Supporting Information

Disclosing Gate-Opening/Closing Events inside a Flexible Metal-Organic Framework loaded with CO_2 by Reactive and Essential Dynamics

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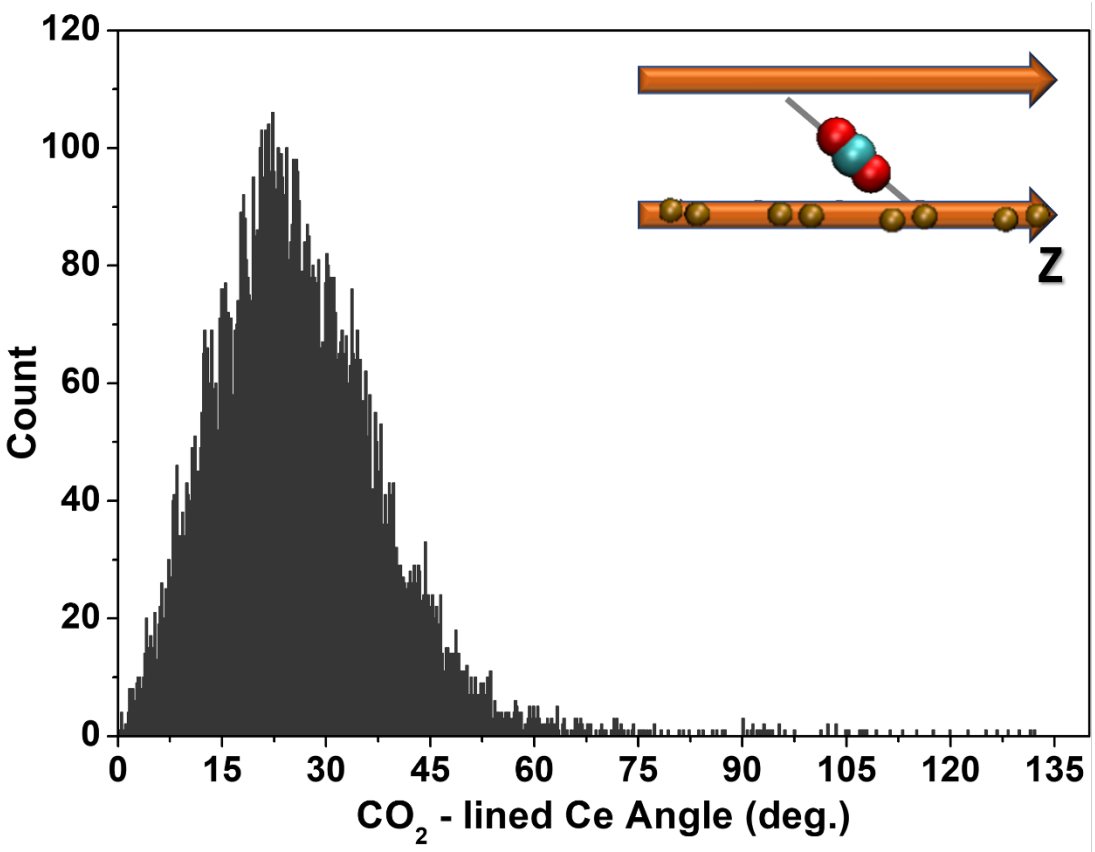


Figure S1. Angle of a CO_2 molecule (traveling in a channel) with the axis of the channel.

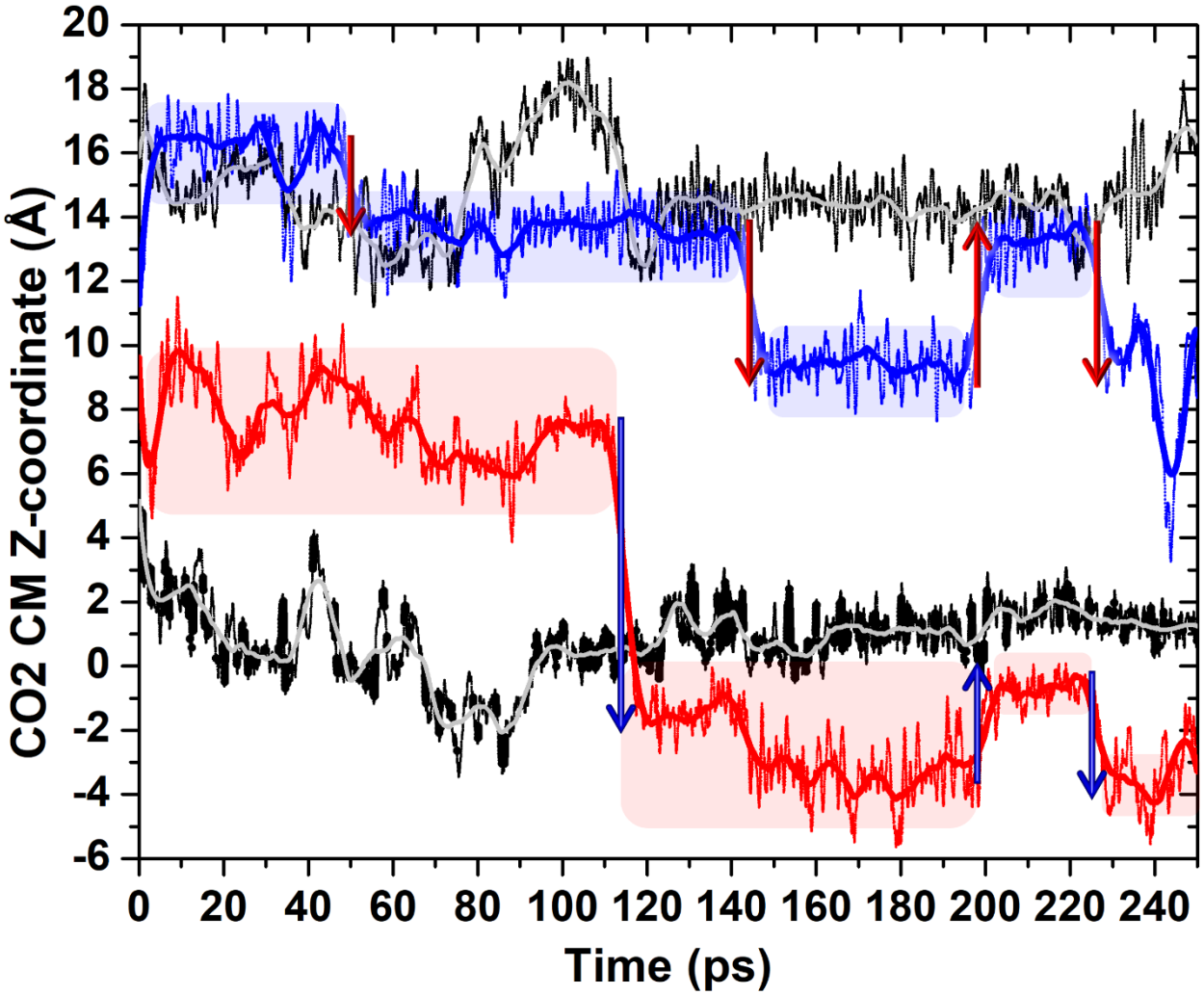


Figure S2. CO_2 (four molecules) motion along the Z direction (inside the channels) as a function of the simulation time. Stationary states are evidenced by the highlighted areas. The arrows indicate diffusion along the channels. The blue plot corresponds to the CO_2 in the Supplementary Video with grey C.

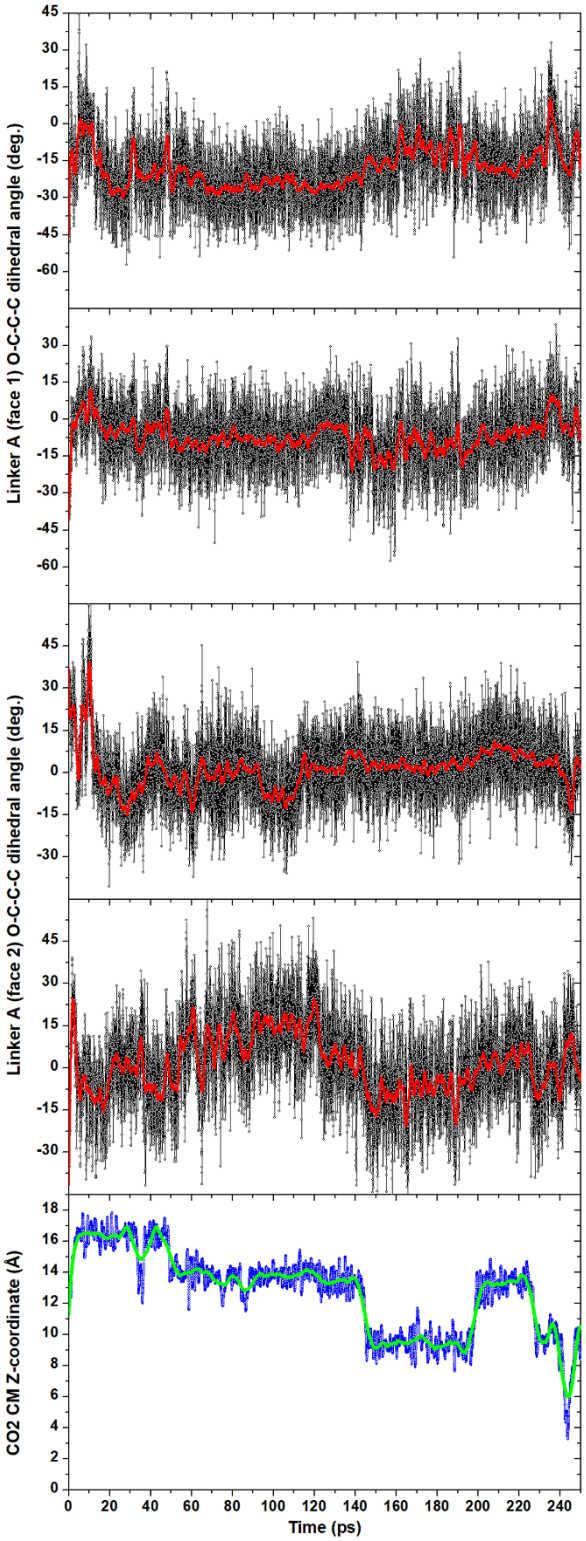


Figure S3. CO_2 motion along the Z direction (inside the channels) as a function of the simulation time compared with the rotations of the rings close by to identify the kicks responsible for diffusion.

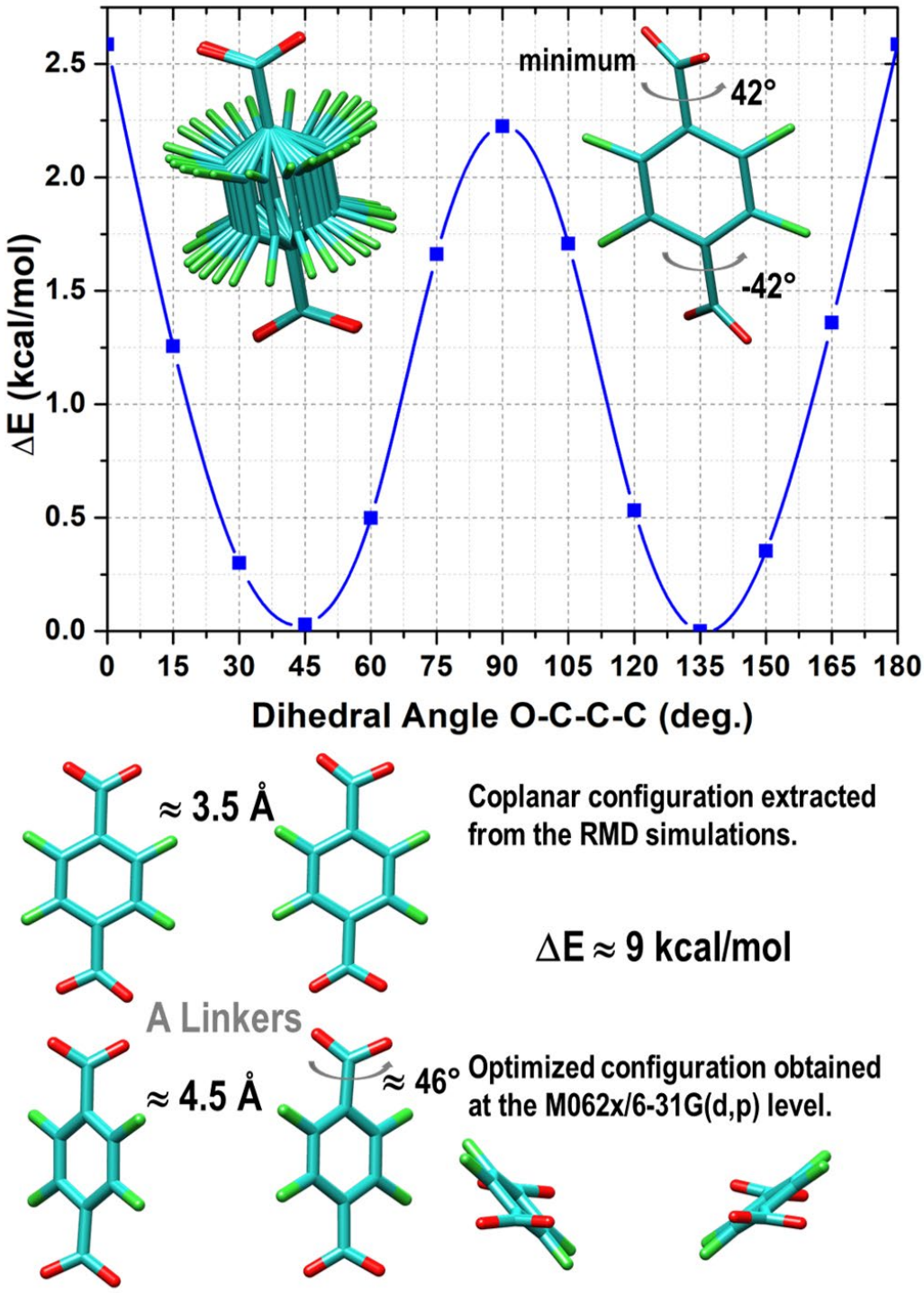


Figure S4. Extracted structures of the A linkers for QC optimizations and rotational barriers estimations. Color code: O red, C dark cyan, F green. **Top:** single linker, torsional energy profile calculated at the M062X/6-31G(d,p) level of theory. **Bottom:** A linker pair, constrained (top), and optimized geometries (bottom) to give a rough estimate of the ring flipping barrier.

Table S1. Weights of the calculated PCA modes for selected A and B linkers

Mode		2A linkers	2A linkers	2 B linkers	4A + 2B linkers
		%	%	%	%
1		60	65	38	55
2		15	9	16	14
3		6	7	11	7
4		6	6	10	5
5		5	4	7	4
6		2	3	5	4
7		1	2	4	3
8		1	2	3	3
9		1	1	3	3
10		1	1	3	2

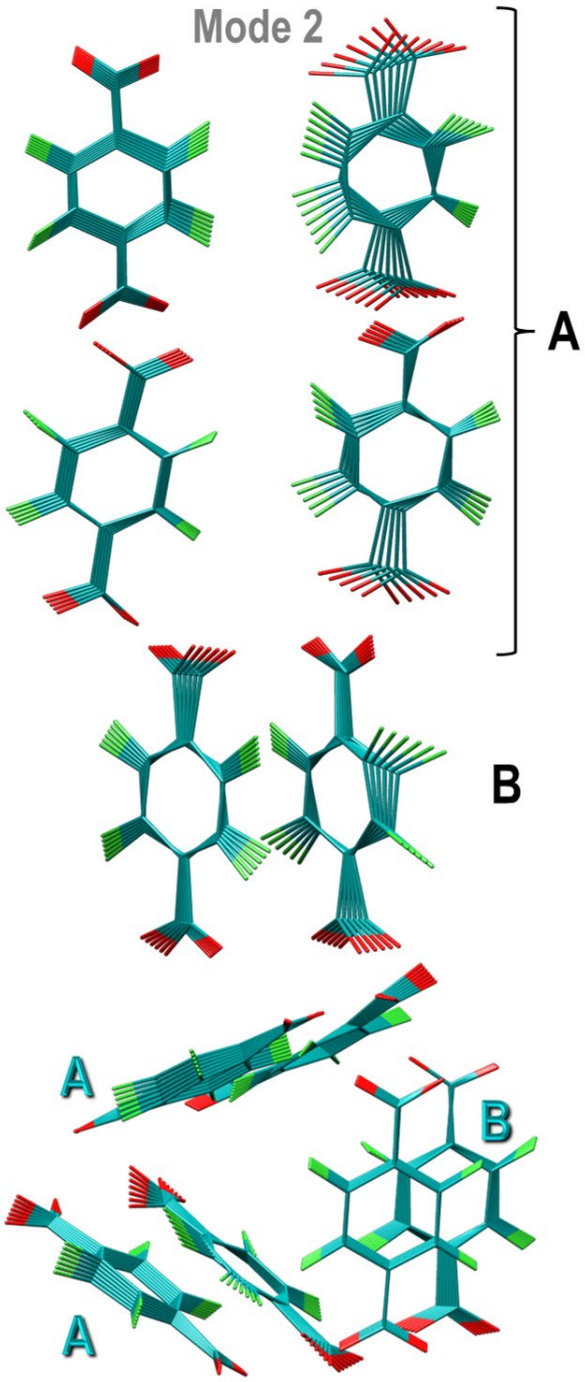


Figure S5. Linkers pairs forming a section of the channel. From top to bottom: type A, type A, type B. **Mode 2** (green slice of the pie plot) identified by PCA (superimposing all the snapshots on the coordinated Ce atoms and carboxyl oxygens – rmsd values are reported in **Figure S3**). Structure color code: O red, C dark cyan, F green.

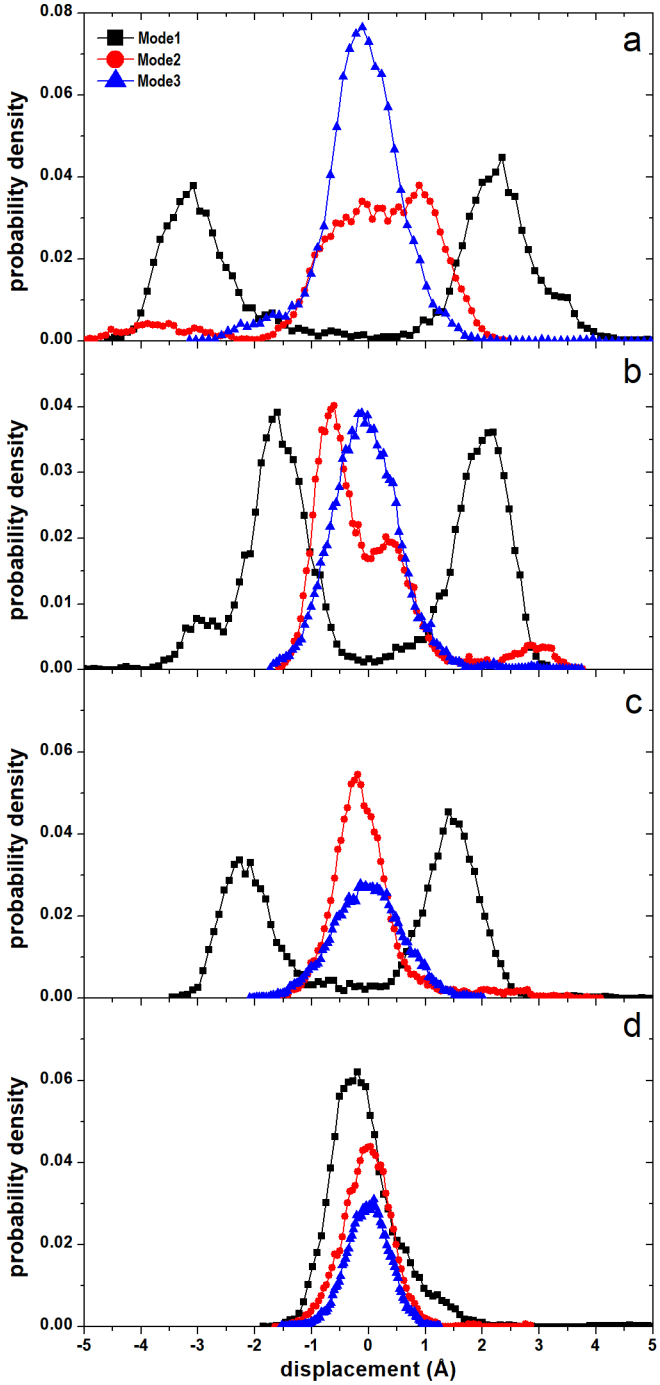


Figure S6. Histograms of the fluctuations of the first three principal components (or modes) of a) all six linkers; b) linker A, c) linker A, d) linker B.

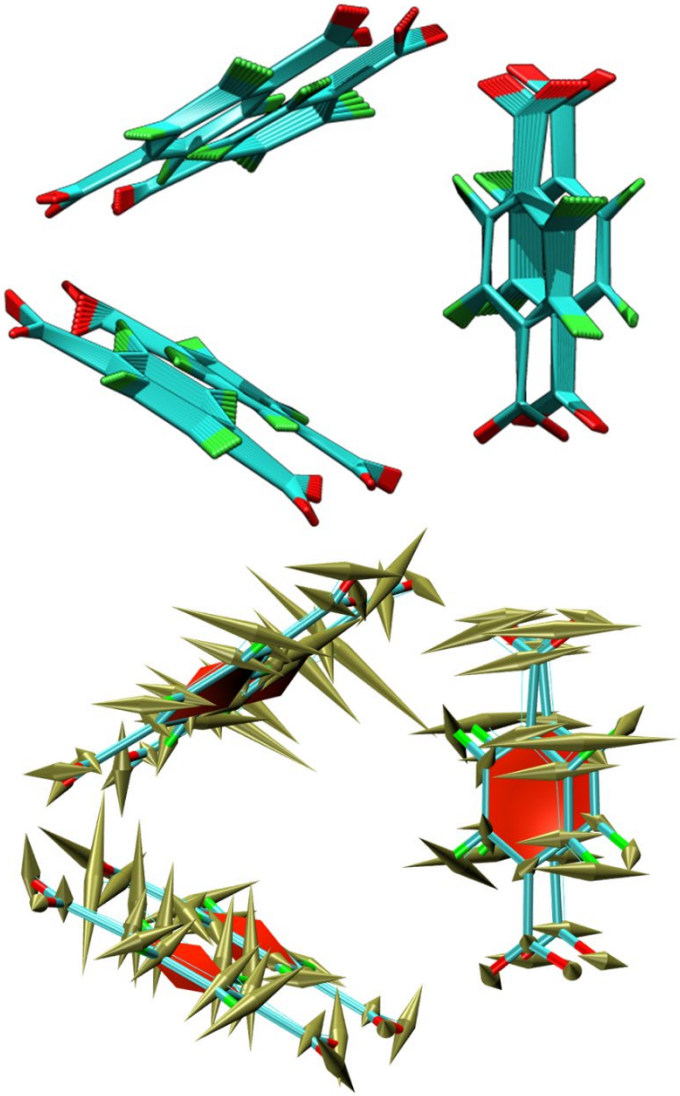


Figure S7. Linkers pairs forming a section of the channel. **Mode 3** identified by PCA (superimposing all the snapshots on the coordinated Ce atoms and carboxyl oxygens – rmsd values are reported in **Figure S5**). Porcupine rendering of the main linker movements. Structure color code: O red, C dark cyan, F green.

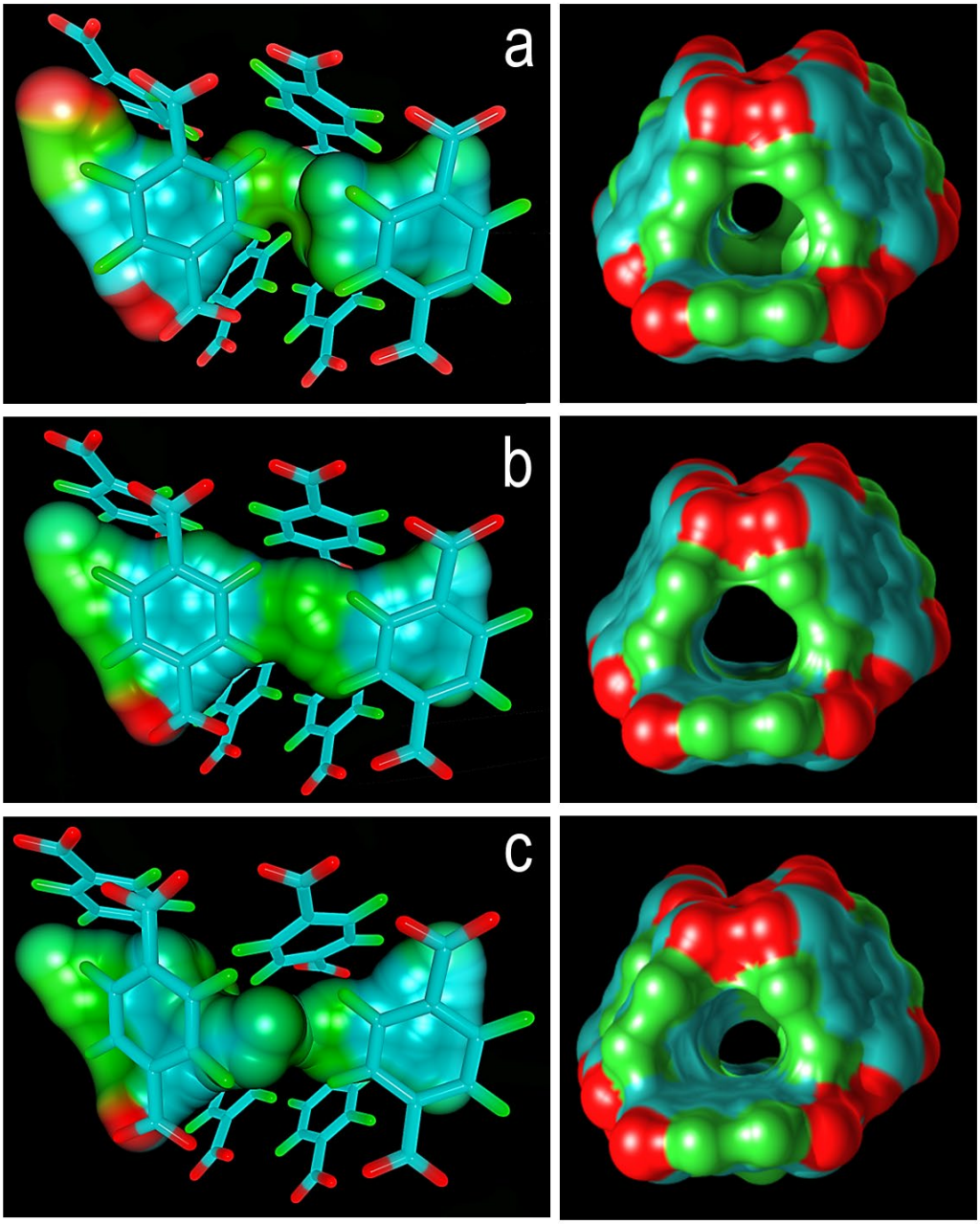


Figure S8. Variability of the channel due to the libration of linkers A (six-linker portion). On the left, the channel has been filled with spheres using CAVER, whereas on the right, the surface accessible to the solvent (SAS) has been visualized to give an idea of the section variations. In a and c are displayed the librations with the maximum amplitude, while in b average structure (considering only the dominant mode – Mode 1). Structure color code: O red, C dark cyan, F green.

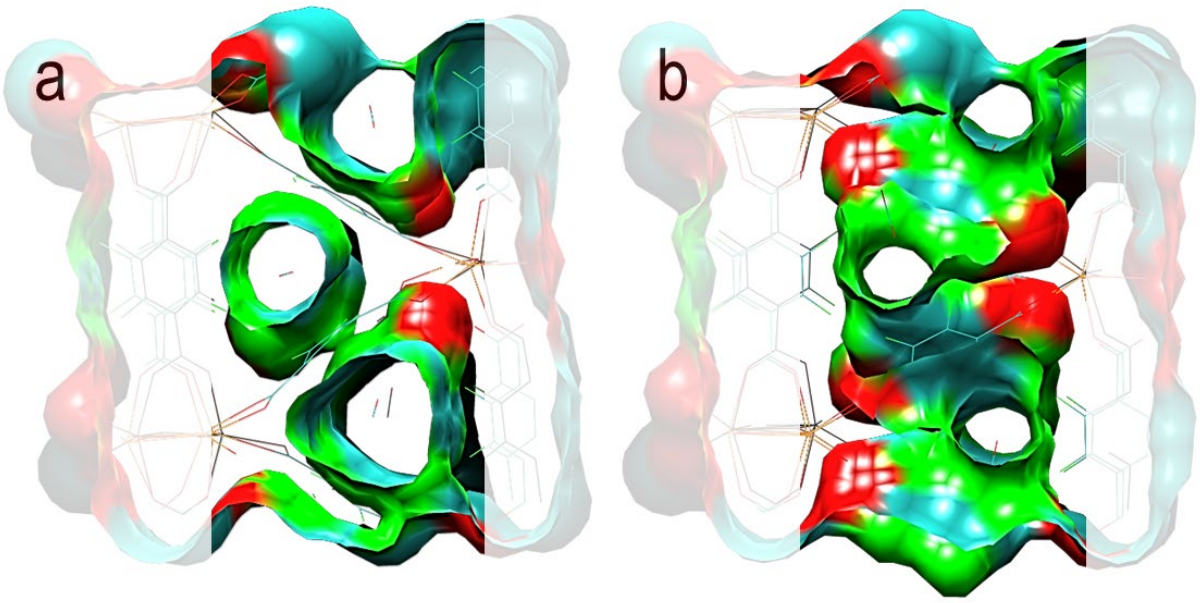


Figure S9. Possible breathing effect in three parallel channels of the MOF structure: **a**) opening stage, **b**) closing stage. Some of the CO_2 molecules are visible inside the open channels. Structure color code: O red, C dark cyan, F green.

Additional Data related to ReaxFF Force field parametrization and validation

Quantum Chemistry DFT optimizations/MD-simulations

All DFT optimizations and MD simulations were carried out by using the Quantum Espresso (QE) suite of programs [*Giannozzi, P.; Baroni, S.; Bonini, N.; Calandra, M.; Car, R.; Cavazzoni, C.; Ceresoli, D.; Chiarotti, G. L.; Cococcioni, M.; Dabo, I.; Dal Corso, A.; De Gironcoli, S.; Fabris, S.; Fratesi, G.; Gebauer, R.; Gerstmann, U.; Gougoussis, C.; Kokalj, A.; Lazzeri, M.; Martin-Samos, L.; Marzari, N.; Mauri, F.; Mazzarello, R.; Paolini, S.; Pasquarello, A.; Paulatto, L.; Sbraccia, C.; Scandolo, S.; Sclauzero, G.; Seitsonen, A. P.; Smogunov, A.; Umari, P.; Wentzcovitch, R. M. QUANTUM ESPRESSO: A Modular and Open-Source Software Project for Quantum Simulations of Materials. J. Phys. Condens. Matter 2009, 21 (39). https://doi.org/10.1088/0953-8984/21/39/395502*], employing PAW (Plane-Augmented-Waves) pseudopotentials [*Blöchl, P. E. Projector Augmented-Wave Method. Phys. Rev. B 1994, 50 (24), 17953–17979. https://doi.org/10.1103/PhysRevB.50.17953*], the PBE XC-functional and plane-waves, as basis sets to build Bloch states. Cutoffs on the wave function and electronic density were set to 40/400 Ry (1 Ry=313.8 Kcal/mol), respectively; the first Brillouin zone in the reciprocal space was sampled at the gamma point only, after verifying that the fully optimized structural parameters converged to a benchmark calculation with 80/800 Ry as cutoff values and a (2x4x6) mesh of k-points; the calculations were spin-restricted by applying Gaussian smearing of the one-particle energy levels of 0.002 Ry. The crystal structure of F4_MIL140A(Ce) was extracted from the experimental cif file and fully optimized following a two-step procedure: first, by using the experimental lattice constants, we optimized the coordinates of all the atoms; then, we optimized also the cell vectors and angles. The same procedure was repeated after removing the water molecules. Born-Oppenheimer MD simulations at ambient temperature were carried out with the QE software (adopting the same values of cutoffs and sampling the reciprocal space at the Gamma point) by choosing an integration time step of about 0.5 fs and the Berendsen thermostat.

Force Field Refinement

Refinement of the force field for describing the FRAMEWORK and its content

We used repeated parametrizations (by means of the fast and efficient Monte Carlo Force Field - MCFF parameter optimizer available in the Amsterdam Density Functional (ADF)package) to obtain a refined force field for the planned simulations. An example of one of these stages is reported below (ffield_bool).
A series of configurations generated by DFT optimizations and dynamics were used to re-tune selected parameters of the force field (highlighted below). The initial values of all the parameters were taken from well-tested ReaxFF force fields available in the literature(refs 29-31).

Training set: DFT optimized structures.
GEOMETRY - Bonds distances and dihedral angles.
The structures and other data are available from the authors upon reasonable request.

Optimized Parameters (MCFFOptimizer in ADF) – ffield file
In the ffield_bool file (see ReaxFF and ADF/ReaxFF manual), the optimized parameters are indicated by **1.0000**

Atoms

1 C	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
2 H	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

		0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
3	O	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
4	Ce	**1.0000**	0.0000	0.0000	**1.0000**	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
5	F	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
6	X	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Bonds

1	1	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
1	2	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
2	2	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
1	3	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
1	4	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
3	3	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
2	3	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
2	4	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
3	**4**	**1.0000**	**1.0000**	0.0000	**1.0000**	0.0000	0.0000	0.0000	**1.0000**
		1.0000	**1.0000**	**1.0000**	0.0000	**1.0000**	**1.0000**	0.0000	0.0000
4	4	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
1	**5**	**1.0000**	**1.0000**	0.0000	**1.0000**	0.0000	0.0000	0.0000	**1.0000**
		1.0000	**1.0000**	**1.0000**	0.0000	**1.0000**	**1.0000**	0.0000	0.0000
2	5	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
3	5	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
5	5	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
4	5	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
		0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Off-diagonal terms

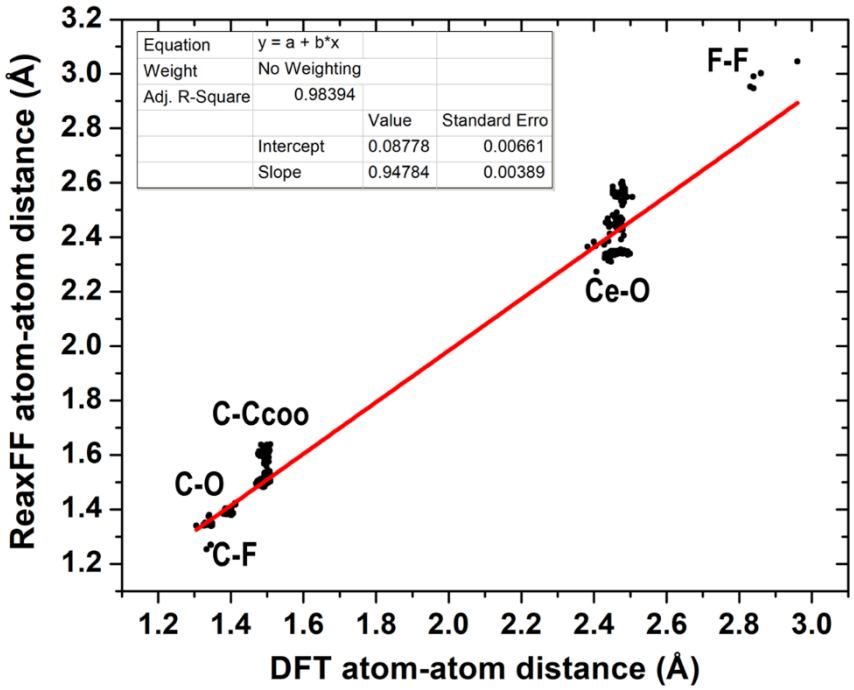
1	2	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
1	3	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
2	3	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
3	**4**	**1.0000**	**1.0000**	**1.0000**	**1.0000**	**1.0000**	0.0000
2	4	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
1	**5**	**1.0000**	**1.0000**	**1.0000**	**1.0000**	**1.0000**	0.0000
2	5	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
3	5	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
4	5	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

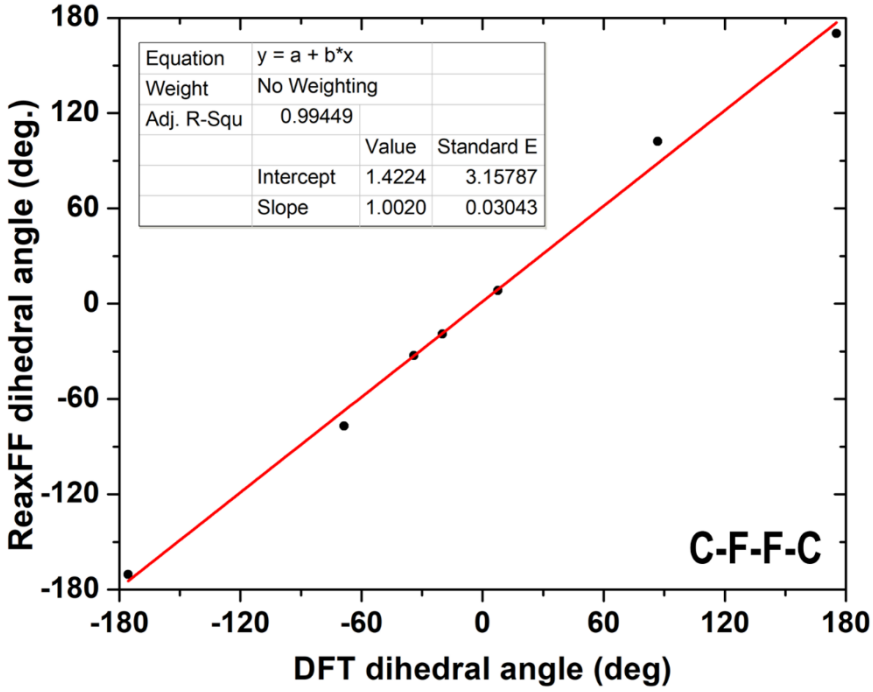
```
Reactive MD-force field used for F4_MIL140A(Ce)
 39        ! Number of general parameters
   50.0000 !Overcoordination parameter
    9.5469 !Overcoordination parameter
   26.5405 !Valency angle conjugation parameter
    1.7224 !Triple bond stabilisation parameter
    6.8702 !Triple bond stabilisation parameter
   60.4850 !C2-correction
    1.0588 !Undercoordination parameter
    4.6000 !Triple bond stabilisation parameter
   12.1176 !Undercoordination parameter
   13.3056 !Undercoordination parameter
  -70.5044 !Triple bond stabilization energy
    0.0000 !Lower Taper-radius
   10.0000 !Upper Taper-radius
    2.8793 !Fe dimer correction
   33.8667 !Valency undercoordination
    6.0891 !Valency angle/lone pair parameter
    1.0563 !Valency angle
    2.0384 !Valency angle parameter
    6.1431 !Fe dimer correction
    6.9290 !Double bond/angle parameter
    0.3989 !Double bond/angle parameter: overcoord
    3.9954 !Double bond/angle parameter: overcoord
   -2.4837 !Fe dimer correction
    5.7796 !Torsion/BO parameter
   10.0000 !Torsion overcoordination
    1.9487 !Torsion overcoordination
   -1.2327 !Reserved
    2.1645 !Conjugation
    1.5591 !vdWaals shielding
    0.1000 !Cutoff for bond order (*100)
    2.1365 !Valency angle conjugation parameter
    0.6991 !Overcoordination parameter
   50.0000 !Overcoordination parameter
    1.8512 !Valency/lone pair parameter
    0.5000 !ACKS2 softness parameter
   20.0000 !Scale factor (d) in dispersion (LJ)
    5.0000 !Reserved
    0.0000 !1: disable undecoord term in val angle
    2.6962 !Valency angle conjugation parameter
  6    ! Nr of atoms; cov.r; valency;a.m;Rvdw;Evdw;gammaEEM;cov.r2;#
            alfa;gammavdW;valency;Eunder;Eover;chiEEM;etaEEM;n.u.
            cov r3;Elp;Heat inc.;bo131;bo132;bo133;softcut;n.u.
            ov/un;val1;n.u.;val3,vval4
 C    1.3674   4.0000  12.0000   2.0453   0.1444   0.7920   1.1706   4.0000
      9.0000   1.5000   4.0000  27.5134  79.5548   6.7897   6.0000   0.0000
      1.1168   0.0000 181.0000  14.2732  24.4406   6.7313   0.8563   0.0000
     -4.1021   5.0000   1.0564   4.0000   2.9663   0.0000   0.0000   0.0000
 H    0.8930   1.0000   1.0080   1.3550   0.0930   0.8203  -0.1000   1.0000
      8.2230  33.2894   1.0000   0.0000 121.1250   3.7248   9.6093   1.0000
     -0.1000   0.0000  61.6606   3.0408   2.4197   0.0003   1.0698   0.0000
    -19.4571   4.2733   1.0338   1.0000   2.8793   0.0000   0.0000   0.0000
 O    1.2450   2.0000  15.9990   2.3890   0.1000   1.0898   1.0548   6.0000
      9.7300  13.8449   4.0000  37.5000 116.0768   8.5000   8.3122   2.0000
      0.9049   0.4056  59.0626   3.5027   0.7640   0.0021   0.9745   0.0000
     -3.5500   2.9000   1.0493   4.0000   2.9225   0.0000   0.0000   0.0000
 Ce   2.6062   3.0000 140.1160   2.8303   0.3338   1.2500   0.0100   3.0000
     11.8468  12.5107   3.0000   0.0078   0.0000  -3.7987   7.2405   0.0000
     -1.2000   0.0000 101.0038   5.3430  10.1260   0.7590   0.0000   0.0000
     -2.5000   2.4588   1.0338   6.0000   2.5791   0.0000   0.0000   0.0000
 F    1.1846   1.0000  18.9984   1.7922   0.1267   0.4038  -0.1000   7.0000
     10.3184   7.5000   1.0000   9.2533   0.2000   9.3891   6.5612   2.0000
     -1.0000   3.5571  18.0000   6.9821   4.1799   1.0561   0.0000   0.0000
     -7.3000   2.6656   1.0493   4.0000   2.9225   0.0000   0.0000   0.0000
 X   -0.1000   2.0000   1.0080   2.0000   0.0000   1.0000  -0.1000   6.0000
     10.0000   2.5000   4.0000   0.0000   0.0000   3.5000  85.0000   0.0000
     -0.1000   0.0000  -2.3700   8.7410  13.3640   0.6690   0.9745   0.0000
    -11.0000   2.7466   1.0338   6.2998   2.8793   0.0000   0.0000   0.0000
 15    ! Nr of bonds; Edis1;LPpen;n.u.;pbe1;pbo5;13corr;pbo6
                       pbe2;pbo3;pbo4;n.u.;pbo1;pbo2;ovcorr
```

```
 1  1  80.8865 107.9944  52.0636   0.5218  -0.3636   1.0000  34.9876   0.7769
        6.1244  -0.1693   8.0804   1.0000  -0.0586   8.1850   1.0000   0.0000
 1  2 169.4760   0.0000   0.0000  -0.6083   0.0000   1.0000   6.0000   0.7652
        5.2290   1.0000   0.0000   1.0000  -0.0500   6.9136   0.0000   0.0000
 2  2 153.3934   0.0000   0.0000  -0.4600   0.0000   1.0000   6.0000   0.7300
        6.2500   1.0000   0.0000   1.0000  -0.0790   6.0552   0.0000   0.0000
 1  3  95.6228 137.8227  68.8810   0.4203  -0.3774   1.0000  18.8662   0.6845
        1.1270  -0.3355   9.0448   1.0000  -0.1842   5.6293   0.0000   0.0000
 1  4   0.0000   0.0000   0.0000   0.5000  -0.3000   1.0000  16.0000   0.5000
        0.5000  -0.2500  15.0000   1.0000  -0.1000   9.0000   0.0000   0.0000
 3  3 142.2858 145.0000  50.8293   0.2506  -0.1000   1.0000  29.7503   0.6051
        0.3451  -0.1055   9.0000   1.0000  -0.1225   5.5000   1.0000   0.0000
 2  3 160.0000   0.0000   0.0000  -0.5725   0.0000   1.0000   6.0000   0.5626
        1.1150   1.0000   0.0000   0.0000  -0.0920   4.2790   0.0000   0.0000
 2  4  93.4841   0.0000   0.0000  -0.6193  -0.5000   0.0000  35.0000   0.2069
        0.2906  -0.5000  25.0000   0.0000  -0.1018   8.8004   0.0000   0.0000
 3  4 137.0329  60.1493   0.0000  -0.2126  -0.5000   0.0000  35.0000   0.1756
        2.7425  -0.3288  10.4385   0.0000  -0.0767   4.8724   0.0000   0.0000
 4  4 134.1649   0.0000   0.0000  -0.7905  -0.2000   0.0000  16.0000   0.1000
        3.0443  -0.2000  15.0000   0.0000  -0.2106   5.0057   0.0000   0.0000
 1  5 242.5403   2.3373   0.0000  -0.7882  -0.5000   1.0000  35.0000   1.0351
        4.3074  -0.2315  14.3578   1.0000  -0.0991   5.1373   1.0000   0.0000
 2  5 154.6080   0.0000   0.0000  -0.1948  -0.2000   0.0000  16.0000   0.1676
       16.3699  -0.2000  15.0000   1.0000  -0.2265   7.1308   0.0000   0.0000
 3  5   0.0000   0.0000   0.0000   0.5000  -0.2000   0.0000  16.0000   0.5000
        1.0001  -0.2000  15.0000   1.0000  -0.1000  15.0000   0.0000   0.0000
 5  5   0.7216   0.0000   0.0000   0.2298  -0.3500   1.0000  25.0000   0.8427
        0.1167  -0.2500  15.0000   1.0000  -0.1506   7.3516   1.0000   0.0000
 4  5  41.1590   0.0000   0.0000   0.6401  -0.2000   0.0000  16.0000   0.4085
        0.0992  -0.2000  15.0000   1.0000  -0.0687   5.9021   0.0000   0.0000
10    ! Nr of off-diagonal terms; Ediss;Ro;gamma;rsigma;rpi;rpi2
 1  2   0.1239   1.4004   9.8467   1.1210  -1.0000  -1.0000
 1  3   0.0628   1.9606  10.0282   1.3240   1.2084   1.0739
 2  3   0.0283   1.2885  10.9190   0.9215  -1.0000  -1.0000
 3  4   0.3863   1.6627  10.4263   1.8027   1.8954  -1.0000
 2  4   0.2410   1.8010   9.0000   2.0472  -1.0000  -1.0000
 1  5   0.1047   1.6152  10.9681   1.3032  -0.9400  -1.0000
 2  5   0.0431   1.7204  10.3632   0.5386  -1.0000  -1.0000
 3  5   0.1547   2.1287   9.6188  -1.0000  -1.0000  -1.0000
 4  5   0.2002   2.1104  11.4482   1.9513  -1.0000  -1.0000
 5  5   0.1068   2.1756   9.4701   1.8620  -0.9330  -1.0000
40    ! Nr of angles;at1;at2;at3;Thetao,o;ka;kb;pv1;pv2
 1  1  1  74.9085  44.7514   0.9144   0.0000   0.0050   0.3556   2.5715
 1  1  2  65.7758  14.5234   6.2481   0.0000   0.5665   0.0000   1.6255
 2  1  2  70.2607  25.2202   3.7312   0.0000   0.0050   0.0000   2.7500
 1  2  2   0.0000   0.0000   6.0000   0.0000   0.0000   0.0000   1.0400
 1  2  1   0.0000   3.4110   7.7350   0.0000   0.0000   0.0000   1.0400
 2  2  2   0.0000  27.9213   5.8635   0.0000   0.0000   0.0000   1.0400
 1  1  5  65.7758  14.5234   6.2481   0.0000   0.5665   0.0000   1.6255
 5  1  5  70.2607  25.2202   3.7312   0.0000   0.0050   0.0000   2.7500
 1  5  5   0.0000   0.0000   6.0000   0.0000   0.0000   0.0000   1.0400
 1  5  1   0.0000   3.4110   7.7350   0.0000   0.0000   0.0000   1.0400
 5  5  5   0.0000  27.9213   5.8635   0.0000   0.0000   0.0000   1.0400
 1  1  3  49.6811   7.1713   4.3889   0.0000   0.7171  10.2661   1.0463
 3  1  3  77.7473  40.1718   2.9802 -25.3063   1.6170 -46.1315   2.2503
 2  1  3  65.0000  13.8815   5.0583   0.0000   0.4985   0.0000   1.4900
 1  3  1  73.5312  44.7275   0.7354   0.0000   3.0000   0.0000   1.0684
 1  3  3  79.4761  36.3701   1.8943   0.0000   0.7351  67.6777   3.0000
 3  3  3  80.7324  30.4554   0.9953   0.0000   1.6310  50.0000   1.0783
 1  3  2  70.1880  20.9562   0.3864   0.0000   0.0050   0.0000   1.6924
 2  3  3  75.6935  50.0000   2.0000   0.0000   1.0000   0.0000   1.1680
 2  3  2  85.8000   9.8453   2.2720   0.0000   2.8635   0.0000   1.5800
 1  2  3   0.0000  25.0000   3.0000   0.0000   1.0000   0.0000   1.0400
 3  2  3   0.0000  15.0000   2.8900   0.0000   0.0000   0.0000   2.8774
 2  2  3   0.0000   8.5744   3.0000   0.0000   0.0000   0.0000   1.0421
 3  4  3  76.2996   3.2695   3.5597   0.0000   1.0000   0.0000   1.4353
 4  3  4  82.2036   3.7033   7.0000   0.0000   1.0000   0.0000   1.0000
 3  4  4  56.2421   7.1704   2.7680   0.0000   1.0000   0.0000   3.9916
 3  3  4  53.6286   3.8270   2.2409   0.0000   1.0000   0.0000   1.2671
 2  3  4  90.0000  10.0000   3.0000   0.0000   1.0000   0.0000   3.1274
 2  4  2  86.0792  36.1486   2.4342   0.0000   1.0000   0.0000   3.1940
```

```
 2  4  3  90.0000  39.9354   0.8289   0.0000   1.0000   0.0000   1.0265
 2  2  4   0.0000   2.5000   2.0000   0.0000   1.0000   0.0000   1.5000
 3  2  4   0.0000   5.0000   2.0000   0.0000   1.0000   0.0000   1.5000
 2  4  4   0.0000   2.5000   2.0000   0.0000   1.0000   0.0000   1.5000
 4  2  4   0.0000   7.5000   2.0000   0.0000   1.0000   0.0000   1.2500
 3  2  5   0.0000   8.5744   3.0000   0.0000   0.0000   0.0000   1.0421
 2  5  2   0.0000  27.9213   5.8635   0.0000   0.0000   0.0000   1.0400
 4  5  4   0.0000   2.0000   1.0000   0.0000   1.0000   0.0000   1.0000
 5  4  5  40.0000   1.0000   1.0000   0.0000   1.0000   0.0000   1.0000
 4  5  5   0.0000  10.0000   1.0000   0.0000   1.0000   0.0000   1.4000
 4  4  5  20.0000   0.0000   1.0000   0.0000   1.0000   0.0000   1.4000
33    ! Nr of torsions;at1;at2;at3;at4;;V1;V2;V3;V2(BO);vconj;n.u;n
 1  1  1  1   2.1207  26.8713   0.5160  -9.0000  -2.8394   0.0000   0.0000
 1  1  1  2  -0.2500  29.2131   0.2945  -4.9581  -2.1802   0.0000   0.0000
 2  1  1  2  -0.2500  31.2081   0.4539  -4.8923  -2.2677   0.0000   0.0000
 1  1  1  5  -0.2500  29.2131   0.2945  -4.9581  -2.1802   0.0000   0.0000
 2  1  1  5  -0.2500  31.2081   0.4539  -4.8923  -2.2677   0.0000   0.0000
 5  1  1  5  -0.2500  31.2081   0.4539  -4.8923  -2.2677   0.0000   0.0000
 1  5  5  1  -0.5529   9.9519   0.1490  -6.0709   0.0000   0.0000   0.0000
 1  1  1  3  -0.3495  22.2142  -0.2959  -2.5000  -1.9066   0.0000   0.0000
 2  1  1  3   0.0646  24.3195   0.6259  -3.9603  -1.0000   0.0000   0.0000
 5  1  1  3   0.0646  24.3195   0.6259  -3.9603  -1.0000   0.0000   0.0000
 3  1  1  3  -0.5456   5.5756   0.8433  -5.1924  -1.0180   0.0000   0.0000
 1  1  3  1   1.7555  27.9267   0.0072  -2.6533  -1.0000   0.0000   0.0000
 1  1  3  2  -1.4358  36.7830  -1.0000  -8.1821  -1.0000   0.0000   0.0000
 2  1  3  1  -1.3959  34.5053   0.7200  -2.5714  -2.1641   0.0000   0.0000
 5  1  3  1  -1.3959  34.5053   0.7200  -2.5714  -2.1641   0.0000   0.0000
 2  1  3  2  -2.5000  70.0597   1.0000  -3.5539  -2.9929   0.0000   0.0000
 5  1  3  5  -2.5000  70.0597   1.0000  -3.5539  -2.9929   0.0000   0.0000
 1  1  3  3   0.6852  11.2819  -0.4784  -2.5000  -2.1085   0.0000   0.0000
 5  1  3  3   0.1933  80.0000   1.0000  -4.0590  -3.0000   0.0000   0.0000
 2  1  3  3   0.1933  80.0000   1.0000  -4.0590  -3.0000   0.0000   0.0000
 3  1  3  1  -1.9889  76.4820  -0.1796  -3.8301  -3.0000   0.0000   0.0000
 3  1  3  5   0.2160  72.7707  -0.7087  -4.2100  -3.0000   0.0000   0.0000
 3  1  3  2   0.2160  72.7707  -0.7087  -4.2100  -3.0000   0.0000   0.0000
 3  1  3  3  -2.5000  71.0772   0.2542  -3.1631  -3.0000   0.0000   0.0000
 1  3  3  1   2.5000  -0.6002   1.0000  -3.4297  -2.8858   0.0000   0.0000
 1  3  3  5  -2.5000  -3.3822   0.7004  -5.4467  -2.9586   0.0000   0.0000
 1  3  3  2  -2.5000  -3.3822   0.7004  -5.4467  -2.9586   0.0000   0.0000
 5  3  3  5   2.5000  -4.0000   0.9000  -2.5000  -1.0000   0.0000   0.0000
 2  3  3  2   2.5000  -4.0000   0.9000  -2.5000  -1.0000   0.0000   0.0000
 1  3  3  3   1.2329  -4.0000   1.0000  -2.5000  -1.7479   0.0000   0.0000
 5  3  3  3   0.8302  -4.0000  -0.7763  -2.5000  -1.0000   0.0000   0.0000
 2  3  3  3   0.8302  -4.0000  -0.7763  -2.5000  -1.0000   0.0000   0.0000
 3  3  3  3  -2.5000  -4.0000   1.0000  -2.5000  -1.0000   0.0000   0.0000
 1    ! Nr of hydrogen bonds;at1;at2;at3;Rhb;Dehb;vhb1
 3  2  3   2.1200  -3.5800   1.4500  19.5000
```

Refinement of a few bond distances and the C-F-F-C dihedral angle





Comparison of the positions of the ligand oxygens sampled through quantum and classical MD simulations at ambient temperature. In both simulations, we sampled 12000 configurations.