Electronic Supplementary Information

Electric Field Induced Rotation of Halogenated Organic Linkers in Isoreticular Metal-Organic Frameworks for Nanofluidic Applications

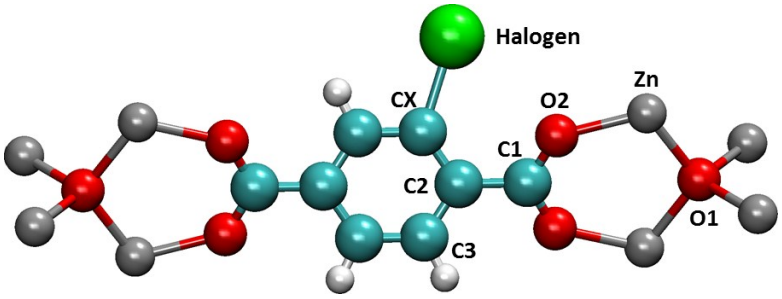
Sadanandam Namsani and A. Ozgur Yazaydin*

Department of Chemical Engineering, University College London, Torrington Place, London, WC1E 7JE, United Kingdom

Table S1: The dipole moment of IRMOF-7 functionalized with different halogens as shown in Figure5.

Halogen type	Total Dipole moment (D)
Br	1.3596
F	1.2498
Cl	1.5576

Table S2: The force field parameters used in this work for to perform MD simulations*



Bond				Bend					Torsion						
i	j	k/k_B (K)	R_0 (Å)	i	j	k	k/k_B (K)	θ_0 (°)	i	j	k	l	k/k_B (K)	ϕ_0 (°)	m (-)
O2	C1	543840.0	1.27	O2	C1	O2	135960.0	132	O2	C1	C2	C3	1258.9	180	2
C1	C2	353750.0	1.44	O2	C1	C2	54882.0	114	C1	C2	C3	H1	1510.7	180	2
C2	C3	483414.0	1.365	C1	C2	C3	34927.0	120	C1	C2	C3	C3	1510.7	180	2
C3	C3	483414.0	1.365	C3	C2	C3	90640.0	120	C2	C3	C3	H1	1510.7	180	2
C3	H1	366000.0	0.95	C3	C3	C2	90640.0	120	C2	C3	C3	C2	1510.7	180	2
CX	Br	232678.1	1.906	C2	C3	H1	37263.0	120	C3	C2	C3	C3	1510.7	180	2
CX	F	420739.8	1.382	C3	C3	H1	37263.0	120	H1	C3	C2	C3	1510.7	180	2
CX	Cl	279858.6	1.751	CX	CX	Br	457551.7	120	H1	C3	C3	H1	1510.7	180	2
				CX	CX	F	108145.8	109.47	H1	C2	C3	H1	1510.7	180	2
				CX	CX	Cl	119660.8	120	CX	CX	CX	Br	1696.3	180	2
									CX	CX	CX	F	716.31	0.0	3
									CX	CX	CX	Cl	1696.3	180	2

*In IRMOF-7 ligand the second benzene ring carbon atoms are treated as C3.

Table S3: Non-bonded interaction parameters used in this work for to perform MD simulations

Atom type	ε/k_B (K)	σ (Å)
Zn	0.42	2.7
O1	700	2.98
O2	70.5	3.11
C1	47.0	3.74
C2	47.86	3.47
C3	47.86	3.47
H1	7.65	2.85
Br	126.395	3.732
F	25.173	2.997
Cl	114.307	3.516
CH_4	148	173

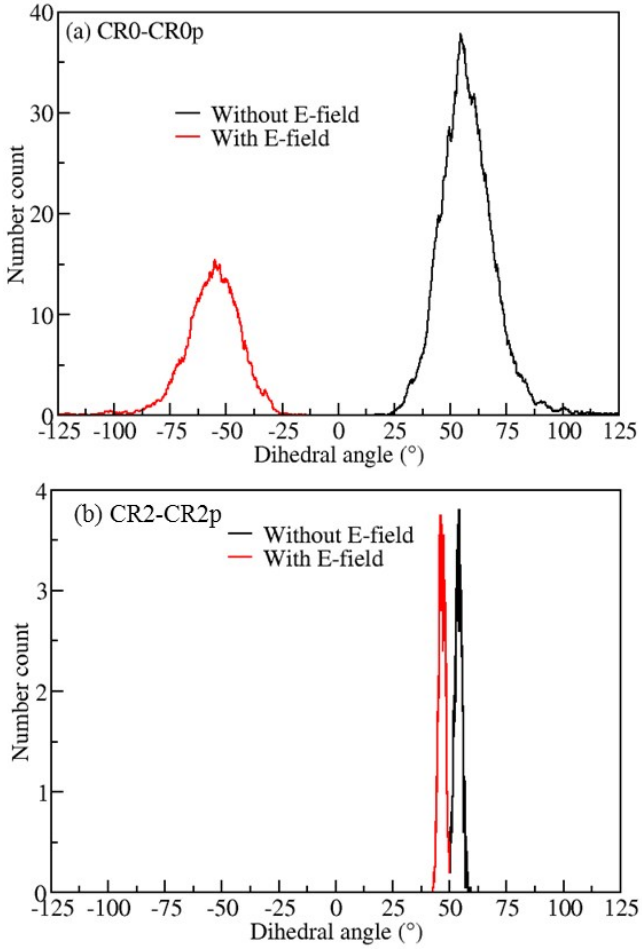


Figure S1. Rotational dihedral angle distributions of (a) CR0-CR0p and (b) CR2-CR2p substituted IRMOF-7-Cl2 with and without E-field (1 V/nm) at 300 K.

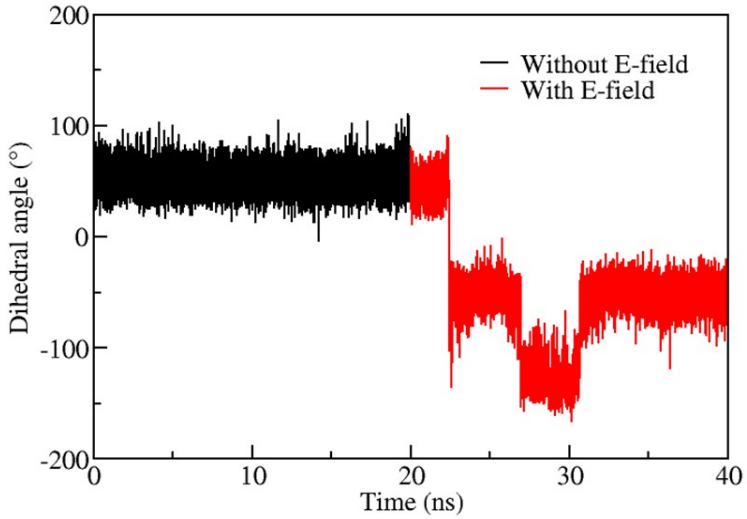


Figure S2. Mean value of rotational dihedral angle of CR0-CR0 substituted IRMOF-7-Cl_2 ligands as a function of MS simulations time

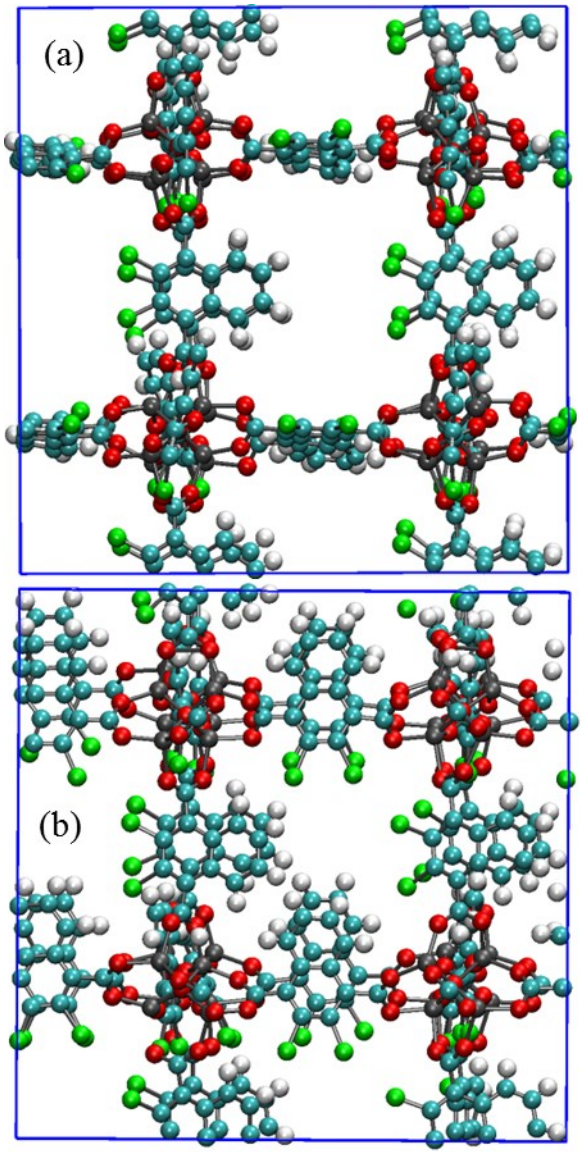


Figure S3. Snapshots of CR0-CR0p substituted IRMOF-7-Cl_2 in the y-direction obtained from methane diffusion simulations (a) before and (b) after the E-field (2 V/nm) is applied. Methane molecules are not shown for clarity.

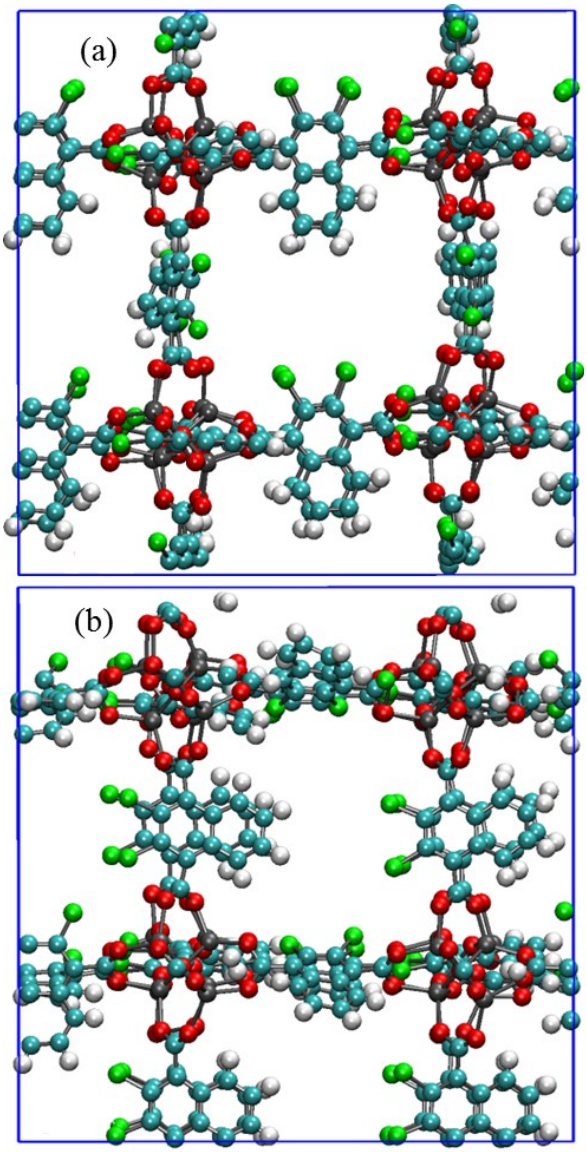


Figure S4. Snapshots of CR0-CR0p substituted IRMOF-7-Cl_2 in the z-direction obtained from methane diffusion simulations (a) before and (b) after the E-field (2 V/nm) is applied. Methane molecules are not shown for clarity.

.

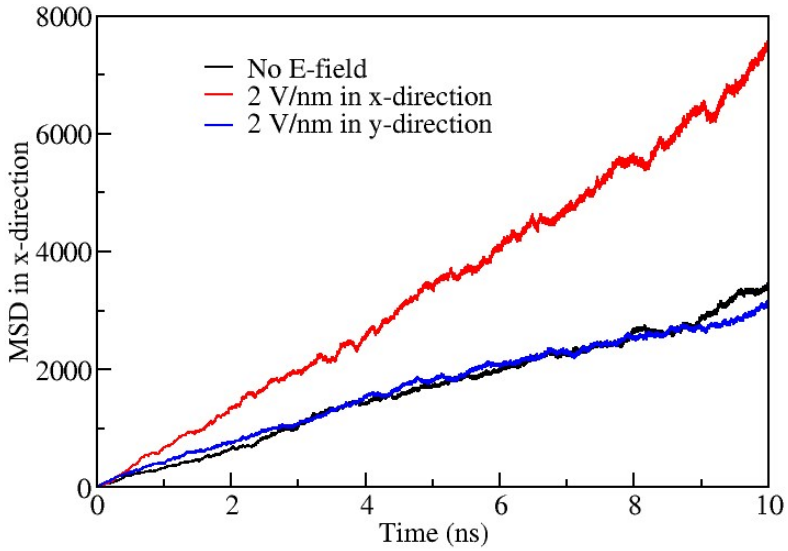


Figure S5. Comparison of MSD for methane molecules in the x-direction from MS simulations; before the E-field applied (black line), after the E-field applied in the x-direction (red line) and after the E-field applied in the y-direction (blue line).