Supporting Information

The DFT/CC correction scheme for the CO_2···H-zeolite interaction

Recently, the DFT/CC method has been proposed for the accurate description of weakly interacting systems.[1, 2] The method is based on the pairwise representability of the DFT error, $\Delta E_{DFT/CC}$, defined as the difference between the CCSD(T) and DFT interaction energies. The above assumption leads to the following equation,

$$\Delta E_{DFT/CC} = \sum_{ij} \varepsilon_{ij}(R_{ij}),$$

where ε_{ij} are the DFT/CC correction functions and R_{ij} are the interatomic distances. The pairwise correction functions are obtained by means of the Reciprocal Power Reproducing Kernel Hilbert Space Interpolation (RP-RKHS); no a priori functional form of correction functions is assumed except for the asymptotic behavior given by the RKHS kernel ($R^{-6} + R^{-8}$). A more detailed description of DFT/CC can be found in Refs.[1, 2]

Correction functions are evaluated from the potential energy surfaces (PES) obtained at the CCSD(T) and DFT levels for a suitable reference set of molecular complexes. For the description of CO_2 interaction with acid zeolites, the pairwise correction functions ε_{ij} were obtained, where *i* stands for C or O atoms of CO_2 molecule and *j* stands for framework O and Si atoms and Brønsted acid group H^+ atom. The framework Al atoms where not explicitly considered, instead correction functions derived for framework Si atoms were used also for Al. Since the reference molecules also contain H atoms (other than a Brønsted acid one) the following correction functions where obtained: ε_{CO}, ε_{CSi}, $\varepsilon_{CH(B)}$, ε_{CH}, ε_{OO}, ε_{OSi}, $\varepsilon_{OH(B)}$, ε_{OH}, where H(B) denotes a Brønsted acid group proton; corresponding reference set is shown in Fig. S1.

The DFT calculations (employing the PBE exchange-correlation functional) where performed with the augmented correlation-consistent valence-quadruple-ς basis set with polarization functions[3] (AVQZ). The CCSD(T)/CBS estimate was obtained using a simple correlation energy dependence on the cardinal number, employing basis sets from Ref. [3] (details given below). All interaction energies were corrected for the basis set superposition error.[4]

The geometry of H_2, CO_2, and H_3O^+ monomers was obtained at the CCSD(T)/AVQZ level and the geometry of $Si(OH)_4$ monomer was optimized at the CCSD(T)/AVTZ level. Correction functions were obtained within the frozen monomer approximation in the following order:

(i) The CO_2···H_2 reference system (Fig. S1a and S1b) provided the ε_{CH} and ε_{OH} correction functions.

(ii) The CO_2···H_2O reference system (Fig. S1c and S1d) provided ε_{CO} and ε_{OO} correction functions, using ε_{CH} and ε_{OH} obtained previously for CO_2···H_2.

(iii) The CO_2···H_3O^+ reference system (Fig. S1e and S1f) provided $\varepsilon_{CH(B)}$ and $\varepsilon_{OH(B)}$ correction functions (for Brønsted acid group proton), using ε_{CO} and ε_{OO} obtained previously for CO_2···H_2O.

(iv) The CO_2···$Si(OH)_4$ reference system (Fig. S1g and S1h) provided ε_{CSi} and ε_{OSi} correction functions, using ε_{CH} and ε_{OH} obtained previously for CO_2···H_2 and ε_{CO} and ε_{OO} obtained previously for CO_2···H_2O.

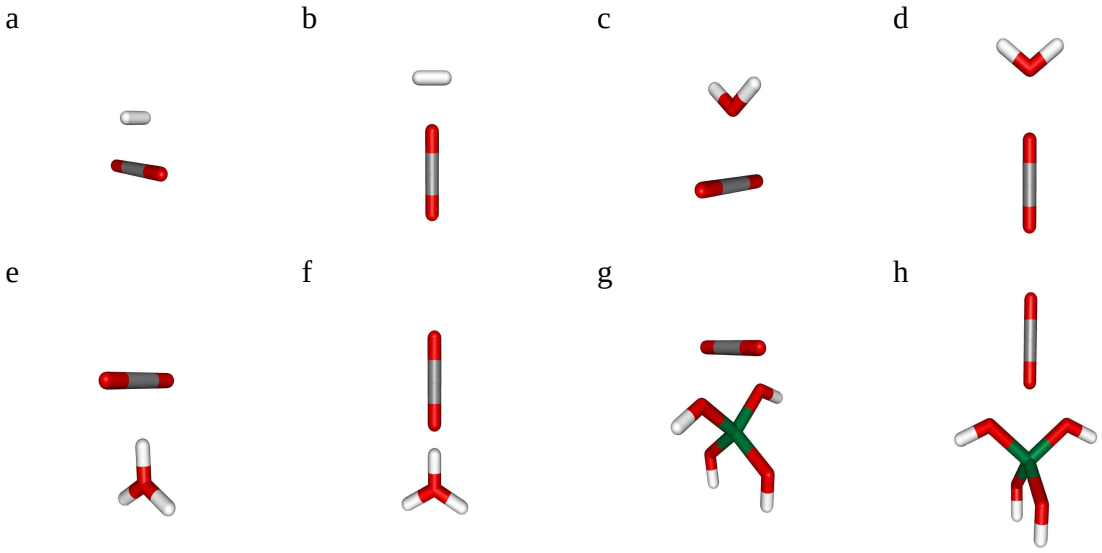

Figure S1 Definition of the reference set used for the generation of the DFT/CC correction functions: $CO_2\cdots H_2$ (a, b), $CO_2\cdots H_2O$ (c, d) $CO_2\cdots H_3O^+$ (e, f), and $CO_2\cdots Si(OH)_4$ (g, h). The C_{2v} symmetry constraints were applied. The C, O, H, and Si atoms are depicted in grey, red, white, and green color, respectively.

All data used for the construction of correction functions are presented in Tables S1-S16 and the correction functions are listed in Table S17. Details about the CCSD(T)/CBS calculations are provided below.

$CO_2\cdots H_2$ and $CO_2\cdots H_2O$

The CBS extrapolation for the CO_2..H_2 and $CO_2\cdots H_2O$ complexes was performed using a simple extrapolation formula, $E_x = E_{CBS} + AX^{-3}$, for the correlation part of the interaction energy (X is the cardinal number of the basis set). The CCSD(T)/AVTZ and CCSD(T)/AVQZ (X= 3, 4) data were used along with HF/AV5Z.

$CO_2\cdots H_3O^+$

The density-fitting MP2 method was employed for the correlation energy extrapolation from AVTZ and AVQZ basis sets (denoted as $E^{MP2\text{-}HF}$). The Hartree-Fock energies were calculated using AV5Z basis set. The CCSD(T)/CBS estimates for the $CO_2\cdots H_3O^+$ complex were obtained according to the formula,

$$E_{CBS}^{CCSD(T)} = E_{AVTZ}^{CCSD(T)} - E_{AVTZ}^{MP2} + E_{CBS}^{MP2-HF} + E_{AV5Z}^{HF}$$

$CO_2\cdots Si(OH)_4$

The density-fitting MP2 method was employed for the correlation energy extrapolation from AVTZ and AVQZ basis sets (denoted as $E^{MP2\text{-}HF}$). The Hartree-Fock energies were calculated using AV5Z basis set. The CCSD(T)/CBS estimates for the $CO_2\cdots Si(OH)_4$ complex were obtained according to the formula,

$$E_{CBS}^{CCSD(T)} = E_{AVDZ}^{CCSD(T)} - E_{AVDZ}^{MP2} + E_{CBS}^{MP2-HF} + E_{AV5Z}^{HF}$$

Transferability check of the DFT/CC correction functions

It is essential to test the reliability of the DFT/CC method; the key assumption of the DFT/CC correction scheme is the transferability of correction functions. Therefore, transferability was checked for the CO_2 interaction with the $(OH)_3Si\text{-}O\text{-}Si(OH)_3$ cluster model (using two different orientations) employing the correction functions obtained for the reference set defined in Fig. S1. Interaction energies calculated at the DFT/CC level (employing correction functions summarized in Table S17) and those calculated at the CCSD(T)/CBS level are depicted in Figure S2. Based on a very good agreement between the results obtained at the CCSD(T)/CBS and DFT/CC levels (Fig. S2) it is concluded that transferability of correction functions is good and that these correction functions can be used for the description of $CO_2\cdots$H-zeolite interactions.

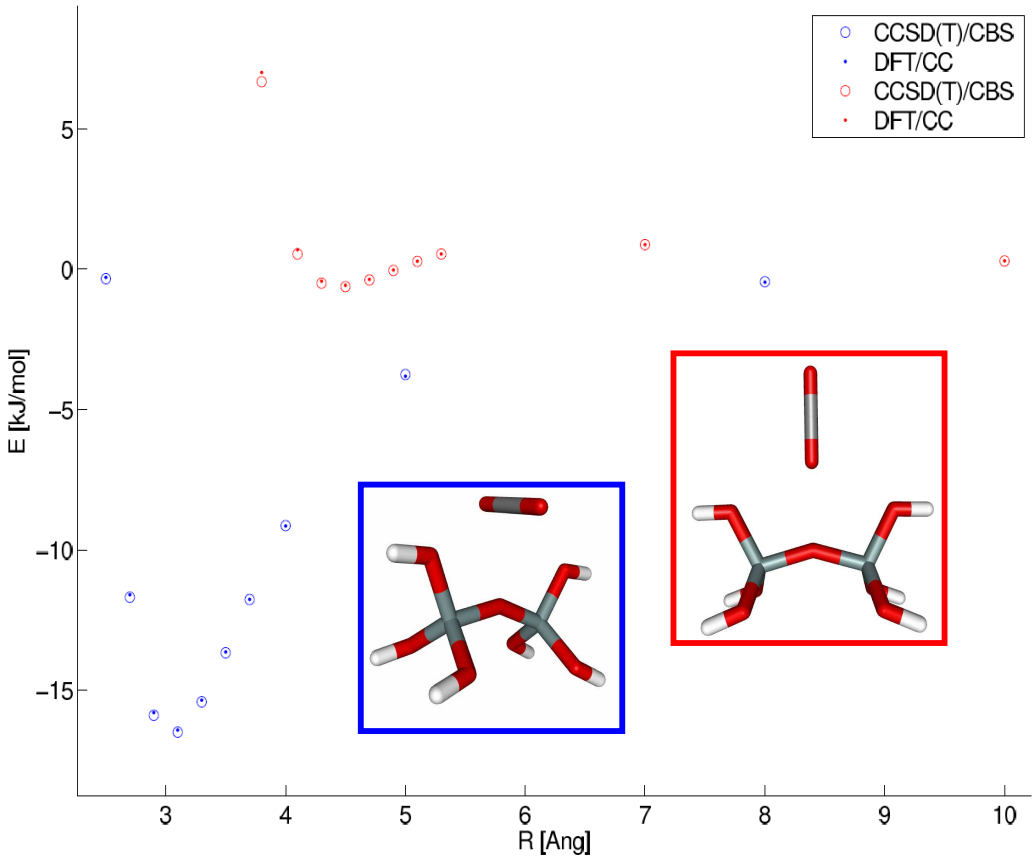

Figure S2. Interaction energies of CO_2 with $(OH)_3Si\text{-}O\text{-}Si(OH)_3$ cluster model calculated at DFT/CC (dots) and CCSD(T)/CBS (circles) levels for the parallel (red) and perpendicular (blue) orientation of CO_2 with respect to the cluster model C_2 axis. *R* is defined as a distance between the C atom of CO_2 and the central O atom of $(OH)_3Si\text{-}O\text{-}Si(OH)_3$ cluster.

References

1 O. Bludsky, M. Rubes, P. Soldan and P. Nachtigall, *J. Chem. Phys.*, 2008, **128**, 114102.
2 M. Rubes, O. Bludsky and P. Nachtigall, *ChemPhysChem*, 2008, **9**, 1702.
3 T. H. Dunning, *J. Chem. Phys.*, 1989, **90**, 1007.
4 S. F. Boys and F. Bernardi, *Mol. Phys.*, 1970, **19**, 553.

Table S1 Interaction energies corrected for BSSE (in Hartrees) for the $CO_2\cdots H_2$ complex.[a]

R	HF/AVTZ	CCSD(T)/AVTZ	HF/AVQZ	CCSD(T)/AVQZ	HF/AV5Z	CCSD(T)/CBS	PBE/AVQZ
1.50	0.09583778	0.08219357	0.09570818	0.08081541	0.09567028	0.07986641	0.07611582
1.80	0.04098015	0.03212223	0.04092021	0.03135960	0.04090095	0.03082757	0.03049951
2.00	0.02210279	0.01570905	0.02207755	0.01521830	0.02206763	0.01486867	0.01546329
2.20	0.01151833	0.00697724	0.01150750	0.00666296	0.01150344	0.00643746	0.00732184
2.40	0.00580734	0.00261499	0.00579906	0.00241008	0.00579821	0.00226573	0.00311981
2.60	0.00282451	0.00059444	0.00281471	0.00045690	0.00281567	0.00036465	0.00106085
2.80	0.00131254	-0.00024090	0.00130165	-0.00033525	0.00130336	-0.00039445	0.00011959
3.10	0.00035933	-0.00054570	0.00034985	-0.00059978	0.00035117	-0.00063100	-0.00034157
3.40	0.00005667	-0.00047693	0.00005032	-0.00050732	0.00005068	-0.00052451	-0.00037315
3.70	-0.00002598	-0.00034714	-0.00002950	-0.00036359	-0.00002977	-0.00037331	-0.00029028
4.00	-0.00004005	-0.00023839	-0.00004166	-0.00024705	-0.00004213	-0.00025267	-0.00019700
4.50	-0.00003065	-0.00012527	-0.00003074	-0.00012811	-0.00003104	-0.00013042	-0.00008871
5.00	-0.00001955	-0.00006822	-0.00001922	-0.00006913	-0.00001932	-0.00007015	-0.00003738
6.00	-0.00000793	-0.00002346	-0.00000778	-0.00002369	-0.00000776	-0.00002394	-0.00000796
7.00	-0.00000362	-0.00000957	-0.00000356	-0.00000971	-0.00000357	-0.00000985	-0.00000274
10.00	-0.00000060	-0.00000123	-0.00000059	-0.00000135	-0.00000060	-0.00000145	-0.00000041
15.00	-0.00000008	-0.00000011	-0.00000008	-0.00000023	-0.00000009	-0.00000033	-0.00000005

[a] Distance between C atom of CO_2 and center of mass of hydrogen (in Å); see Fig. S1a.

Table S2 Difference between CCSD(T)/CBS and PBE/AVQZ interaction energies, ΔE, and C-H and O-H contributions to $\Delta E_{DFT/CC}$ evaluated using correction functions given in Table S17 (in Hartrees) for the $CO_2\cdots H_2$ complex.[a]

R	ΔE	E_{CH}	E_{OH}
1.50	0.00375058	0.00406775	-0.00031717
1.80	0.00032807	0.00116440	-0.00083634
2.00	-0.00059461	0.00019559	-0.00079021
2.20	-0.00088438	-0.00025543	-0.00062895
2.40	-0.00085408	-0.00040907	-0.00044501
2.60	-0.00069620	-0.00040965	-0.00028655
2.80	-0.00051404	-0.00034366	-0.00017038
3.10	-0.00028943	-0.00021669	-0.00007274
3.40	-0.00015135	-0.00011465	-0.00003670
3.70	-0.00008304	-0.00005225	-0.00003079
4.00	-0.00005566	-0.00002096	-0.00003470
4.50	-0.00004171	-0.00000474	-0.00003697
5.00	-0.00003276	-0.00000237	-0.00003039
6.00	-0.00001598	-0.00000111	-0.00001487
7.00	-0.00000711	-0.00000066	-0.00000645
10.00	-0.00000104	-0.00000051	-0.00000053
15.00	-0.00000027	-0.00000021	-0.00000006

[a] Distance between C atom of CO_2 and center of mass of hydrogen (in Å); see Fig. S1a.

Table S3 Interaction energies corrected for BSSE (in Hartrees) for the $CO_2 \cdots H_2$ complex.[a]

R	HF/AVTZ	CCSD(T)/AVTZ	HF/AVQZ	CCSD(T)/AVQZ	HF/AV5Z	CCSD(T)/CBS	PBE/AVQZ
2.60	0.11911420	0.10684647	0.11906953	0.10592231	0.11905045	0.10526144	0.10188577
2.80	0.06310838	0.05486618	0.06305399	0.05421088	0.06304678	0.05376515	0.05301082
3.00	0.03275316	0.02716217	0.03270784	0.02672129	0.03270385	0.02642865	0.02669788
3.20	0.01675284	0.01294104	0.01672863	0.01266104	0.01672467	0.01247042	0.01303486
3.40	0.00848630	0.00587529	0.00847978	0.00570421	0.00847692	0.00558125	0.00613099
3.60	0.00428281	0.00248432	0.00428498	0.00238105	0.00428380	0.00230293	0.00273085
3.80	0.00217182	0.00092479	0.00217559	0.00086185	0.00217567	0.00081323	0.00110632
4.00	0.00111985	0.00024870	0.00112228	0.00020945	0.00112304	0.00017980	0.00036333
4.20	0.00059626	-0.00001752	0.00059715	-0.00004257	0.00059814	-0.00006050	0.00004771
4.40	0.00033375	-0.00010301	0.00033378	-0.00011928	0.00033472	-0.00013023	-0.00006720
4.70	0.00015905	-0.00010892	0.00015866	-0.00011781	0.00015937	-0.00012330	-0.00009069
5.00	0.00009016	-0.00007941	0.00008964	-0.00008450	0.00009014	-0.00008733	-0.00006251
5.50	0.00004708	-0.00003801	0.00004648	-0.00004012	0.00004672	-0.00004099	-0.00001633
6.00	0.00002953	-0.00001685	0.00002902	-0.00001780	0.00002908	-0.00001807	0.00000367
7.00	0.00001384	-0.00000278	0.00001355	-0.00000315	0.00001350	-0.00000327	0.00000790
10.00	0.00000236	0.00000056	0.00000232	0.00000041	0.00000230	0.00000031	0.00000164
15.00	0.00000031	0.00000016	0.00000031	0.00000003	0.00000030	-0.00000006	0.00000022

[a] Distance between C atom of CO_2 and center of mass of hydrogen (in Å); see Fig. S1b.

Table S4 Difference between CCSD(T)/CBS and PBE/AVQZ interaction energies, ΔE, and C-H and O-H contributions to $\Delta E_{DFT/CC}$ evaluated using correction functions given in Table S17 (in Hartrees) for the $CO_2 \cdots H_2$ complex.[a]

R	ΔE	E_{CH}	E_{OH}
2.60	0.00337566	-0.00040965	0.00378532
2.80	0.00075433	-0.00034366	0.00109799
3.00	-0.00026923	-0.00025807	-0.00001115
3.20	-0.00056444	-0.00017840	-0.00038604
3.40	-0.00054975	-0.00011465	-0.00043509
3.60	-0.00042792	-0.00006899	-0.00035893
3.80	-0.00029309	-0.00003901	-0.00025409
4.00	-0.00018353	-0.00002096	-0.00016257
4.20	-0.00010822	-0.00001114	-0.00009707
4.40	-0.00006303	-0.00000614	-0.00005689
4.70	-0.00003261	-0.00000322	-0.00002939
5.00	-0.00002482	-0.00000237	-0.00002245
5.50	-0.00002466	-0.00000160	-0.00002306
6.00	-0.00002174	-0.00000111	-0.00002063
7.00	-0.00001117	-0.00000066	-0.00001051
10.00	-0.00000133	-0.00000051	-0.00000082
15.00	-0.00000028	-0.00000021	-0.00000007

[a] Distance between C atom of CO_2 and center of mass of hydrogen (in Å); see Fig. S1b.

Table S5 Interaction energies corrected for BSSE (in Hartrees) for the $CO_2\cdots H_2O$ complex.[a]

R	HF/AVTZ	CCSD(T)/AVTZ	HF/AVQZ	CCSD(T)/AVQZ	HF/AV5Z	CCSD(T)/CBS	PBE/AVQZ
2.00	0.03848429	0.03216494	0.03837318	0.03091808	0.03835308	0.03006920	0.03284316
2.20	0.01705948	0.01230358	0.01698110	0.01151644	0.01696874	0.01098688	0.01385740
2.40	0.00630013	0.00285351	0.00624402	0.00235973	0.00623634	0.00203267	0.00453944
2.60	0.00125338	-0.00118906	0.00121524	-0.00149594	0.00120912	-0.00169816	0.00029105
2.80	-0.00089928	-0.00260047	-0.00092306	-0.00279058	-0.00092945	-0.00291835	-0.00142889
3.00	-0.00166136	-0.00282750	-0.00167451	-0.00294650	-0.00168105	-0.00303029	-0.00195260
3.20	-0.00179699	-0.00258386	-0.00180224	-0.00265913	-0.00180830	-0.00271629	-0.00194970
3.40	-0.00167729	-0.00219943	-0.00167669	-0.00224715	-0.00168186	-0.00228759	-0.00174179
3.60	-0.00147368	-0.00181347	-0.00146926	-0.00184376	-0.00147332	-0.00187315	-0.00147887
3.80	-0.00126025	-0.00147593	-0.00125398	-0.00149538	-0.00125684	-0.00151703	-0.00122559
4.00	-0.00106563	-0.00119775	-0.00105902	-0.00121063	-0.00106081	-0.00122663	-0.00100315
4.20	-0.00089822	-0.00097466	-0.00089221	-0.00098360	-0.00089318	-0.00099548	-0.00081810
4.40	-0.00075806	-0.00079771	-0.00075302	-0.00080428	-0.00075345	-0.00081318	-0.00066711
4.60	-0.00064209	-0.00065772	-0.00063806	-0.00066278	-0.00063818	-0.00066954	-0.00054673
4.80	-0.00054650	-0.00054669	-0.00054331	-0.00055068	-0.00054330	-0.00055590	-0.00045084
5.00	-0.00046766	-0.00045815	-0.00046507	-0.00046126	-0.00046503	-0.00046538	-0.00037482
5.50	-0.00032439	-0.00030462	-0.00032259	-0.00030614	-0.00032264	-0.00030863	-0.00024670
6.00	-0.00023202	-0.00021103	-0.00023062	-0.00021173	-0.00023073	-0.00021338	-0.00017152
8.00	-0.00007616	-0.00006438	-0.00007564	-0.00006446	-0.00007573	-0.00006498	-0.00005503
10.00	-0.00003193	-0.00002608	-0.00003170	-0.00002611	-0.00003176	-0.00002637	-0.00002307
12.00	-0.00001565	-0.00001252	-0.00001552	-0.00001256	-0.00001557	-0.00001273	-0.00001131
15.00	-0.00000651	-0.00000511	-0.00000646	-0.00000515	-0.00000650	-0.00000526	-0.00000471
20.00	-0.00000210	-0.00000159	-0.00000208	-0.00000164	-0.00000210	-0.00000172	-0.00000152

[a] Distance between C atom of CO_2 and O atom from water (in Å); see Fig. S1c.

Table S6 Difference between CCSD(T)/CBS and PBE/AVQZ interaction energies, ΔE, and C-H, O-H, C-O, and O-O contributions to $\Delta E_{DFT/CC}$ evaluated using correction functions given in Table S17 (in Hartrees) for the $CO_2\cdots H_2O$ complex.[a]

R	ΔE	E_{CH}	E_{OH}	E_{CO}	E_{OO}
2.00	-0.00277396	-0.00039083	-0.00024029	-0.00083624	-0.00130660
2.20	-0.00287052	-0.00031630	-0.00014208	-0.00145556	-0.00095658
2.40	-0.00250678	-0.00023293	-0.00008136	-0.00163237	-0.00056012
2.60	-0.00198921	-0.00015885	-0.00004864	-0.00155801	-0.00022371
2.80	-0.00148947	-0.00010118	-0.00003424	-0.00137514	0.00002110
3.00	-0.00107769	-0.00006046	-0.00003065	-0.00116516	0.00017858
3.20	-0.00076659	-0.00003404	-0.00003238	-0.00096655	0.00026639
3.40	-0.00054580	-0.00001833	-0.00003529	-0.00079871	0.00030654
3.60	-0.00039428	-0.00000986	-0.00003714	-0.00066488	0.00031759
3.80	-0.00029144	-0.00000555	-0.00003726	-0.00055937	0.00031075
4.00	-0.00022349	-0.00000358	-0.00003586	-0.00047904	0.00029499
4.20	-0.00017738	-0.00000274	-0.00003319	-0.00041774	0.00027628
4.40	-0.00014608	-0.00000231	-0.00002984	-0.00037136	0.00025745
4.60	-0.00012281	-0.00000197	-0.00002635	-0.00033416	0.00023966
4.80	-0.00010506	-0.00000169	-0.00002298	-0.00030369	0.00022333
5.00	-0.00009056	-0.00000145	-0.00001987	-0.00027778	0.00020853
5.50	-0.00006193	-0.00000102	-0.00001346	-0.00022502	0.00017758
6.00	-0.00004186	-0.00000077	-0.00000891	-0.00018518	0.00015299
8.00	-0.00000994	-0.00000057	-0.00000156	-0.00009090	0.00008307
10.00	-0.00000330	-0.00000046	-0.00000036	-0.00004692	0.00004447
12.00	-0.00000142	-0.00000033	-0.00000014	-0.00002403	0.00002302
15.00	-0.00000055	-0.00000018	-0.00000005	-0.00000887	0.00000860
20.00	-0.00000021	-0.00000005	-0.00000001	-0.00000201	0.00000197

[a] Distance between C atom of CO_2 and O atom from water (in Å); see Fig. S1c.

Table S7 Interaction energies corrected for BSSE (in Hartrees) for the $CO_2\cdots H_2O$ complex.[a]

R	HF/AVTZ	CCSD(T)/AVTZ	HF/AVQZ	CCSD(T)/AVQZ	HF/AV5Z	CCSD(T)/CBS	PBE/AVQZ
3.00	0.08033767	0.06909543	0.08033075	0.06811290	0.08033650	0.06740672	0.06833609
3.20	0.03997724	0.03259885	0.03996128	0.03200337	0.03997172	0.03159091	0.03324675
3.40	0.02035172	0.01529737	0.02034586	0.01494834	0.02035619	0.01470825	0.01623906
3.60	0.01080844	0.00724089	0.01080918	0.00703915	0.01081787	0.00690008	0.00807440
3.80	0.00612375	0.00354746	0.00612400	0.00342997	0.00613188	0.00335193	0.00416788
4.00	0.00377262	0.00187714	0.00376926	0.00180792	0.00377646	0.00176707	0.00229975
4.20	0.00254582	0.00112895	0.00253798	0.00108704	0.00254408	0.00106827	0.00140365
4.40	0.00186594	0.00079220	0.00185430	0.00076428	0.00185900	0.00075709	0.00096744
4.60	0.00145730	0.00063302	0.00144365	0.00061217	0.00144694	0.00061022	0.00074597
4.80	0.00118817	0.00054714	0.00117455	0.00053057	0.00117667	0.00053053	0.00062347
5.00	0.00099535	0.00049018	0.00098324	0.00047701	0.00098453	0.00047753	0.00054581
5.50	0.00068068	0.00038532	0.00067331	0.00037871	0.00067386	0.00037980	0.00042110
6.00	0.00048791	0.00030161	0.00048299	0.00029819	0.00048343	0.00029972	0.00032824
8.00	0.00016135	0.00011424	0.00015985	0.00011356	0.00015989	0.00011420	0.00011714
10.00	0.00006742	0.00004972	0.00006683	0.00004945	0.00006681	0.00004966	0.00004909
12.00	0.00003287	0.00002470	0.00003259	0.00002455	0.00003256	0.00002461	0.00002393
15.00	0.00001358	0.00001037	0.00001348	0.00001028	0.00001345	0.00001026	0.00000989
20.00	0.00000433	0.00000337	0.00000430	0.00000330	0.00000427	0.00000325	0.00000315

[a] Distance between C atom of CO_2 and O atom from water (in Å); see Fig. S1d.

Table S8 Difference between CCSD(T)/CBS and PBE/AVQZ interaction energies, ΔE, and C-H, O-H, C-O, and O-O contributions to $\Delta E_{DFT/CC}$ evaluated using correction functions given in Table S17 (in Hartrees) for the $CO_2\cdots H_2O$ complex.[a]

R	ΔE	E_{CH}	E_{OH}	E_{CO}	E_{OO}
3.00	-0.00092937	-0.00006046	-0.00031943	-0.00116516	0.00061568
3.20	-0.00165584	-0.00003404	-0.00021992	-0.00096655	-0.00043532
3.40	-0.00153082	-0.00001833	-0.00013892	-0.00079871	-0.00057485
3.60	-0.00117432	-0.00000986	-0.00008307	-0.00066488	-0.00041652
3.80	-0.00081594	-0.00000555	-0.00004969	-0.00055937	-0.00020133
4.00	-0.00053268	-0.00000358	-0.00003220	-0.00047904	-0.00001787
4.20	-0.00033538	-0.00000274	-0.00002458	-0.00041774	0.00010967
4.40	-0.00021035	-0.00000231	-0.00002239	-0.00037136	0.00018571
4.60	-0.00013575	-0.00000197	-0.00002260	-0.00033416	0.00022299
4.80	-0.00009294	-0.00000169	-0.00002309	-0.00030369	0.00023553
5.00	-0.00006827	-0.00000145	-0.00002292	-0.00027778	0.00023389
5.50	-0.00004130	-0.00000102	-0.00001936	-0.00022502	0.00020411
6.00	-0.00002852	-0.00000077	-0.00001399	-0.00018518	0.00017141
8.00	-0.00000294	-0.00000057	-0.00000268	-0.00009090	0.00009121
10.00	0.00000056	-0.00000046	-0.00000052	-0.00004692	0.00004843
12.00	0.00000067	-0.00000033	-0.00000017	-0.00002403	0.00002530
15.00	0.00000037	-0.00000018	-0.00000006	-0.00000887	0.00000939
20.00	0.00000010	-0.00000005	-0.00000001	-0.00000201	0.00000210

[a] Distance between C atom of CO_2 and O atom from water (in Å); see Fig. S1d.

Table S9 Interaction energies corrected for BSSE (in Hartrees) for the $CO_2\cdots H_3O^+$ complex.[a]

R	HF/AVTZ	MP2/AVTZ	CCSD(T)/AVTZ	HF/AVQZ	MP2/AVQZ	HF/AV5Z	CCSD(T)/CBS	PBE/AVQZ
2.60	0.03530690	0.02043589	0.02154919	0.03519569	0.01994653	0.03518065	0.02076885	0.01756492
2.80	0.02123376	0.01055652	0.01124727	0.02117075	0.01026854	0.02116009	0.01078445	0.00881708
3.00	0.01372381	0.00596342	0.00642410	0.01369857	0.00581089	0.01369134	0.00617145	0.00492033
3.20	0.00957143	0.00385753	0.00419224	0.00956255	0.00377714	0.00955805	0.00405517	0.00321844
3.40	0.00714183	0.00287323	0.00313556	0.00713932	0.00282972	0.00713745	0.00306026	0.00246884
3.60	0.00561549	0.00237488	0.00259132	0.00561507	0.00234991	0.00561607	0.00254945	0.00211350
3.80	0.00458466	0.00208243	0.00226638	0.00458202	0.00206375	0.00458601	0.00223999	0.00191273
4.00	0.00384307	0.00187763	0.00203613	0.00383409	0.00185688	0.00384057	0.00201329	0.00176844
4.20	0.00328192	0.00171195	0.00184951	0.00326464	0.00168531	0.00327234	0.00182374	0.00164307
4.40	0.00284005	0.00156564	0.00168548	0.00281547	0.00153351	0.00282296	0.00165534	0.00152361
4.60	0.00248105	0.00143095	0.00153563	0.00245224	0.00139629	0.00245847	0.00150293	0.00140692
4.80	0.00218268	0.00130566	0.00139732	0.00215305	0.00127170	0.00215751	0.00136469	0.00129415
5.00	0.00193104	0.00118981	0.00127029	0.00190304	0.00115871	0.00190569	0.00123958	0.00118655
5.20	0.00171687	0.00108384	0.00115476	0.00169170	0.00105644	0.00169280	0.00112682	0.00108528
5.40	0.00153343	0.00098782	0.00105053	0.00151130	0.00096404	0.00151129	0.00102554	0.00099152
6.00	0.00111968	0.00075399	0.00079845	0.00110475	0.00073827	0.00110365	0.00078105	0.00075685
7.00	0.00070898	0.00049902	0.00052596	0.00070068	0.00049035	0.00069999	0.00051633	0.00049810
10.00	0.00024938	0.00018590	0.00019456	0.00024691	0.00018336	0.00024686	0.00019192	0.00018432
15.00	0.00007637	0.00005879	0.00006129	0.00007570	0.00005811	0.00007571	0.00006060	0.00005830

[a] Distance between C atom of CO_2 and O atom from H_3O^+ (in Å); see Fig. S1e.

Table S10 Difference between CCSD(T)/CBS and PBE/AVQZ interaction energies, ΔE, and C-H(B), O-H(B), C-O, and O-O contributions to $\Delta E_{DFT/CC}$ evaluated using correction functions given in Table S17 (in Hartrees) for the $CO_2\cdots H_3O^+$ complex;[a] H(B) denotes the Brønsted acid group proton.

R	ΔE	$E_{CH(B)}$	$E_{OH(B)}$	E_{CO}	E_{OO}
2.60	0.00320393	0.00737656	-0.00239090	-0.00155801	-0.00022371
2.80	0.00196737	0.00584280	-0.00252139	-0.00137514	0.00002110
3.00	0.00125112	0.00478697	-0.00254927	-0.00116516	0.00017858
3.20	0.00083673	0.00405010	-0.00251320	-0.00096655	0.00026639
3.40	0.00059142	0.00352455	-0.00244095	-0.00079871	0.00030654
3.60	0.00043594	0.00313274	-0.00234951	-0.00066488	0.00031759
3.80	0.00032727	0.00282126	-0.00224537	-0.00055937	0.00031075
4.00	0.00024484	0.00256132	-0.00213243	-0.00047904	0.00029499
4.20	0.00018067	0.00233432	-0.00201220	-0.00041774	0.00027628
4.40	0.00013172	0.00213501	-0.00188938	-0.00037136	0.00025745
4.60	0.00009601	0.00195975	-0.00176924	-0.00033416	0.00023966
4.80	0.00007054	0.00180510	-0.00165420	-0.00030369	0.00022333
5.00	0.00005303	0.00166857	-0.00154629	-0.00027778	0.00020853
5.20	0.00004155	0.00154745	-0.00144631	-0.00025479	0.00019520
5.40	0.00003401	0.00143903	-0.00135383	-0.00023435	0.00018317
6.00	0.00002421	0.00116890	-0.00111251	-0.00018518	0.00015299
7.00	0.00001822	0.00085399	-0.00082162	-0.00012765	0.00011350
10.00	0.00000761	0.00037482	-0.00036477	-0.00004692	0.00004447
15.00	0.00000230	0.00010048	-0.00009791	-0.00000887	0.00000860

[a] Distance between C atom of CO_2 and O atom from H_3O^+ (in Å); see Fig. S1e.

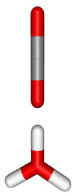

Table S11 Interaction energies corrected for BSSE (in Hartrees) for the $CO_2\cdots H_3O^+$ complex.[a]

R	HF/AVTZ	MP2/AVTZ	CCSD(T)/AVTZ	HF/AVQZ	MP2/AVQZ	HF/AV5Z	CCSD(T)/CBS	PBE/AVQZ
3.00	0.14166102	0.13279271	0.13354482	0.14105304	0.13045051	0.14090614	0.12979022	0.12802453
3.20	0.03407510	0.02697429	0.02735316	0.03385272	0.02576474	0.03378248	0.02535301	0.02367887
3.40	-0.00475463	-0.01001910	-0.00994031	-0.00484484	-0.01067117	-0.00488867	-0.01104622	-0.01232528
3.60	-0.01735533	-0.02094742	-0.02106684	-0.01742560	-0.02133235	-0.01745210	-0.02170788	-0.02253242
3.80	-0.01969910	-0.02197110	-0.02218401	-0.01978261	-0.02222021	-0.01979946	-0.02257083	-0.02304567
4.00	-0.01832037	-0.01963538	-0.01986739	-0.01840235	-0.01979939	-0.01841701	-0.02010592	-0.02035441
4.20	-0.01590103	-0.01656085	-0.01677340	-0.01595654	-0.01665530	-0.01597179	-0.01691149	-0.01702636
4.40	-0.01345493	-0.01368647	-0.01386705	-0.01348114	-0.01372968	-0.01349660	-0.01393812	-0.01397468
4.60	-0.01131120	-0.01127351	-0.01142299	-0.01131722	-0.01128586	-0.01133161	-0.01145434	-0.01143975
4.80	-0.00953481	-0.00933455	-0.00945826	-0.00952740	-0.00932908	-0.00953977	-0.00946657	-0.00941409
5.00	-0.00809339	-0.00780053	-0.00790431	-0.00807614	-0.00778402	-0.00808609	-0.00789829	-0.00781701
5.20	-0.00692710	-0.00658673	-0.00667538	-0.00690331	-0.00656379	-0.00691077	-0.00666052	-0.00655931
5.40	-0.00597770	-0.00561822	-0.00569526	-0.00595088	-0.00559269	-0.00595617	-0.00567595	-0.00556373
6.00	-0.00400976	-0.00367147	-0.00372604	-0.00398697	-0.00365055	-0.00398929	-0.00370882	-0.00360139
7.00	-0.00230337	-0.00205555	-0.00209074	-0.00228888	-0.00204160	-0.00229040	-0.00207871	-0.00201426
10.00	-0.00069368	-0.00059794	-0.00061095	-0.00068926	-0.00059344	-0.00068951	-0.00060664	-0.00059085
15.00	-0.00018990	-0.00015999	-0.00016404	-0.00018868	-0.00015874	-0.00018874	-0.00016283	-0.00015877

[a] Distance between C atom of CO_2 and O atom from H_3O^+ (in Å); see Fig. S1f.

Table S12 Difference between CCSD(T)/CBS and PBE/AVQZ interaction energies, ΔE, and C-H(B), O-H(B), C-O, and O-O contributions to $\Delta E_{DFT/CC}$ evaluated using correction functions given in Table S17 (in Hartrees) for the $CO_2\cdots H_3O^+$ complex;[a] H(B) denotes the Brønsted acid group proton.

R	ΔE	$E_{CH(B)}$	$E_{OH(B)}$	E_{CO}	E_{OO}
3.00	0.00176569	0.00460465	-0.00185606	-0.00116516	0.00061566
3.20	0.00167414	0.00385334	-0.00047598	-0.00096655	-0.00043533
3.40	0.00127907	0.00332775	-0.00048258	-0.00079871	-0.00057485
3.60	0.00082454	0.00294406	-0.00092223	-0.00066488	-0.00041651
3.80	0.00047484	0.00264425	-0.00134021	-0.00055937	-0.00020132
4.00	0.00024849	0.00239682	-0.00160886	-0.00047904	-0.00001786
4.20	0.00011486	0.00217980	-0.00172665	-0.00041774	0.00010967
4.40	0.00003656	0.00199078	-0.00174298	-0.00037136	0.00018572
4.60	-0.00001460	0.00182611	-0.00170479	-0.00033416	0.00022299
4.80	-0.00005247	0.00168152	-0.00164088	-0.00030369	0.00023553
5.00	-0.00008128	0.00155459	-0.00156711	-0.00027778	0.00023389
5.20	-0.00010122	0.00144273	-0.00148924	-0.00025479	0.00022409
5.40	-0.00011222	0.00134311	-0.00140948	-0.00023435	0.00021100
6.00	-0.00010743	0.00109553	-0.00117330	-0.00018518	0.00017141
7.00	-0.00006445	0.00081795	-0.00087083	-0.00012765	0.00012361
10.00	-0.00001578	0.00039297	-0.00040917	-0.00004692	0.00004843
15.00	-0.00000405	0.00011809	-0.00012240	-0.00000887	0.00000939

[a] Distance between C atom of CO_2 and O atom from H_3O^+ (in Å); see Fig. S1f.

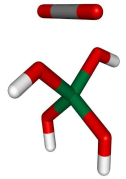

Table S13 Interaction energies corrected for BSSE (in Hartrees) for the $CO_2 \cdots Si(OH)_4$ complex.

R	MP2/AVDZ	CCSD(T)/AVDZ	HF/AVTZ	MP2/AVTZ	HF/AVQZ	MP2/AVQZ	HF/AV5Z	CCSD(T)/CBS	PBE/AVQZ
2.40	0.14596698	0.14750059	0.15666306	0.13544058	0.15628585	0.13208906	0.15617723	0.13134361	0.13611612
2.80	0.04039226	0.04077528	0.04813944	0.03580161	0.04797644	0.03427161	0.04792153	0.03360219	0.04032678
3.20	0.00524184	0.00512779	0.01006423	0.00342550	0.00998463	0.00275613	0.00995300	0.00218007	0.00753350
3.40	-0.00070086	-0.00089822	0.00294808	-0.00184119	0.00290354	-0.00226712	0.00287810	-0.00276825	0.00157923
3.60	-0.00319785	-0.00341797	-0.00050100	-0.00392612	-0.00051954	-0.00419112	-0.00054034	-0.00461191	-0.00121539
3.80	-0.00393712	-0.00414648	-0.00197759	-0.00440721	-0.00198007	-0.00457074	-0.00199634	-0.00491389	-0.00232652
4.00	-0.00385583	-0.00403916	-0.00245022	-0.00416038	-0.00244413	-0.00426132	-0.00245594	-0.00453456	-0.00259821
4.20	-0.00344319	-0.00359644	-0.00244728	-0.00364192	-0.00243705	-0.00370414	-0.00244492	-0.00391813	-0.00247519
4.40	-0.00293996	-0.00306503	-0.00224389	-0.00307177	-0.00223194	-0.00310984	-0.00223685	-0.00327632	-0.00219648
4.60	-0.00245551	-0.00255667	-0.00197596	-0.00254443	-0.00196371	-0.00256753	-0.00196660	-0.00269738	-0.00188276
4.80	-0.00203196	-0.00211384	-0.00170622	-0.00209204	-0.00169456	-0.00210603	-0.00169626	-0.00220831	-0.00158039
5.00	-0.00167866	-0.00174527	-0.00146048	-0.00171820	-0.00144993	-0.00172675	-0.00145100	-0.00180839	-0.00131479
5.20	-0.00139051	-0.00144513	-0.00124684	-0.00141493	-0.00123759	-0.00142029	-0.00123838	-0.00148636	-0.00108721
5.40	-0.00115755	-0.00120274	-0.00106532	-0.00117092	-0.00105740	-0.00117438	-0.00105805	-0.00122852	-0.00090022
6.00	-0.00096936	-0.00100710	-0.00067837	-0.00068990	-0.00067343	-0.00069063	-0.00067382	-0.00073291	-0.00052591
6.50	-0.00069246	-0.00071956	-0.00048007	-0.00046466	-0.00047652	-0.00046451	-0.00047673	-0.00049430	-0.00035384
7.00	-0.00032953	-0.00034317	-0.00034881	-0.00032445	-0.00034624	-0.00032410	-0.00034635	-0.00033946	-0.00024987
8.00	-0.00017640	-0.00018428	-0.00019704	-0.00017272	-0.00019565	-0.00017242	-0.00019573	-0.00018118	-0.00013833
9.00	-0.00010328	-0.00010825	-0.00011982	-0.00010076	-0.00011897	-0.00010054	-0.00011907	-0.00010607	-0.00008372
10.00	-0.00006473	-0.00006809	-0.00007719	-0.00006298	-0.00007664	-0.00006282	-0.00007672	-0.00006655	-0.00005388
12.00	-0.00002949	-0.00003127	-0.00003645	-0.00002858	-0.00003618	-0.00002851	-0.00003623	-0.00003050	-0.00002543
15.00	-0.00001160	-0.00001254	-0.00001477	-0.00001121	-0.00001464	-0.00001118	-0.00001468	-0.00001223	-0.00001030

[a] Distance between C atom of CO_2 and Si atom from $Si(OH)_4$ (in Å); see Fig. S1g.

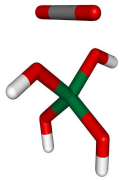

Table S14 Difference between CCSD(T)/CBS and PBE/AVQZ interaction energies, ΔE, and C-H, O-H, C-O, O-O, CSi, and OSi contributions to $\Delta E_{DFT/CC}$ evaluated using correction functions given in Table S17 (in Hartrees) for the $CO_2 \cdots Si(OH)_4$ complex.[a]

R	ΔE	E_{CH}	E_{OH}	E_{CO}	E_{OO}	E_{CSi}	E_{OSi}
2.40	-0.00477251	-0.00036980	-0.00023217	-0.00202259	-0.00232509	0.00113350	-0.00095637
2.80	-0.00672459	-0.00025324	-0.00012398	-0.00378045	-0.00142741	0.00056908	-0.00170859
3.20	-0.00535343	-0.00014141	-0.00006904	-0.00397765	-0.00019347	0.00059843	-0.00157029
3.40	-0.00434748	-0.00009799	-0.00005665	-0.00365491	0.00028244	0.00058871	-0.00140907
3.60	-0.00339652	-0.00006462	-0.00005080	-0.00323718	0.00062363	0.00058081	-0.00124836
3.80	-0.00258736	-0.00004064	-0.00004907	-0.00280632	0.00083923	0.00056966	-0.00110021
4.00	-0.00193635	-0.00002455	-0.00004905	-0.00240559	0.00095290	0.00055351	-0.00096361
4.20	-0.00144294	-0.00001462	-0.00004905	-0.00206094	0.00099484	0.00052311	-0.00083617
4.40	-0.00107985	-0.00000886	-0.00004815	-0.00177663	0.00099127	0.00048349	-0.00072115
4.60	-0.00081462	-0.00000570	-0.00004620	-0.00154396	0.00095835	0.00044783	-0.00062473
4.80	-0.00062792	-0.00000413	-0.00004331	-0.00135848	0.00091032	0.00041662	-0.00054887
5.00	-0.00049360	-0.00000338	-0.00003961	-0.00120964	0.00085733	0.00039065	-0.00048961
5.20	-0.00039915	-0.00000296	-0.00003553	-0.00109098	0.00080445	0.00036832	-0.00044150
5.40	-0.00032830	-0.00000263	-0.00003145	-0.00099269	0.00075390	0.00034508	-0.00040093
6.00	-0.00020700	-0.00000190	-0.00002074	-0.00077365	0.00062173	0.00027414	-0.00030703
6.50	-0.00014046	-0.00000153	-0.00001416	-0.00063988	0.00053338	0.00023294	-0.00024990
7.00	-0.00008959	-0.00000129	-0.00000952	-0.00053398	0.00046034	0.00019936	-0.00020594
8.00	-0.00004285	-0.00000110	-0.00000420	-0.00037593	0.00034139	0.00014195	-0.00014381
9.00	-0.00002236	-0.00000101	-0.00000185	-0.00027017	0.00025056	0.00010190	-0.00010258
10.00	-0.00001267	-0.00000090	-0.00000090	-0.00019418	0.00018353	0.00007366	-0.00007382
12.00	-0.00000506	-0.00000066	-0.00000031	-0.00010028	0.00009632	0.00003790	-0.00003788
15.00	-0.00000193	-0.00000037	-0.00000011	-0.00003723	0.00003609	0.00001394	-0.00001401

[a] Distance between C atom of CO_2 and Si atom from $Si(OH)_4$ (in Å); see Fig. S1g

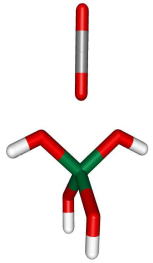

Table S15 Interaction energies corrected for BSSE (in Hartrees) for the $CO_2 \cdots Si(OH)_4$ complex.[a]

R	MP2/AVDZ	CCSD(T)/AVDZ	HF/AVTZ	MP2/AVTZ	HF/AVQZ	MP2/AVQZ	HF/AV5Z	CCSD(T)/CBS	PBE/AVQZ
3.40	0.19078802	0.19677776	0.21793500	0.18197360	0.21783420	0.17932563	0.21780145	0.18342387	0.18241210
3.80	0.06021478	0.06261715	0.07434950	0.05688446	0.07431678	0.05569502	0.07430185	0.05723836	0.06077595
4.00	0.03166825	0.03314574	0.04198082	0.02965599	0.04197593	0.02889705	0.04196199	0.02981034	0.03346971
4.20	0.01604104	0.01695062	0.02363633	0.01480579	0.02364906	0.01433503	0.02363700	0.01487975	0.01810126
4.40	0.00787243	0.00844523	0.01351880	0.00708529	0.01353686	0.00679829	0.01352883	0.00714045	0.00972469
4.60	0.00379501	0.00417145	0.00802805	0.00326143	0.00804495	0.00309029	0.00804092	0.00332549	0.00527648
4.80	0.00185735	0.00211783	0.00506067	0.00147231	0.00507345	0.00137351	0.00507191	0.00155102	0.00296945
5.00	0.00098440	0.00117348	0.00344007	0.00069924	0.00344657	0.00064285	0.00344614	0.00078561	0.00179916
5.20	0.00061544	0.00075851	0.00252751	0.00040646	0.00252721	0.00037269	0.00252712	0.00049126	0.00121511
5.40	0.00047360	0.00058604	0.00198451	0.00032306	0.00197886	0.00030064	0.00197877	0.00040075	0.00092460
5.60	0.00042717	0.00051855	0.00163562	0.00031894	0.00162698	0.00030244	0.00162669	0.00038780	0.00077389
5.80	0.00041525	0.00049147	0.00139151	0.00033603	0.00138195	0.00032324	0.00138160	0.00039674	0.00068849
6.00	0.00041139	0.00047611	0.00120724	0.00035152	0.00119798	0.00034145	0.00119771	0.00040531	0.00063205
6.50	0.00038786	0.00043277	0.00088422	0.00035315	0.00087669	0.00034736	0.00087691	0.00039376	0.00052903
7.00	0.00034068	0.00037292	0.00066697	0.00031729	0.00066081	0.00031348	0.00066134	0.00034795	0.00043445
8.00	0.00023715	0.00025491	0.00039728	0.00022426	0.00039353	0.00022230	0.00039390	0.00024172	0.00027644
9.00	0.00015994	0.00017047	0.00024887	0.00015206	0.00024661	0.00015093	0.00024675	0.00016243	0.00017537
10.00	0.00010907	0.00011566	0.00016297	0.00010405	0.00016155	0.00010336	0.00016160	0.00011053	0.00011510
12.00	0.00005448	0.00005735	0.00007795	0.00005212	0.00007732	0.00005181	0.00007732	0.00005491	0.00005506
15.00	0.00002271	0.00002364	0.00003158	0.00002177	0.00003135	0.00002164	0.00003134	0.00002263	0.00002230

[a] Distance between C atom of CO_2 and Si atom from $Si(OH)_4$ (in Å); see Fig. S1h.

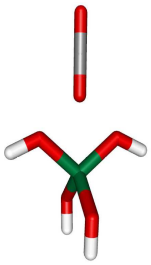

Table S16 Difference between CCSD(T)/CBS and PBE/AVQZ interaction energies, ΔE, and C-H, O-H, C-O, O-O, CSi, and OSi contributions to $\Delta E_{DFT/CC}$ evaluated using correction functions given in Table S17 (in Hartrees) for the $CO_2\cdots Si(OH)_4$ complex.[a]

R	ΔE	E_{CH}	E_{OH}	E_{CO}	E_{OO}	E_{CSi}	E_{OSi}
3.40	0.00101178	-0.00009799	-0.00027520	-0.00365491	0.00284700	0.00058871	0.00160416
3.80	-0.00353759	-0.00004064	-0.00016306	-0.00280632	-0.00042273	0.00056966	-0.00067450
4.00	-0.00365937	-0.00002455	-0.00011883	-0.00240559	-0.00069558	0.00055351	-0.00096832
4.20	-0.00322151	-0.00001462	-0.00008542	-0.00206094	-0.00051128	0.00052311	-0.00107235
4.40	-0.00258424	-0.00000886	-0.00006230	-0.00177663	-0.00018370	0.00048349	-0.00103623
4.60	-0.00195100	-0.00000570	-0.00004748	-0.00154396	0.00015007	0.00044783	-0.00095176
4.80	-0.00141843	-0.00000413	-0.00003887	-0.00135848	0.00041579	0.00041662	-0.00084936
5.00	-0.00101354	-0.00000338	-0.00003439	-0.00120964	0.00059609	0.00039065	-0.00075286
5.20	-0.00072386	-0.00000296	-0.00003236	-0.00109098	0.00069905	0.00036832	-0.00066497
5.40	-0.00052385	-0.00000263	-0.00003129	-0.00099269	0.00074248	0.00034508	-0.00058469
5.60	-0.00038609	-0.00000234	-0.00003024	-0.00090951	0.00074674	0.00031994	-0.00051086
5.80	-0.00029175	-0.00000211	-0.00002876	-0.00083772	0.00072774	0.00029563	-0.00044630
6.00	-0.00022674	-0.00000190	-0.00002685	-0.00077365	0.00069488	0.00027414	-0.00039349
6.50	-0.00013527	-0.00000153	-0.00002069	-0.00063988	0.00059722	0.00023294	-0.00030328
7.00	-0.00008649	-0.00000129	-0.00001470	-0.00053398	0.00050745	0.00019936	-0.00024336
8.00	-0.00003472	-0.00000110	-0.00000676	-0.00037593	0.00037078	0.00014195	-0.00016364
9.00	-0.00001294	-0.00000101	-0.00000301	-0.00027017	0.00027354	0.00010190	-0.00011422
10.00	-0.00000456	-0.00000090	-0.00000136	-0.00019418	0.00019947	0.00007366	-0.00008124
12.00	-0.00000015	-0.00000066	-0.00000038	-0.00010028	0.00010500	0.00003790	-0.00004170
15.00	0.00000033	-0.00000037	-0.00000012	-0.00003723	0.00003937	0.00001394	-0.00001532

[a] Distance between C atom of CO_2 and Si atom from $Si(OH)_4$ (in Å); see Fig. S1h.

Table 17 The DFT/CC correction funcitons ε_{ij} (in Hartrees) as a function of atom-atom distances; *i* stands for C and O atoms of CO_2 and *j* stands for framework O and Si framework atoms, for Brønsted acid group proton H(B) and for H atom.[a]

R_{CH}	ε_{CH}	R_{OH}	ε_{OH}	$R_{CH(B)}$	$\varepsilon_{CH(B)}$	$R_{OH(B)}$	$\varepsilon_{OH(B)}$	R_{CO}	ε_{CO}	R_{OO}	ε_{OO}	R_{CSi}	ε_{CSi}	R_{OSi}	E_{OSi}
1.545199	0.00203387	1.484013	0.00190043	1.630840	0.00502352	0.867730	-0.00045426	2.000000	-0.00083624	1.836887	0.00046807	2.400000	0.00113350	2.236890	0.00196146
1.837836	0.00058220	1.678407	0.00055690	1.830840	0.00372104	1.067730	0.00101251	2.200000	-0.00145556	2.036887	-0.00057321	2.800000	0.00056908	2.636890	-0.00040414
2.034119	0.00009780	1.873981	0.00000309	2.030840	0.00286262	1.267730	0.00105550	2.400000	-0.00163237	2.236887	-0.00070300	3.200000	0.00059843	2.836890	-0.00072747
2.231063	-0.00012771	2.070401	-0.00018379	2.230840	0.00229493	1.467730	0.00062452	2.600000	-0.00155801	2.436887	-0.00053554	3.400000	0.00058871	3.036890	-0.00085543
2.428506	-0.00020454	2.267447	-0.00020821	2.430840	0.00191535	1.667730	0.00017899	2.800000	-0.00137514	2.636887	-0.00031203	3.600000	0.00058081	3.236890	-0.00083949
2.626336	-0.00020483	2.464969	-0.00017046	2.630840	0.00165051	1.867730	-0.00014472	3.000000	-0.00116516	2.836887	-0.00012107	3.800000	0.00056966	3.436890	-0.00077246
2.824472	-0.00017183	2.662861	-0.00011872	2.830840	0.00145064	2.067730	-0.00033563	3.200000	-0.00096655	3.036887	0.00001318	4.000000	0.00055351	3.636890	-0.00068549
3.122121	-0.00010834	2.861046	-0.00007382	3.030840	0.00129082	2.267730	-0.00043165	3.400000	-0.00079871	3.236887	0.00009527	4.200000	0.00052311	3.836890	-0.00060272
3.420181	-0.00005733	3.059468	-0.00004197	3.230840	0.00115479	2.467730	-0.00047484	3.600000	-0.00066488	3.436887	0.00013801	4.400000	0.00048349	4.036890	-0.00052706
3.718554	-0.00002612	3.258082	-0.00002275	3.430840	0.00103882	2.667730	-0.00049059	3.800000	-0.00055937	3.636887	0.00015556	4.600000	0.00044783	4.236890	-0.00045769
4.017168	-0.00001048	3.556295	-0.00001016	3.630840	0.00094073	2.867730	-0.00049183	4.000000	-0.00047904	3.836887	0.00015855	4.800000	0.00041662	4.436890	-0.00039365
4.515268	-0.00000237	3.854785	-0.00000766	3.830840	0.00085714	3.067730	-0.00048332	4.200000	-0.00041774	4.336887	0.00013919	5.000000	0.00039065	4.636890	-0.00033793
5.013745	-0.00000118	4.352730	-0.00000919	4.030840	0.00078533	3.267730	-0.00046791	4.400000	-0.00037136	4.836887	0.00011586	5.200000	0.00036832	4.836890	-0.00029312
6.011459	-0.00000056	4.851097	-0.00000879	4.230840	0.00072303	3.867730	-0.00039899	4.600000	-0.00033416	6.836887	0.00006156	5.400000	0.00034508	5.336890	-0.00021981
7.009825	-0.00000033	5.848669	-0.00000463	4.430840	0.00066823	4.867730	-0.00028092	4.800000	-0.00030369	8.836887	0.00003287	6.000000	0.00027414	5.836890	-0.00017340
10.006880	-0.00000025	8.844674	-0.00000034	5.030840	0.00053314	7.867730	-0.00010892	5.000000	-0.00027778	10.836887	0.00001734	6.500000	0.00023294	6.836890	-0.00011384
15.004587	-0.00000011	13.841863	-0.00000002	6.030840	0.00037438	12.867730	-0.00003051	5.500000	-0.00022502	13.836887	0.00000637	7.000000	0.00019936	7.836890	-0.00007845
				9.030840	0.00016220			6.000000	-0.00018518	18.836887	0.00000137	8.000000	0.00014195	8.836890	-0.00005557
				14.030840	0.00004324			8.000000	-0.00009090			9.000000	0.00010190	10.836890	-0.00002865
								10.000000	-0.00004692			10.000000	0.00007366	13.836890	-0.00001044
								12.000000	-0.00002403			12.000000	0.00003790		
								15.000000	-0.00000887			15.000000	0.00001394		
								20.000000	-0.00000201						

[a] Distances in Å, correction functions in Hartree.