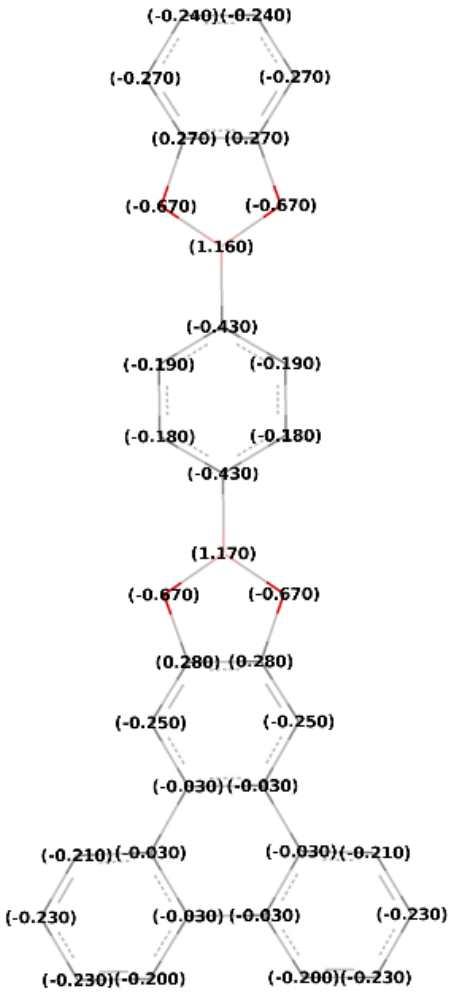

Fig. S2. (b) Natural atomic charges on COF-8.

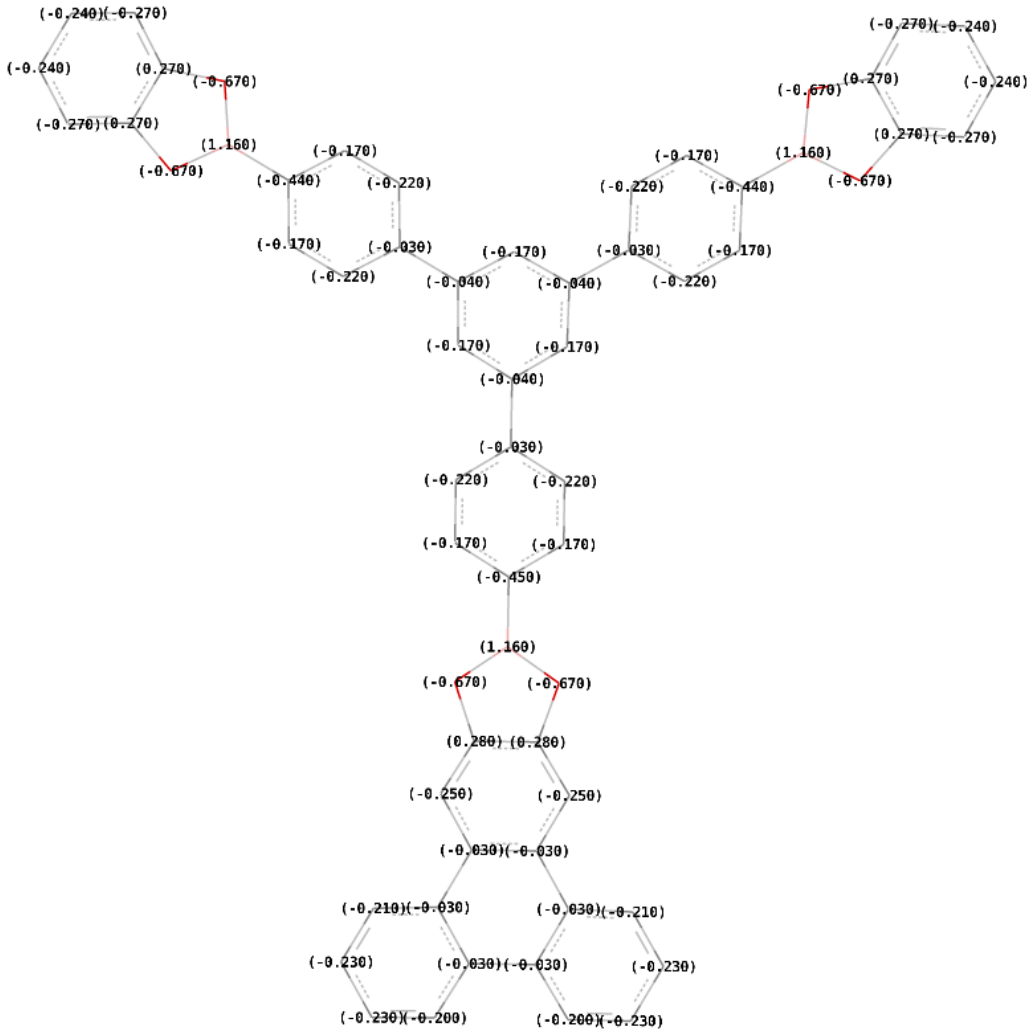

Fig. S2. (c) Natural atomic charges on COF-10.

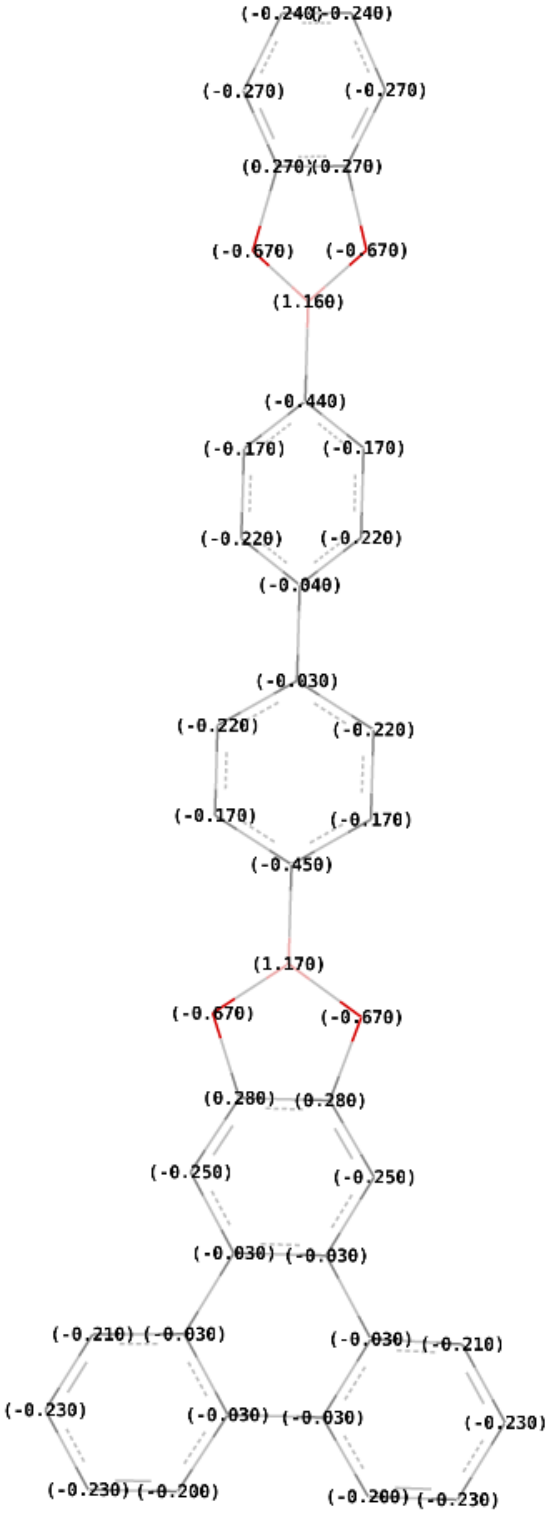

Fig. S2. (d) Natural atomic charges on TP-COF.

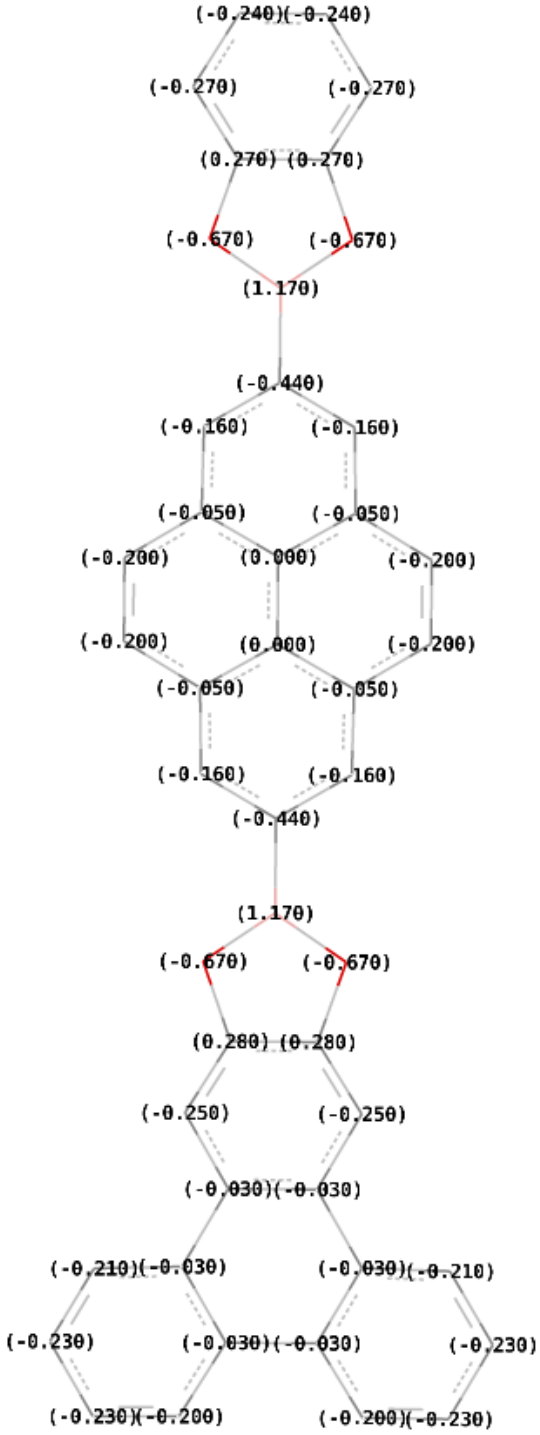

Fig. S3. Snapshot of CO_2 located between two COF layers.

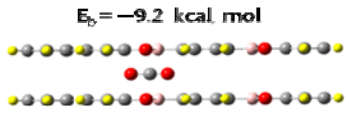

Fig. S4. (a) Binding sites and energies (E_b in kcal/mol) of COF-8.

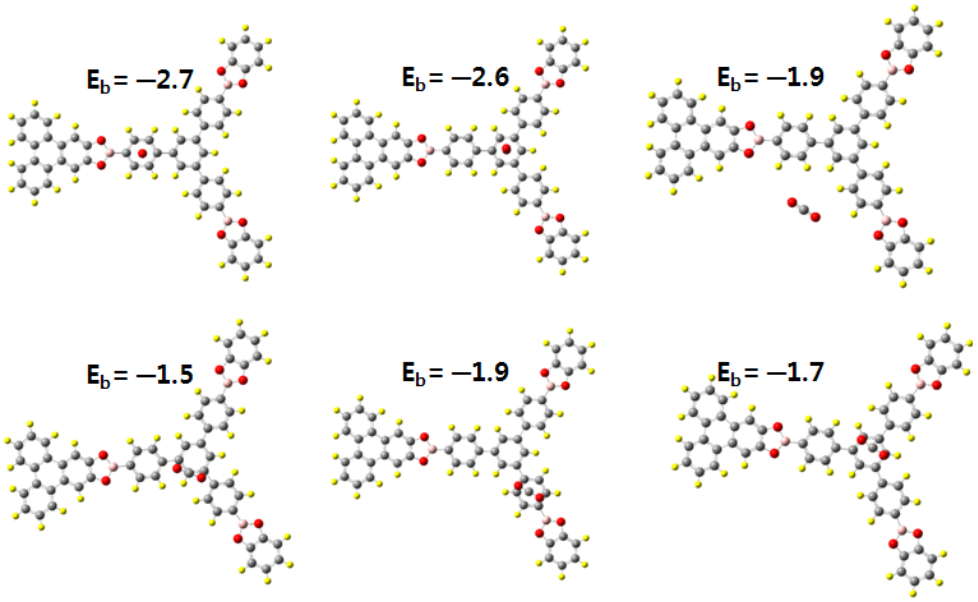

Fig. S4. (b) Binding sites and energies (E_b in kcal/mol) of COF-10.

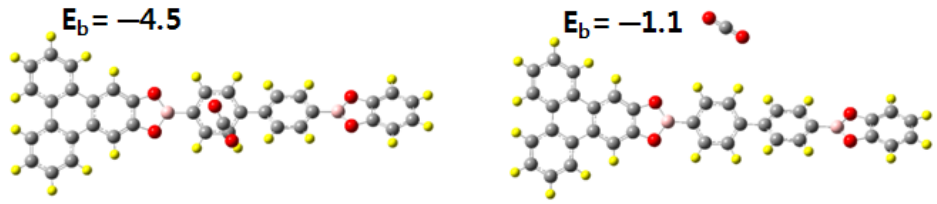

Fig. S4. (c) Binding sites and energies (in kcal/mol) of TP-COF.

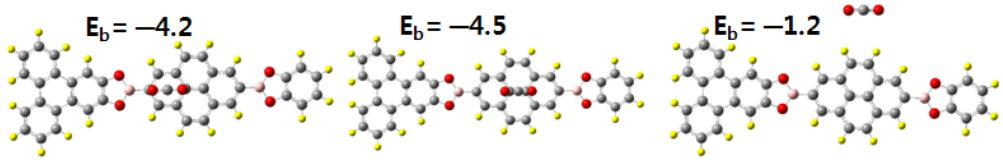

Fig. S5. (a) Density distributions (red dots) for CO_2 in COF-5 at fixed loadings of 50, 100, 200, and 300 CO_2 molecules per a 2x2x6 cell.

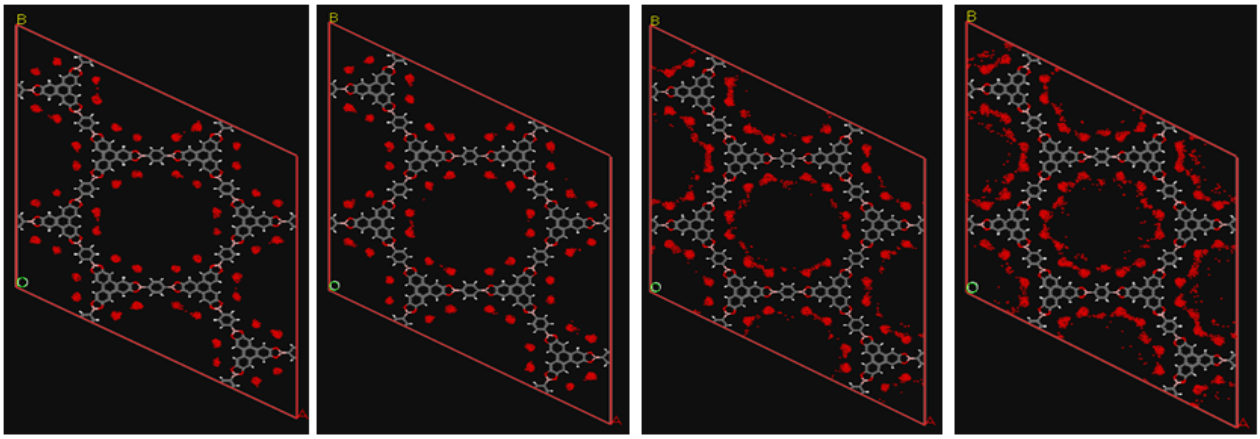

Fig. S5. (b) The density distribution (red dots) of CO_2 in COF-8, COF-10 and TP-COF at a fixed loading of 50 CO_2 molecules per 2x2x6 cell.

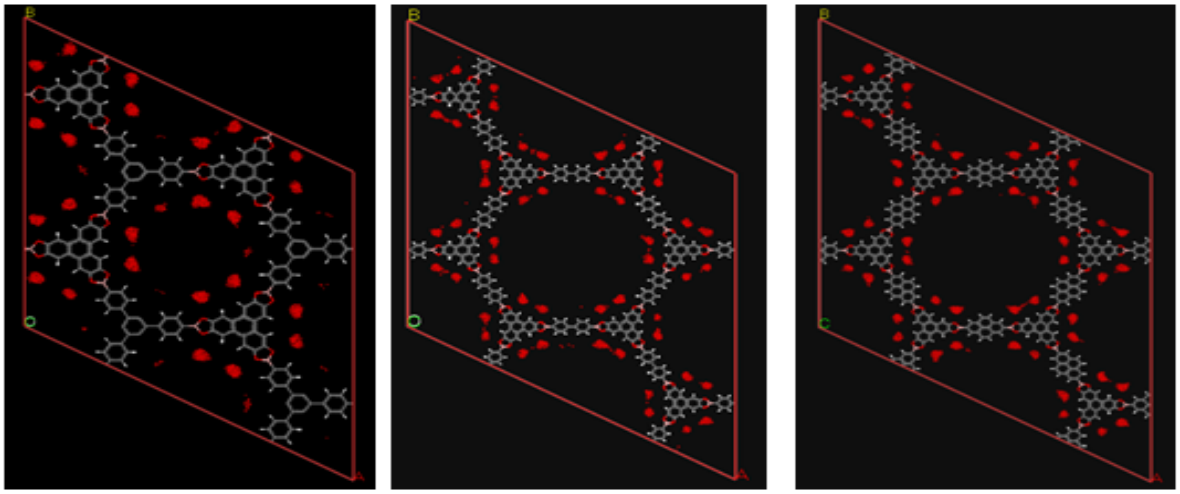

Table S1. Crystalline structure data of COFs.

Material	*a*=*b* (in *Å*)	*C* (in *Å*)
P6/mmm		
COF-5	30.240 (29.70 [a])	3.389 (3.460)
COF-10	37.669 (36.028 [b])	3.447 (3.526)
TP-COF	37.427 (37.542 [c])	3.453 (3.378)
P-6m2		
COF-8	22.569 (22.013 [b])	3.461 (3.630)

[a]Experimental values from Ref.[1]. [b]Experimental values from Ref.[2]. [c]Experimental values from Ref.[3].

Table S4. Crystalline structure data of new COFs.

Material		
P6/mmm		
2D COF-05	a=b=41.492	α=β=90
	c=3.442	γ=120
I-43d		
3D COF-05 (*ctn*)	a=b=c=67.8928	α=β=γ=90
P-43m		
3D COF-05 (*bor*)	a=b=c=44.5711	α=β=γ=90

References

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2. A. P. Côté, H. M. El-Kaderi, H. Furukawa, J. R. Hunt and O. M. Yaghi, *J. Am. Chem. Soc.,* 2007, **129**, 12914.

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