Electronic Supplementary Information

for

Design of Electric Field Controlled Molecular Gates Mounted on Metal-Organic Frameworks

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Table S1. Details of convergence criteria for DFT geometry optimisation simulations

Energy tolerance	2.0 e-6 eV/atom
Max. force tolerance	0.05 eV/Angstrom
Max. stress tolerance	0.1 GPa
Max. displacement tolerance	0.002 Angstrom

Table S2. Comparison of binding energies obtained for the closed and open configurations (Figure 2) using Tkatchenko-Scheffler (TS) and Grimme* dispersion corrections.

Closed (with dispersion)	Binding energy, kJ mol^{-1}
TS	-357.2816
Grimme	-317.3923

Open (with dispersion)	Binding energy, kJ mol^{-1}
TS	-278.4649
Grimme	-253.9022

* *J. Comput. Chem.*, **27**(15), 1787-1799, (2006).

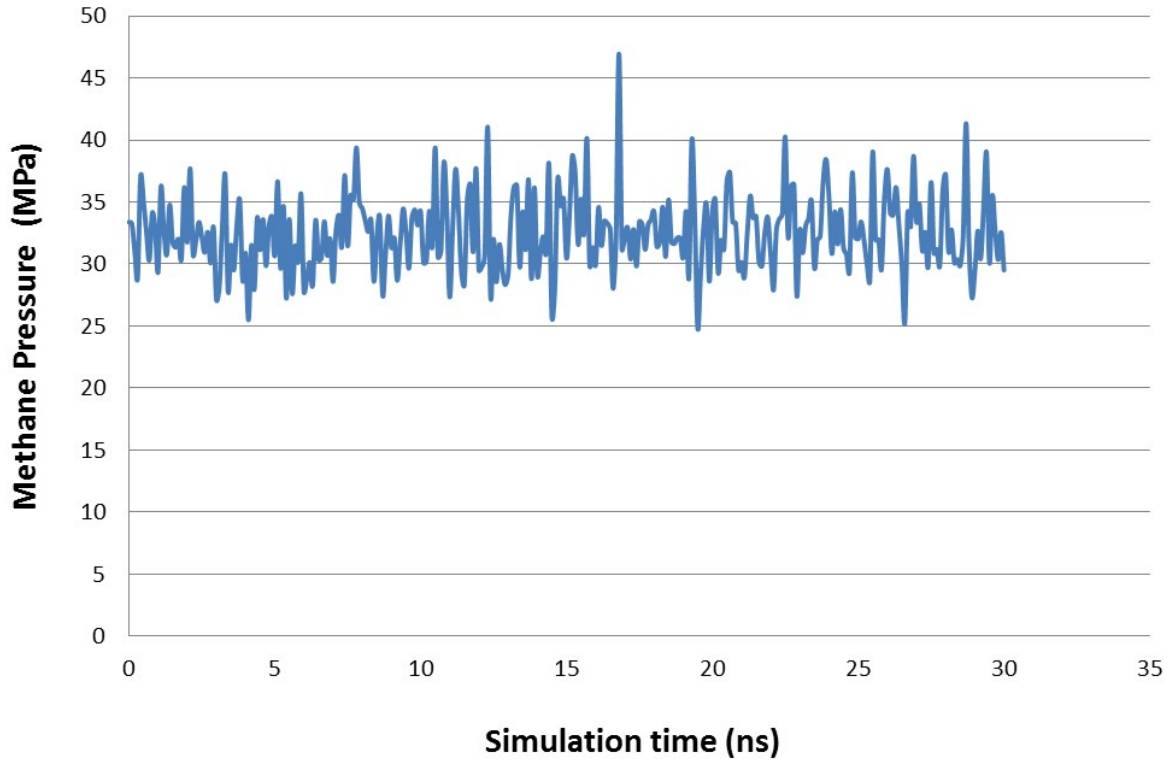


Figure S1. Pressure variation with simulation time for methane molecules between the molecular gates and the carbon wall.

Force Field Information

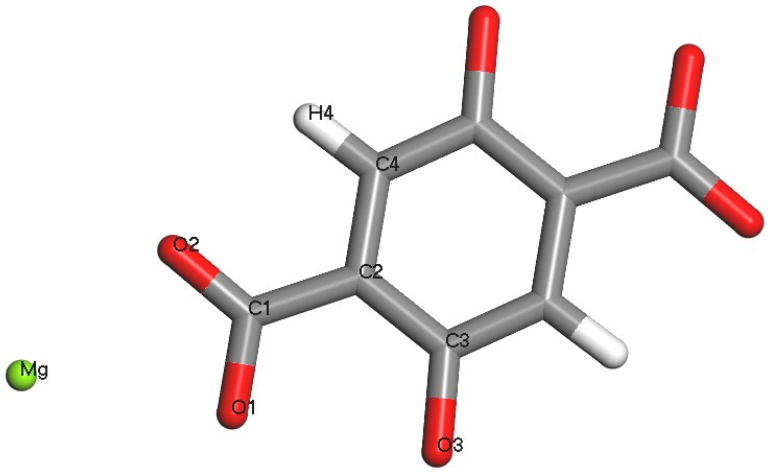
The total energy, U, is calculated in the following form

$$U = \frac{K_{bond}}{2}(r_{ij} - r_{ij,bond})^2 + \frac{K_{angle}}{2}(\theta_{ijk} - \theta_{ijk,angle})^2 + \frac{K_{torsion}}{2}(1 + \cos(n\theta_{ijkl} - \theta_{ijkl,} + \frac{q_i q_j}{4\pi\varepsilon_0 r_{ij}}$$

Lennard Jones parameters

Atoms	σ_i, nm	ε_i, kJ mol^{-1}
Mg	0.2691	0.4647
C	0.3431	0.4396
O	0.3118	0.2512
H	0.2571	0.1842
F	0.2997	0.2093
Methane (CH_4)	0.3730	1.2300

Partial Atomic Charges for Mg-MOF-74



Atoms	Charges, q_i
Mg	1.566
C1	0.936
C2	-0.325
C3	0.457
C4	-0.235
O1	-0.915
O2	-0.768
O3	-0.907
H4	0.191

Intramolecular force field terms for Mg-MOF-74

Bond

i	j	K_{bond}, kJ mol^{-1} nm^{-2}	$r_{ij,bond}$, nm
C1	**O1**	501905.602	0.1346
C1	**O2**	451545.168	0.1394
C3	**O3**	674291.146	0.1219
C1	**C2**	325952.190	0.1461
C2	**C3**	387408.861	0.1379
C2	**C4**	387408.836	0.1379
C3	**C4**	387408.861	0.1379
C4	**H4**	299306.278	0.1081

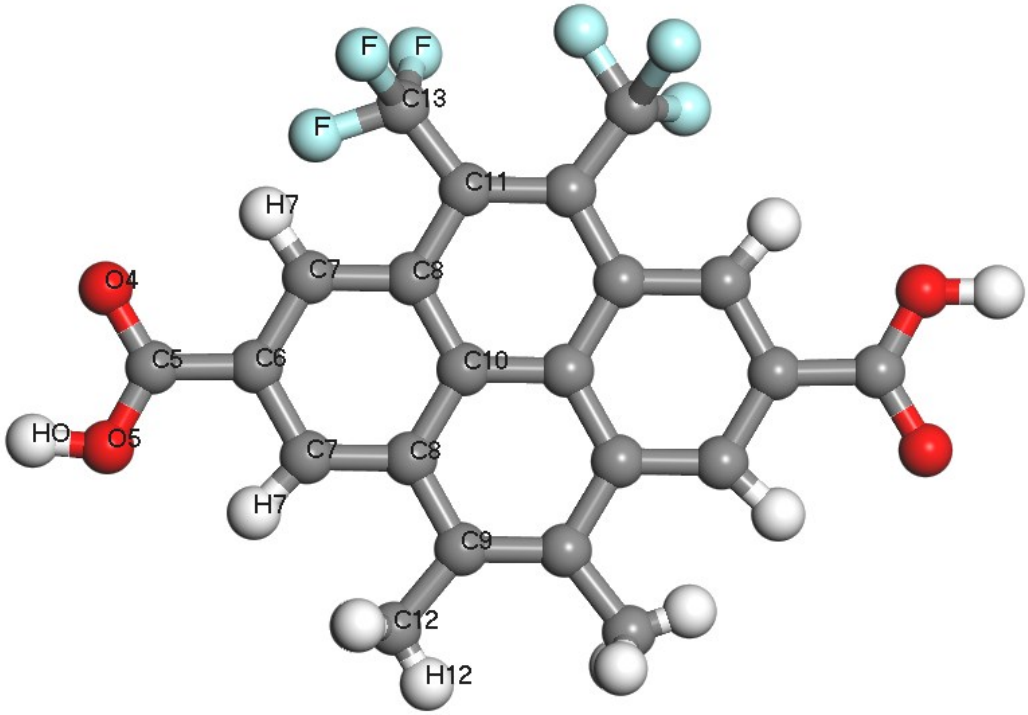
Angle

i	j	k	K_{angle}, kJ mol^{-1} rad^{-2}	$\theta_{ijk,angle}$, degree
O1	**C1**	**O2**	2162.321	120.000
O1	**C1**	**C2**	1373.527	120.000
O2	**C1**	**C2**	1563.552	120.000
C1	**C2**	**C3**	1102.913	120.000
C1	**C2**	**C4**	1102.913	120.000
C2	**C3**	**O3**	1508.734	120.000
C2	**C4**	**H4**	620.3582	120.000
C2	**C4**	**C3**	1205.193	120.000
C2	**C3**	**C4**	1205.193	120.000
C4	**C2**	**C3**	1205.193	120.000
O3	**C3**	**C4**	1508.734	120.000

Torsion

i	j	k	l	n	$K_{torsion}$, kJ mol^{-1}	$\theta_{ijkl,torsion}$, degree
O1	**C1**	**C2**	**C3**	2	5.234	180.000
O1	**C1**	**C2**	**C4**	2	5.234	180.000
O2	**C1**	**C2**	**C3**	2	5.234	180.000
O2	**C1**	**C2**	**C4**	2	5.234	180.000
O5	**C5**	**C6**	**C7**	2	5.234	180.000
C1	**C2**	**C3**	**O3**	2	5.234	180.000
C1	**C2**	**C3**	**C4**	2	14.104	180.000
C1	**C2**	**C4**	**H4**	2	14.104	180.000
C2	**C3**	**C4**	**C2**	2	14.104	180.000
C2	**C4**	**C3**	**O3**	2	14.104	180.000
C3	**C2**	**C4**	**H4**	2	14.104	180.000
C3	**C4**	**C2**	**C1**	2	14.104	180.000
C4	**C2**	**C3**	**O3**	2	14.104	180.000
C4	**C3**	**C2**	**C4**	2	14.104	180.000

Partial atomic charges for the gate molecule (4,5-dimethyl -9,10- bis(triflоromethyl)pyrene-2,7-dicarboxylic acid)



Atoms	Charges, q_i
C5	0.794
C6	-0.089
C7	-0.162
C8	0.120
C9	0.007
C10	-0.030
C11	-0.172
C12	-0.267
C13	0.634
O4	-0.605
O5	-0.515
HO	0.342
H7	0.132
H12	0.108
F	-0.201

Intramolecular force field terms for the gate molecule

Bond

i	j	K_{bond}, kJ mol^{-1} nm^{-2}	$r_{ij,bond}$, nm
O4	**C5**	479397.137	0.1366
O5	**C5**	479397.137	0.1366
O5	**HO**	504455.078	0.0966
C5	**C6**	327968.383	0.1458
C6	**C7**	387408.836	0.1379
C7	**H7**	299306.278	0.1081
C7	**C8**	387408.836	0.1379
C8	**C10**	387408.836	0.1379
C8	**C11**	387408.836	0.1379
C8	**C9**	387408.836	0.1379
C9	**C9**	387408.836	0.1379
C9	**C12**	309776.253	0.1486
C10	**C10**	387408.836	0.1379
C11	**C11**	387408.836	0.1379
C11	**C13**	309776.253	0.1486
C12	**H12**	277224.263	0.1109
C13	**F**	349820.315	0.1382

Angle

i	j	k	K_{angle}, kJ mol^{-1} rad^{-2}	θ_{angle}, degree
O4	**C5**	**O5**	1794.000	120.000
O4	**C5**	**C6**	1348.928	120.000
O5	**C5**	**C6**	1348.928	120.000
C5	**C6**	**C7**	1106.499	120.000
C6	**C7**	**H7**	620.3582	120.000
C6	**C7**	**C8**	1205.193	120.000
C7	**C8**	**C10**	1205.193	120.000
C7	**C8**	**C11**	1205.193	120.000
C7	**C6**	**C7**	1205.193	120.000
C8	**C10**	**C8**	1205.193	120.000
C8	**C10**	**C10**	1205.193	120.000
C8	**C11**	**C11**	1205.193	120.000
C8	**C11**	**C13**	1073.514	120.000
C8	**C9**	**C9**	1205.193	120.000
C8	**C9**	**C12**	1073.514	120.000
C9	**C9**	**C12**	1073.514	120.000
C9	**C8**	**C7**	1205.193	120.000
C9	**C8**	**C10**	1205.193	120.000
C9	**C12**	**H12**	494.503	109.470
C10	**C8**	**C11**	1205.193	120.000
C11	**C11**	**C13**	1073.514	120.000
C11	**C13**	**F**	927.0964	109.470
HO	**O5**	**C5**	737.4562	104.510
H4	**C4**	**C3**	620.358	120.000
H7	**C7**	**C8**	620.358	120.000

H12	**C12**	**H12**	306.579	109.47
F	**C13**	**F**	942.705	109.47

Torsion

i	j	k	l	n	$K_{torsion}$, kJ mol^{-1}	$\theta_{ijkl,torsion}$, degree
O4	**C5**	**C6**	**C7**	2	5.234	180.000
C5	**C6**	**C7**	**H7**	2	14.104	180.000
C5	**C6**	**C7**	**C8**	2	14.104	180.000
C6	**C7**	**C8**	**C9**	2	14.104	180.000
C6	**C7**	**C8**	**C10**	2	14.104	180.000
C6	**C7**	**C8**	**C11**	2	14.104	180.000
C7	**C6**	**C7**	**C8**	2	14.104	180.000
C7	**C6**	**C7**	**H7**	2	14.104	180.000
C7	**C8**	**C9**	**C9**	2	14.104	180.000
C7	**C8**	**C9**	**C12**	2	14.104	180.000
C7	**C8**	**C10**	**C8**	2	14.104	180.000
C7	**C8**	**C10**	**C10**	2	14.104	180.000
C7	**C8**	**C11**	**C11**	2	14.104	180.000
C7	**C8**	**C11**	**C13**	2	14.104	180.000
C8	**C9**	**C9**	**C8**	2	14.104	180.000
C8	**C9**	**C9**	**C12**	2	14.104	180.000
C8	**C9**	**C12**	**H12**	6	0.349	-180.000
C8	**C10**	**C8**	**C7**	2	14.104	180.000
C8	**C10**	**C8**	**C9**	2	14.104	180.000
C8	**C10**	**C8**	**C11**	2	14.104	180.000
C8	**C10**	**C10**	**C8**	2	14.104	180.000
C8	**C11**	**C11**	**C8**	2	14.104	180.000
C8	**C11**	**C11**	**C13**	2	14.104	180.000
C8	**C11**	**C13**	**F**	6	0.349	-180.000
C9	**C9**	**C12**	**H12**	2	14.104	180.000
C9	**C9**	**C8**	**C10**	2	14.104	180.000
C9	**C8**	**C10**	**C10**	2	14.104	180.000
C10	**C8**	**C11**	**C11**	2	14.104	180.000
C10	**C10**	**C8**	**C11**	2	14.104	180.000
C11	**C11**	**C13**	**F**	6	0.349	-180.000
HO	**O5**	**C5**	**C6**	2	10.467	180.000
HO	**O5**	**C5**	**O4**	2	1.047	0.000
H7	**C7**	**C8**	**C9**	2	14.104	180.000
H7	**C7**	**C8**	**C10**	2	14.104	180.000
H7	**C7**	**C8**	**C11**	2	14.104	180.000