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Supplementary Information for

Mechanochemical synthesis of a fluorenone-based metal organic framework with polarized fluorescence: an experimental and computational study

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Table S1: Atomic coordinates for Zn-FDC

Atoms	x	y	z
Zn1	-0.30794	-0.26001	0.96973
C2	-1.57481	1.32627	-0.39734
C3	-1.46024	1.34374	-0.04919
C4	-1.51170	1.34556	-0.34631
C5	-1.24472	1.30854	-0.11571
C6	-1.37256	1.33609	-0.19692
C7	-1.59404	1.34638	-0.13468
C8	-1.69383	1.36438	-0.22339
C9	-1.65101	1.35000	-0.31257
C10	-1.39003	1.34324	-0.24931
C11	-1.21356	1.30873	-0.16361
C12	-1.58548	1.35227	-0.26474
C13	-1.25184	1.34040	-0.28228
C14	-1.55781	1.34788	-0.18213
C15	-1.31211	1.34279	-0.33032
C16	-1.43412	1.33174	-0.10043
O17	-1.46488	1.27581	-0.42867
O18	-1.74950	1.34642	-0.41290
O19	-1.35512	1.46577	-0.02279
O20	-1.59135	1.23711	-0.03056
O21	-1.86157	1.41790	-0.22284
O22	0.80167	0.52557	0.49819
O23	0.06974	1.11247	0.53305
H24	0.87897	0.55956	0.52805
H25	0.97884	1.60139	0.93568
H26	0.89846	0.31770	0.72737
H27	0.79747	0.33379	0.64496
H28	0.19400	0.35011	0.67681
H29	0.87864	0.28067	0.90954
H30	0.92938	0.27527	0.82638
H31	0.25846	0.36134	0.87526
H32	0.03047	0.80298	0.48474
H33	2.29597	0.57720	0.49359

a=6.8770Å, *b*=6.3848 Å, *c*=28.7917 Å, *ß*=95.1270°

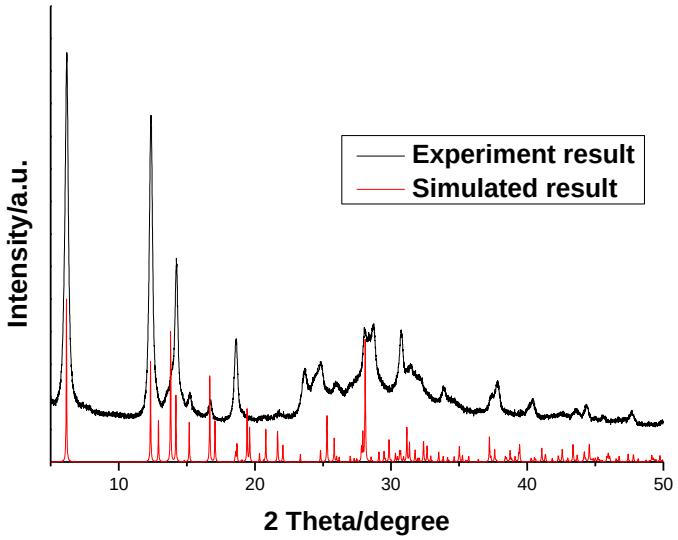

Fig. S1. Experimental and simulated XRD profile for Zn-FDC MOF.

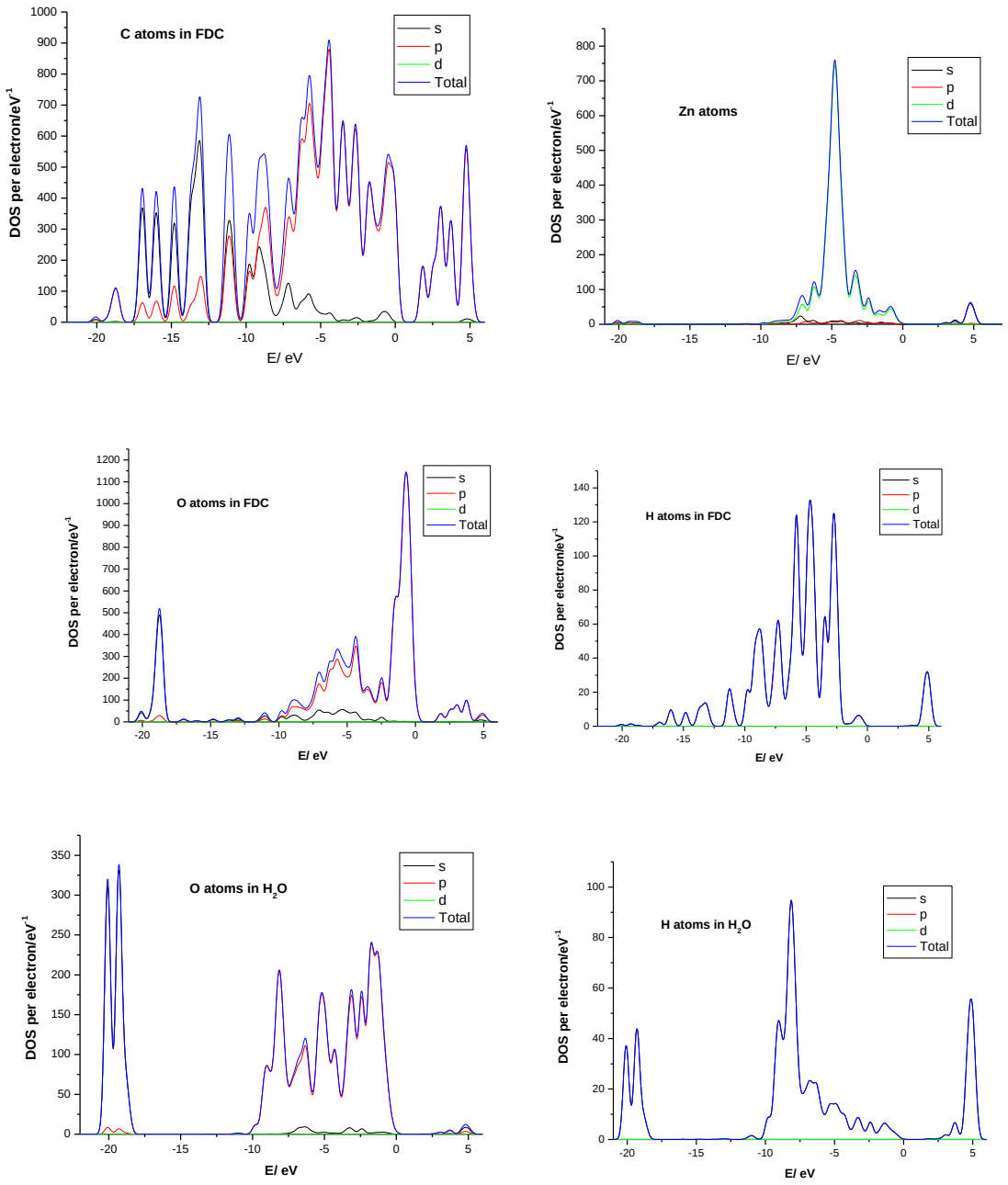

Fig. S2. Total and partial electronic density of states (TDOS and PDOS) profiles for different atoms in Zn-FDC.

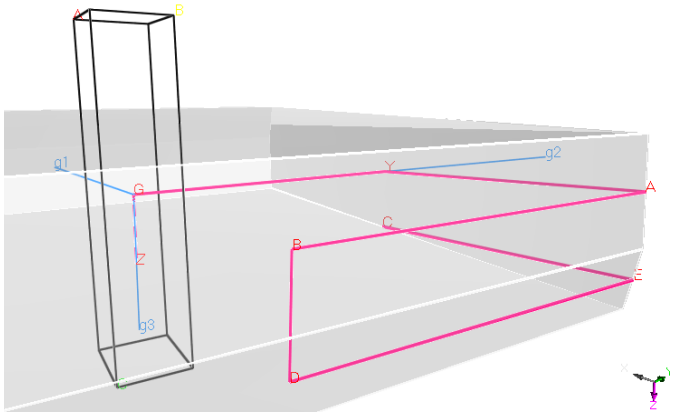

Fig. S3. The real space (black line) and reciprocal space (red line) in the first Brillouin Zone (BZ) for Zn-FDC MOF. G (0,0,0); Z (0,0,0.5); Y (0,0.5,0); A (-0.5,0.5,0); B (-0.5,0,0); D (-0.5,0,0.5); E (-0.5,0.5,0.5); C(0,0.5,0.5) are the selected reciprocal points in the first BZ.

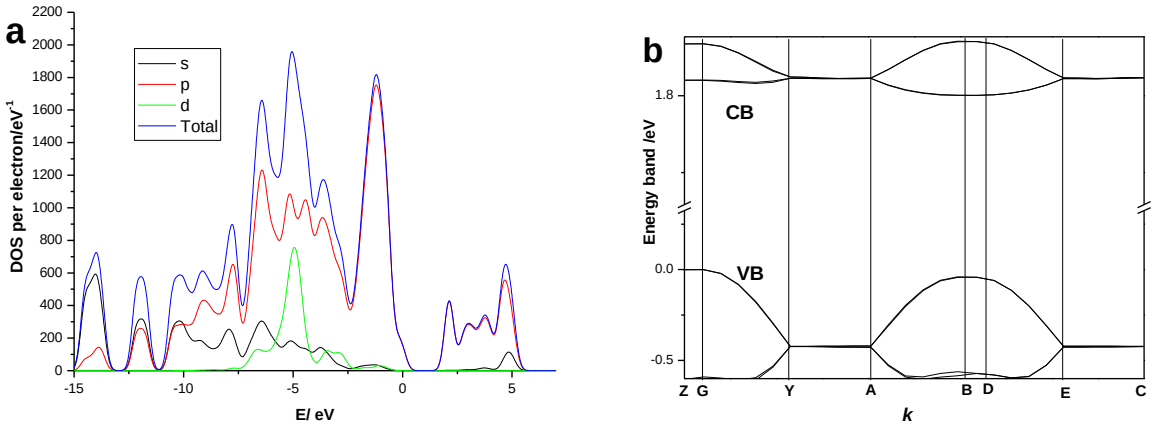

Fig. S4. a) Total and partial electronic density of state (TDOS and PDOS) and b) band structure for Zn-FDC MOF. G (0,0,0); Z (0,0,0.5); Y (0,0.5,0); A (-0.5,0.5,0); B (-0.5,0,0); D (-0.5,0,0.5); E (-0.5,0.5,0.5); C(0,0.5,0.5) are the selected reciprocal points in the first BZ. The Brillouin zone is sampled by 4×4×1 *k*-points.