Electronic Supplementary Material (ESI) for Catalysis Science & Technology.

Electronic Supplementary Information (ESI)
The Effect of Topology in Lewis Pair Functionalized Metal Organic Frameworks on CO_2 Adsorption and Hydrogenation

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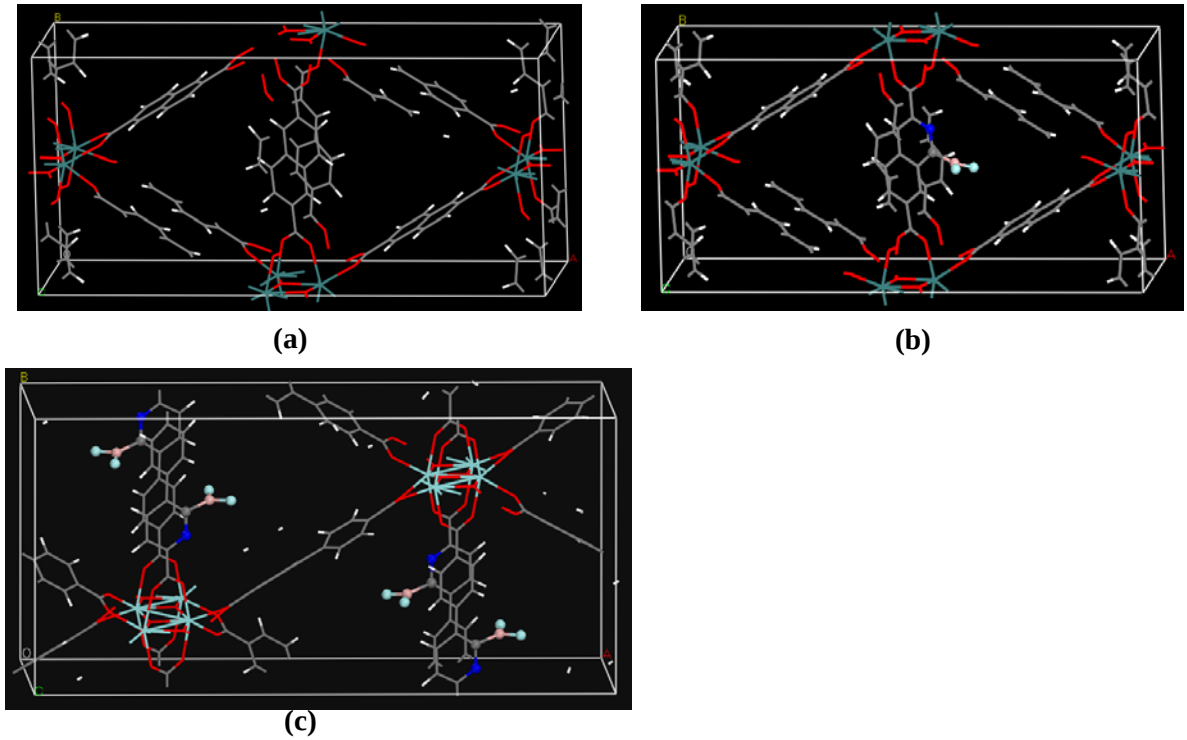
1. Unit cell optimization



(a) **(b)**

(c)

Figure S1. Optimized structures of the unit cells of (a) MIL-140B, (b) MIL-140B-NBF_2 and (c) MIL-140C-$(NBF_2)_4$.

Table S1. Lattice constants of the unit cells of MIL-140B, MIL-140C, MIL-140B-NBF_2, and MIL-140C-NBF_2. Values computed from CP2K are from this work. Values denoted as Exp and Sim are experimental and Rietveld analysis (structure profile refinement) data from Guillerm et al.,[1] respectively.

	a(Å)	b(Å)	c(Å)	α(°)	β(°)	γ(°)
MIL-140B						
Exp[1]	26.71	13.30	7.79	90.00	92.56	90.00
Sim[1]	27.65	13.41	7.85	90.00	90.13	90.00
CP2K	28.24	13.46	7.85	90.00	93.43	90.00
MIL-140C						
Exp[1]	31.03	15.51	7.82	90.00	93.26	90.00
Sim[1]	31.06	15.59	7.85	90.00	95.17	90.00
CP2K	31.89	15.61	7.93	90.00	95.17	90.00
MIL-140B-NBF_2						
CP2K	28.22	13.44	7.85	90.00	93.43	90.00
MIL-140C-NBF_2						
CP2K	31.92	15.57	7.90	90.20	95.29	90.00

Table S1 shows the lattice constants of MIL-140B/C obtained from different methods. Exp and Sim represent the experimental data and simulated data from FullProf software, both reported by Guillerm et al.[1] CP2K represents the data calculated in this work using the CP2K software package.[2]

Table S2. The calculated pore volume, porosity, density for NBF_2 functionalized or unfunctionalized MIL-140B/C.

Material	Pore volume ($cm^3\ g^{-1}$)	Porosity (%)	Density ($g\ cm^{-3}$)
MIL-140B	0.23	33.5%	1.43
MIL-140B-NBF_2	0.22	31.8%	1.46
MIL-140C	0.38	44.2%	1.17
MIL-140C-NBF_2	0.36	42.6%	1.19

2. Charge distribution of the functionalized ligand with CO_2 adsorption

The density derived electrostatic and chemical (DDEC) method[3, 4] was used to analyze the atomic charge distributions for MIL-140B, MIL-140B-NBF_2, MIL-140C and MIL-140C-NBF_2. These charges were used in the GCMC simulations. The charges for these materials are given at the end of this file.

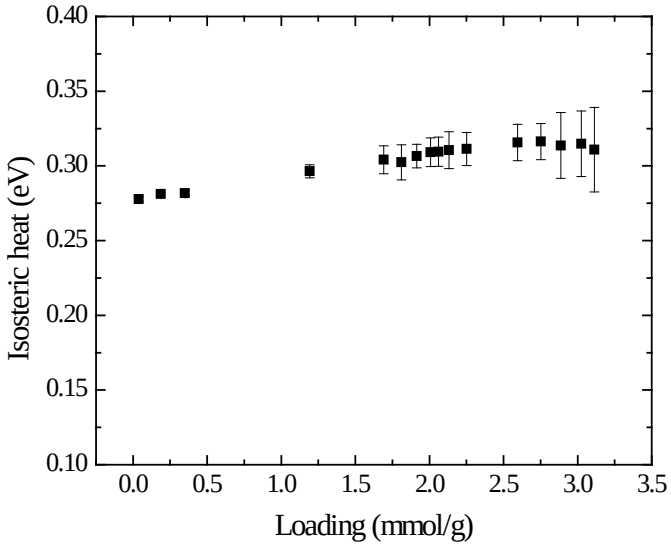


Figure S2. Isosteric heats for CO_2 adsorption in MIL-140B as a function of loading as computed from GCMC simulations.

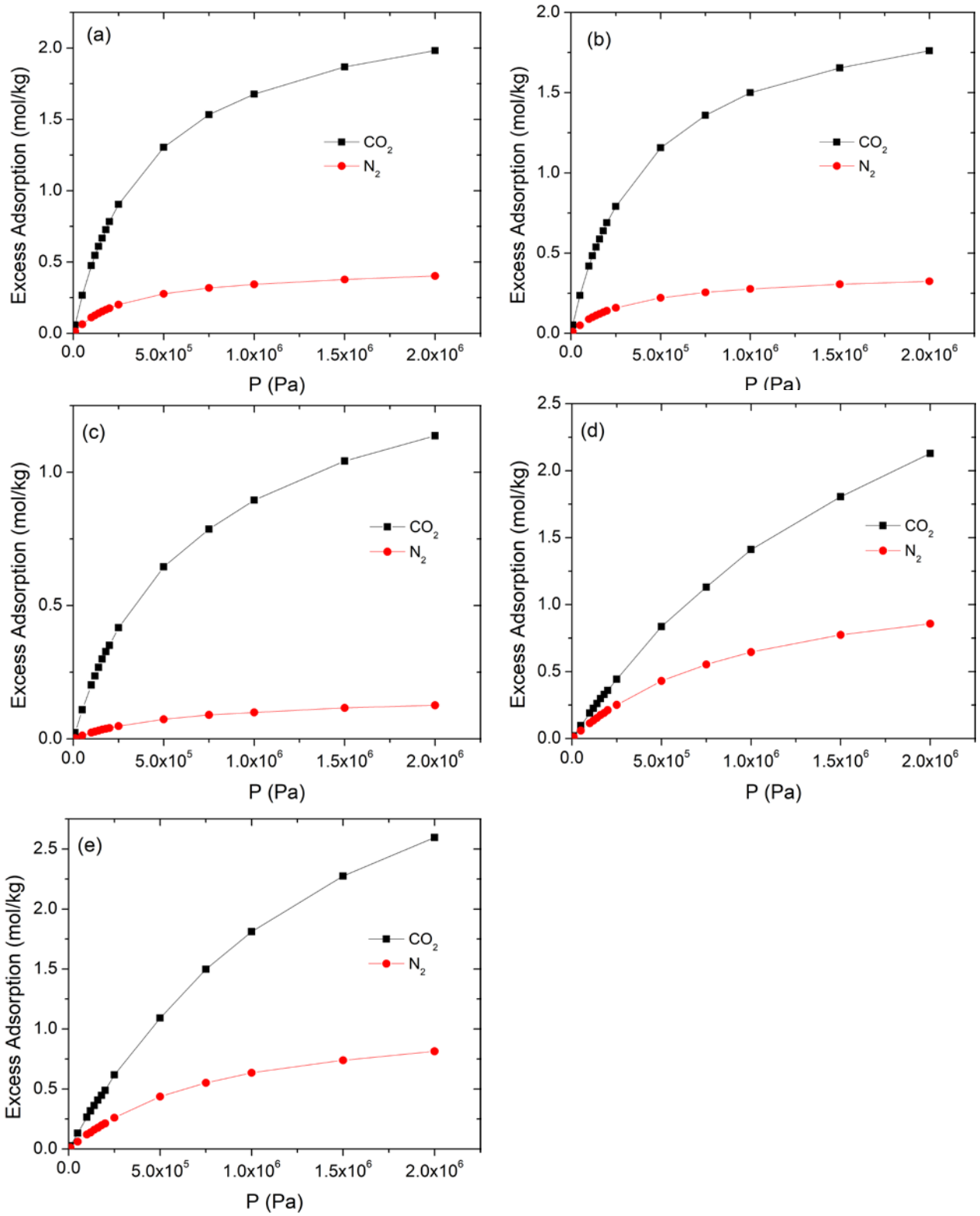


Figure S3. CO_2 and N_2 adsorption isotherms at 298 K computed from GCMC simulations for a bulk gas phase concentration of 15 mol% CO_2 and 85 mol% N_2 in (a) MIL-140B, (b) MIL-140B-NBF_2, (c) MIL-140B-$(NBF_2)_4$ (d) MIL-140C, (e) MIL-140C-NBF_2.

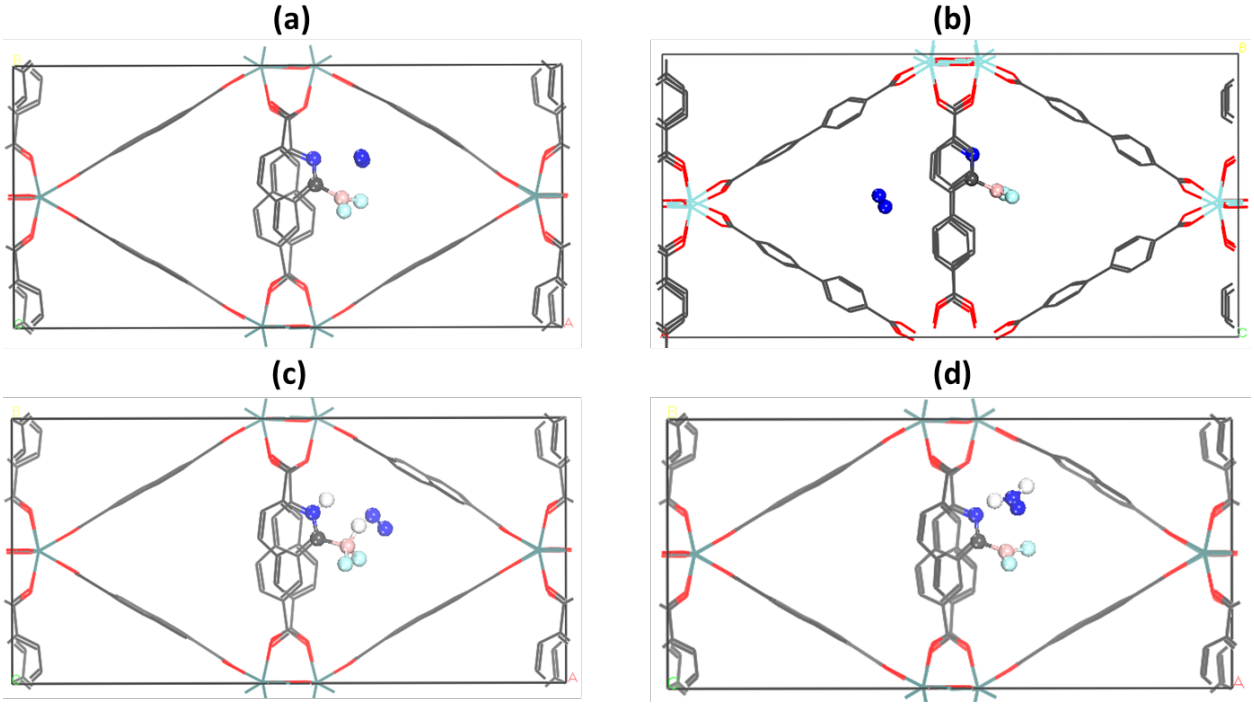


Figure S4. The optimized structure of N_2 physisorption (a) in MIL-140B-NBF_2 and (b) in MIL-140C-NBF_2; (c) and (d) are initial and final structure for N_2 hydrogenation in MIL-140B-NBF_2. The final structure in (d) is 2.5 eV higher in energy than the initial structure in (c). The product state was shown in (d) is the lowest energy structure among all sampled structures, including binding one H to each N in N_2.

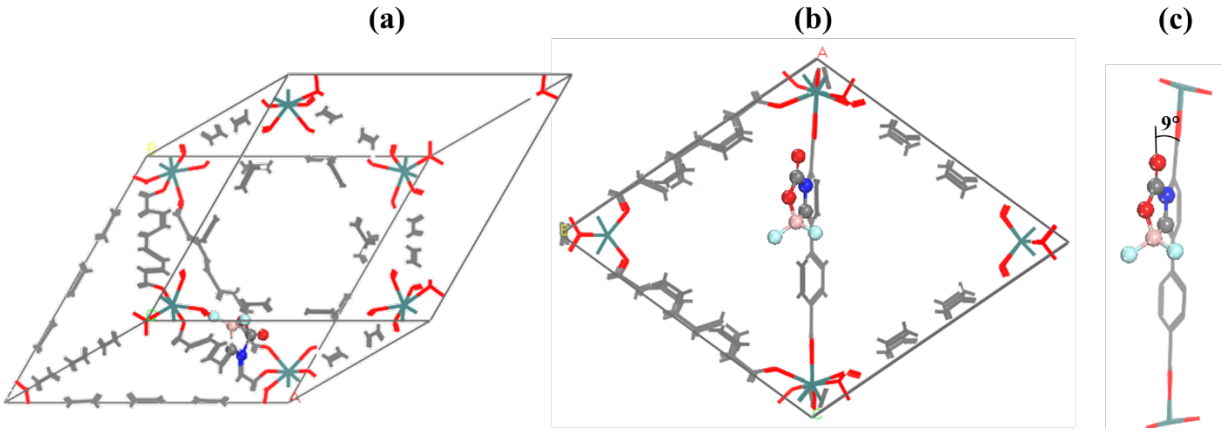


Figure S5. Optimized structures of CO_2 chemisorption in UiO-67-NBF_2: (a) and (b) primitive cell of UiO-67-NBF_2 with CO_2 chemisorbed. (c) The torsion angle of CO_2 refers to the NBF_2 functionalized bpdc linker.

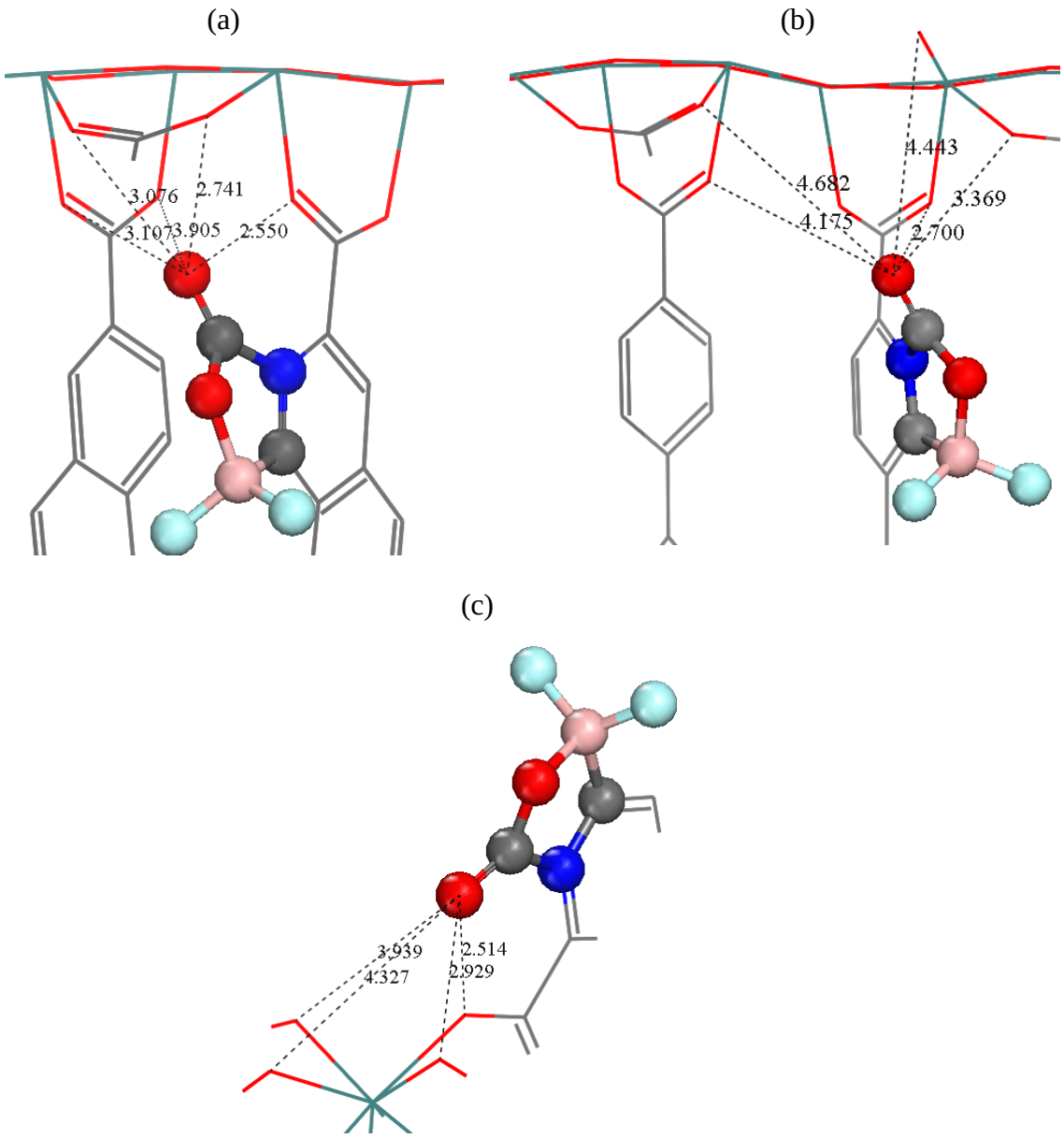


Figure S6. The distance between the unbound O atom of chemisorbed CO_2 and O atoms of the carboxylate linkers for (a) MIL-140B-NBF_2, (b) MIL-140C-NBF_2 and (c) UiO-67-NBF_2.

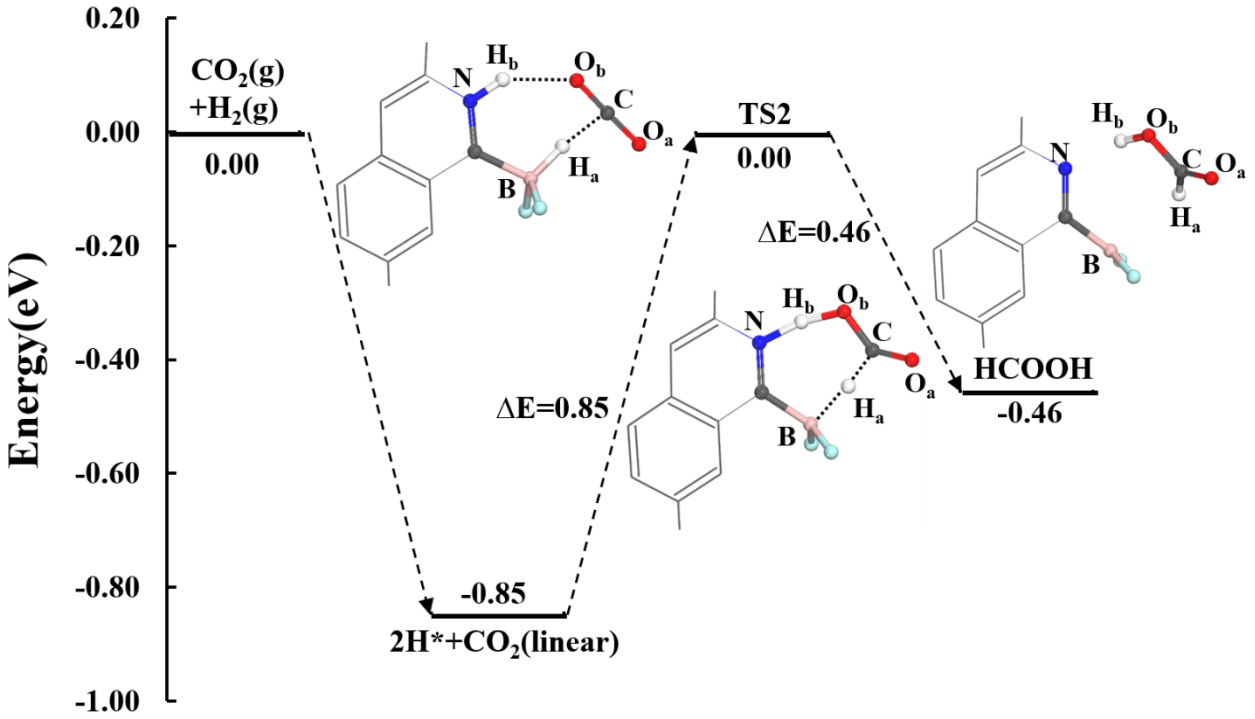


Figure S7 Relative energy profile for physisorbed CO_2 (linear) reacting with chemisorbed H atoms in MIL-140B-NBF_2.

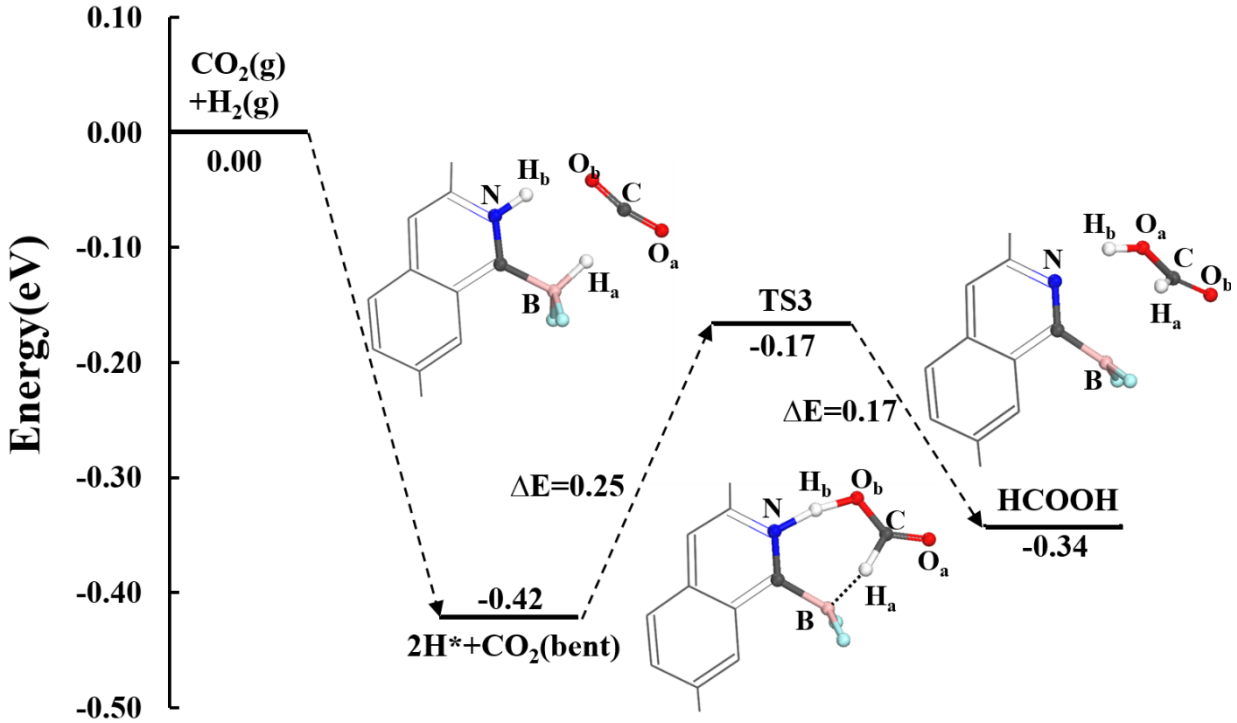


Figure S8. Relative energy profile for physisorbed CO_2 (bent) reacting with chemisorbed H atoms in MIL-140B-NBF_2.

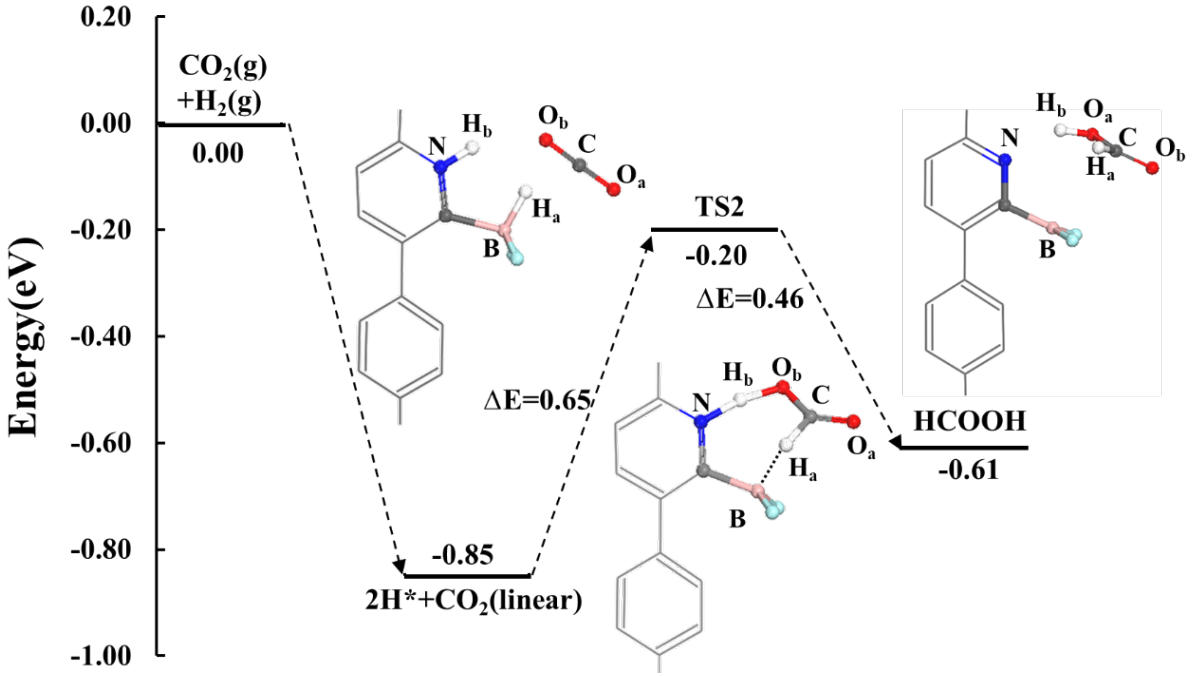


Figure S9. Relative energy profile for physisorbed CO_2 (linear) reacting with chemisorbed H atoms in MIL-140C-NBF_2.

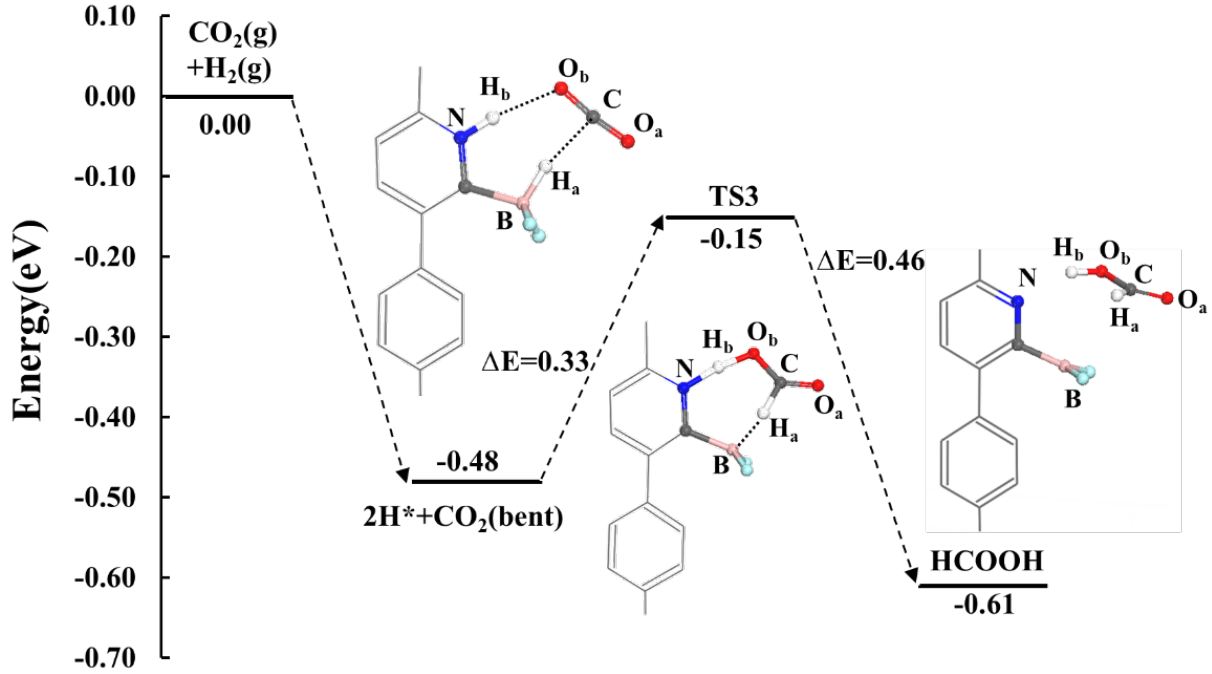


Figure S10. Relative energy profile for physisorbed CO_2 (bent) reacting with chemisorbed H atoms in MIL-140C-NBF_2.

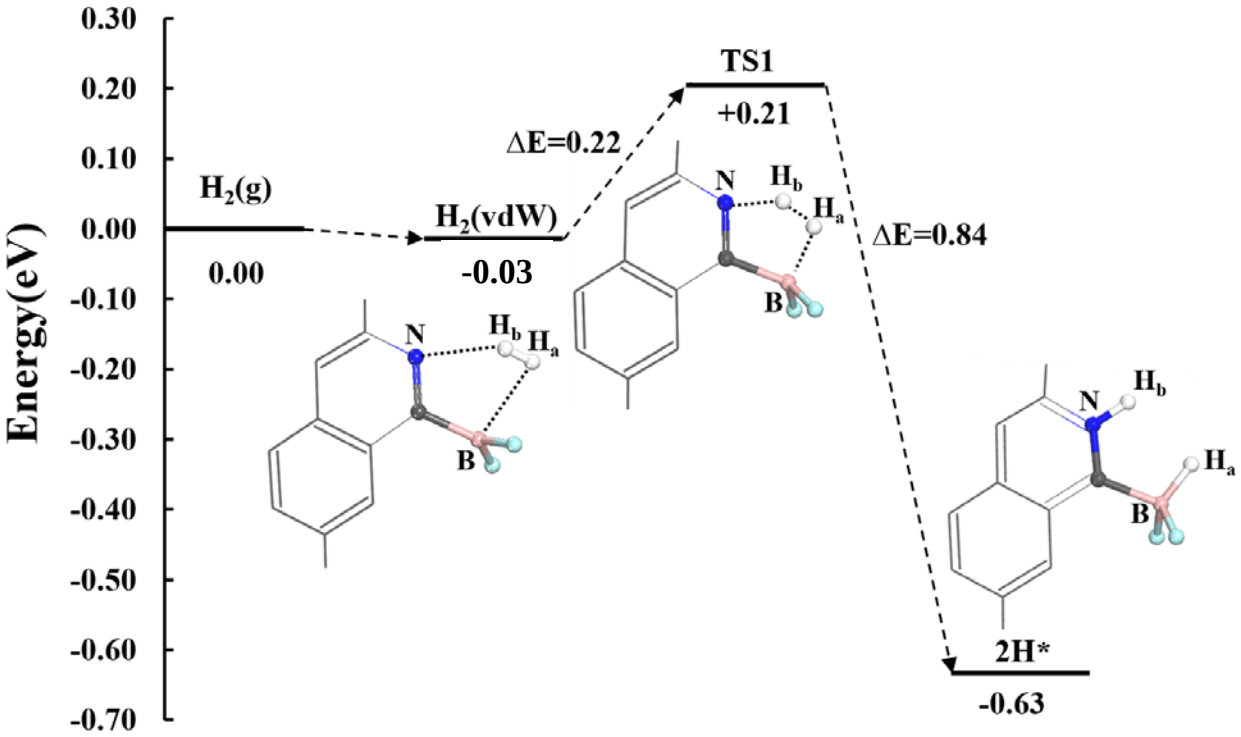


Figure S11. Relative energy profile for the dissociation of H_2 in MIL-140B-NBF_2.

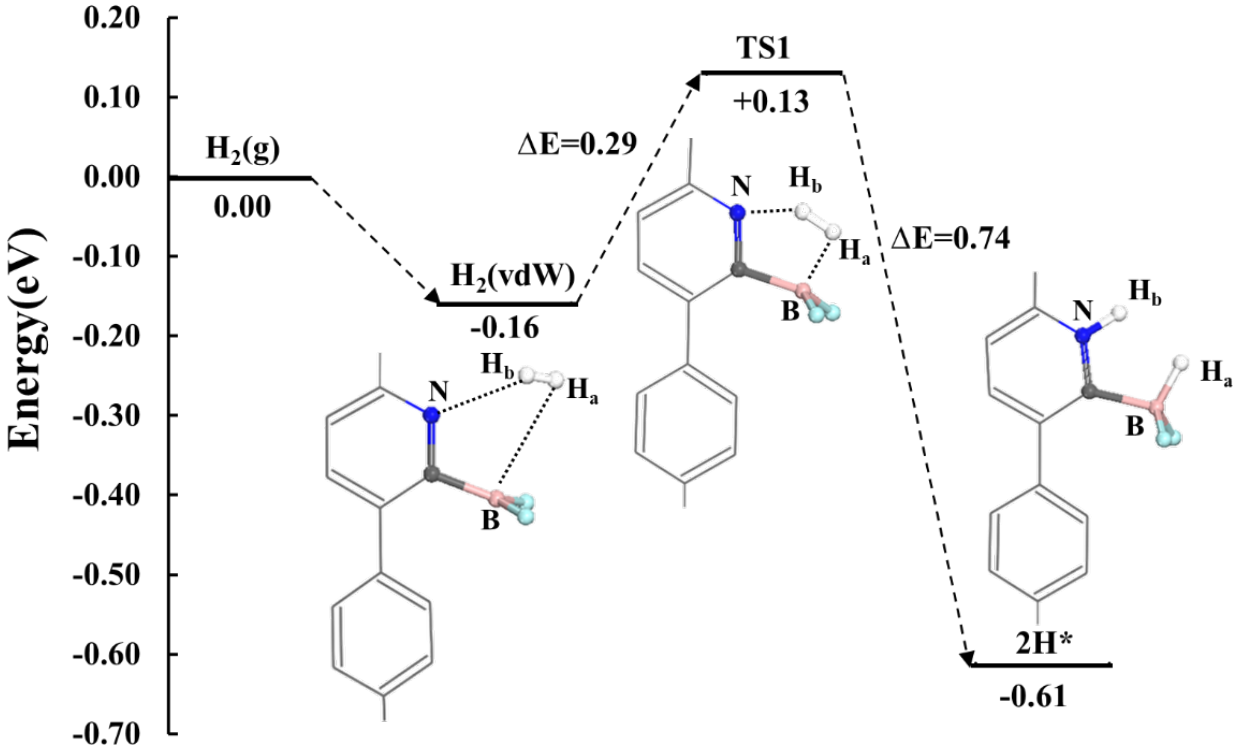


Figure S12. Relative energy profile for the dissociation of H_2 in MIL-140C-NBF_2.

References

1. V. Guillerm, F. Ragon, M. Dan-Hardi, T. Devic, M. Vishnuvarthan, B. Campo, A. Vimont, G. Clet, Q. Yang, G. Maurin, G. Férey, A. Vittadini, S. Gross and C. Serre, *Angew. Chem. Int. Ed.*, 2012, **51**, 9267-9271.
2. J. VandeVondele, M. Krack, F. Mohamed, M. Parrinello, T. Chassaing and J. Hutter, *Comput. Phys. Commun.*, 2005, **167**, 103-128.
3. T. A. Manz and D. S. Sholl, *J. Chem. Theory Comput.*, 2010, **6**, 2455-2468.
4. T. A. Manz and D. S. Sholl, *J. Chem. Theory Comput.*, 2012, **8**, 2844-2867.

MIL-140B atom positions and DDEC charges

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MIL-140B-NBF2 atom positions and DDEC charges

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MIL-140C atom positions and DDEC charges

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MIL-140C-NBF2 atom positions and DDEC charges

225
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