Electronic Supplementary Materials

Enhanced pseudocapacitive performance of a Pb-based MOF/FCNT composite for high-stability supercapacitor applications: A step ahead towards energy storage

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Table S1. Selected bond lengths (Å)) for YK-2.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Pb1	O4[1]	2.536(2)	N1	C1	1.334(5)
Pb1	O4	2.536(2)	N1	C6	1.339(5)
Pb1	N1	2.565(3)	C1	C2	1.370(6)
Pb1	N1[1]	2.565(3)	C2	C3	1.490(6)
O1	C3	1.298(6)	C2	C4	1.389(6)
O2	C3	1.210(6)	C4	C5	1.385(5)
O3	C7	1.240(6)	C5	C6	1.386(5)
O4	C7	1.256(7)	C6	C7	1.509(6)

Table S2. Selected bond angles (degree) for YK-2

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O4	Pb1	O4[1]	115.41(11)	C4	C2	C3	121.5(4)
N1[1]	Pb1	O4	70.10(9)	O2	C3	O1	125.1(5)
N1[1]	Pb1	O4[1]	62.83(9)	C2	C3	O1	113.6(4)
N1	Pb1	O4	62.83(9)	C2	C3	O2	121.3(4)
N1	Pb1	O4[1]	70.10(9)	C5	C4	C2	119.9(4)
N1[1]	Pb1	N1	83.55(14)	C6	C5	C4	118.6(4)
C7	O4	Pb1[1]	119.2(2)	C5	C6	N1	121.2(4)

C1	N1	Pb1	121.6(3)	C7	C6	N1	115.4(4)
C6	N1	Pb1	117.3(3)	C7	C6	C5	123.3(4)
C6	N1	C1	119.5(4)	O4	C7	O3	125.4(4)
C2	C1	N1	123.1(4)	C6	C7	O3	117.5(5)
C3	C2	C1	120.8(4)	C6	C7	O4	117.0(4)
C4	C2	C1	117.7(4)				

Table S3. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for YK-2 (U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor).

Atom	***x***	***y***	***z***	**U(eq)**
Pb1	5000	5034.99(14)	2500	25.22(15)
O1	8232(2)	7172(3)	1695(4)	50.5(10)
O2	8444.5(17)	9068(3)	2621(4)	56.4(9)
O3	4606(2)	8191(3)	5658(4)	52.1(10)
O4	4666.4(19)	6281(2)	4790(3)	31.9(6)
N1	6012.0(19)	6795(3)	3403(3)	29.3(8)
C1	6728(3)	6974(5)	2800(6)	33.9(12)
C2	7193(3)	8032(4)	3015(5)	29.3(10)
C3	8020(3)	8147(5)	2409(6)	33.5(12)
C4	6879(2)	8971(4)	3853(5)	42.2(11)
C5	6128(3)	8806(4)	4464(5)	42.2(11)
C6	5718(3)	7684(4)	4248(5)	26.4(9)
C7	4928(2)	7369(6)	4944(4)	29.6(13)

Table S4. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for YK-2.

The Anisotropic displacement factor exponent takes the form: -$2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{12}**	**U_{13}**	**U_{23}**
Pb1	20.4(2)	19.74(19)	38.6(2)	-0	15.51(13)	0
O1	38(2)	38(2)	83(3)	-7.9(17)	39.9(19)	-14.2(17)
O2	34.6(19)	40.0(19)	103(3)	-18.2(15)	40.9(17)	-17.0(17)
O3	44(2)	31.6(19)	92(2)	-7.9(15)	53.4(19)	-18.2(17)
O4	30.6(16)	23.1(16)	46.3(17)	-5.7(14)	22.1(12)	-1.0(12)
N1	26(2)	27.9(18)	39(2)	-4.6(14)	21.4(16)	-6.6(14)
C1	27(3)	32(3)	47(3)	-5(2)	21(2)	-8(2)
C2	21(3)	27(2)	44(3)	-2.7(18)	19(2)	-1.7(18)
C3	24(3)	30(3)	50(3)	-3.1(19)	18(2)	0.3(19)
C4	34(3)	28(2)	71(3)	-11.4(19)	28(2)	-8(2)
C5	37(3)	24(2)	71(3)	-4.8(19)	28(2)	-10(2)
C6	21(3)	25(2)	36(2)	1.8(18)	14.0(19)	0.4(18)
C7	24(3)	30(3)	38(3)	3.3(16)	18(2)	0.0(15)

Table S5. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for YK-2.

Atom	*x*	*y*	*z*	U(eq)
H1	8820(40)	7210(50)	1450(60)	80(20)
H1a	6920(3)	6352(5)	2205(6)	40.7(14)
H4	7172(2)	9709(4)	4003(5)	50.6(13)
H5	5904(3)	9435(4)	5006(5)	50.6(13)

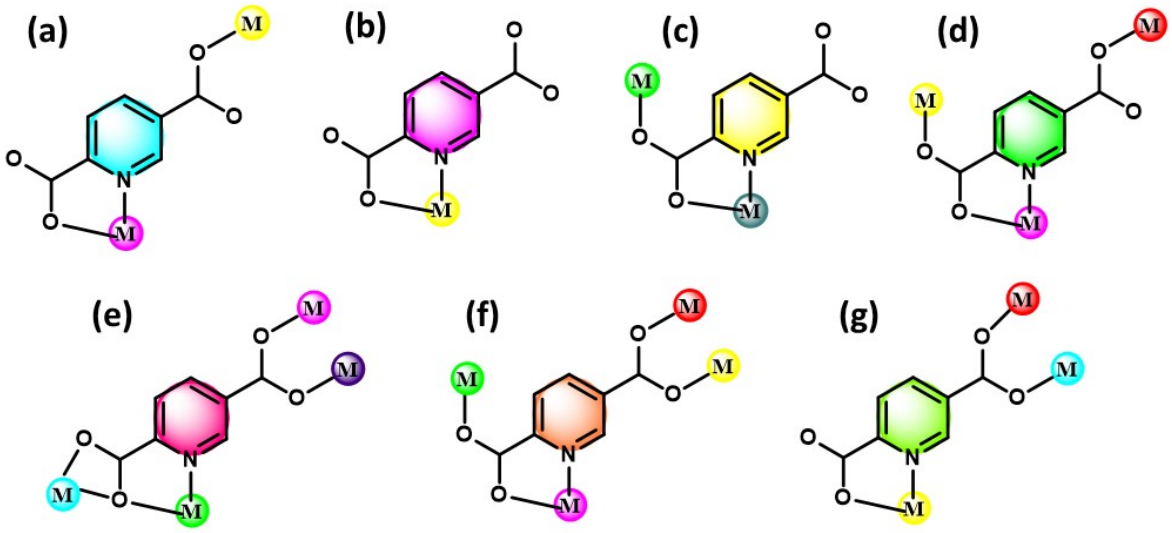

Fig. S1. Various coordination modes of H_2pdc ligand.

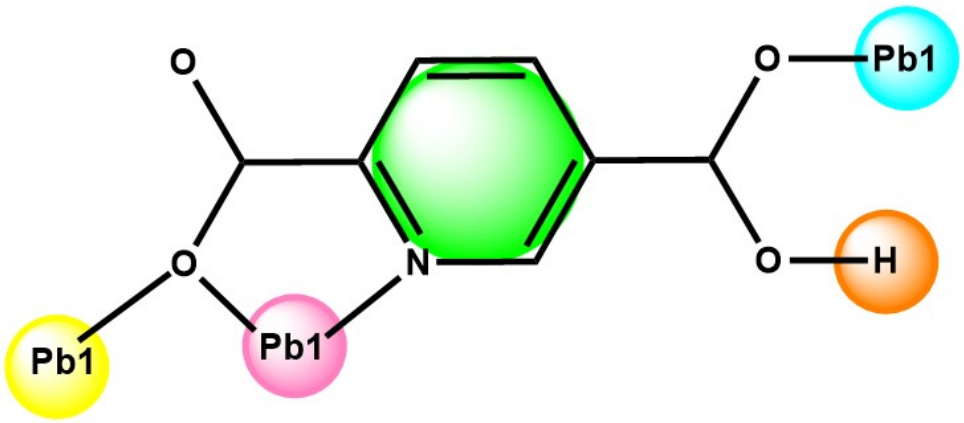

Fig. S2. Coordination mode of H_2pdc ligand in YK-2.

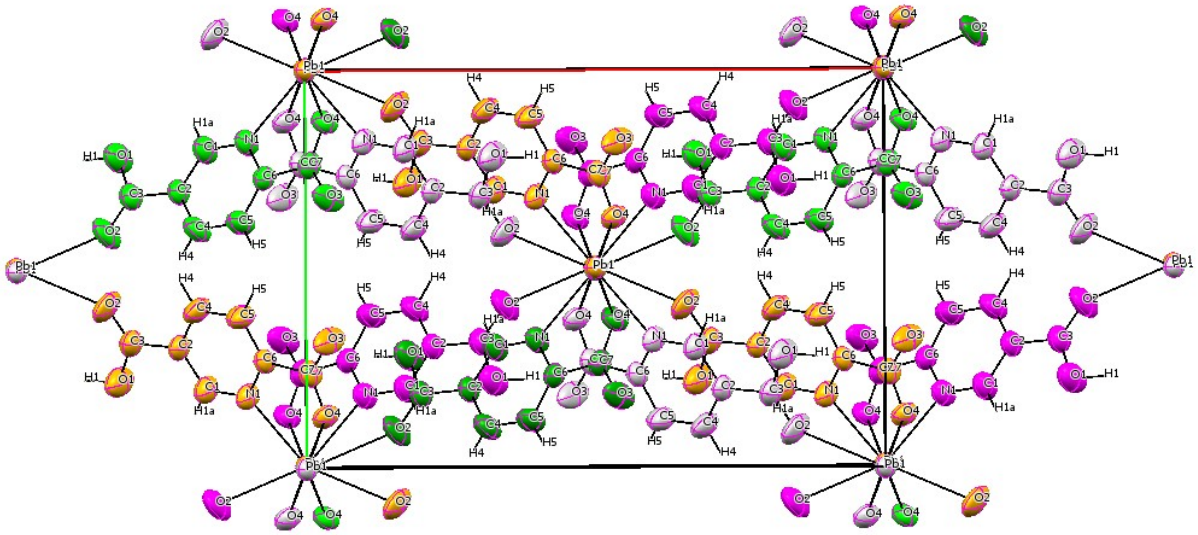

Fig. S3. ORTEP view with 50% probability level.

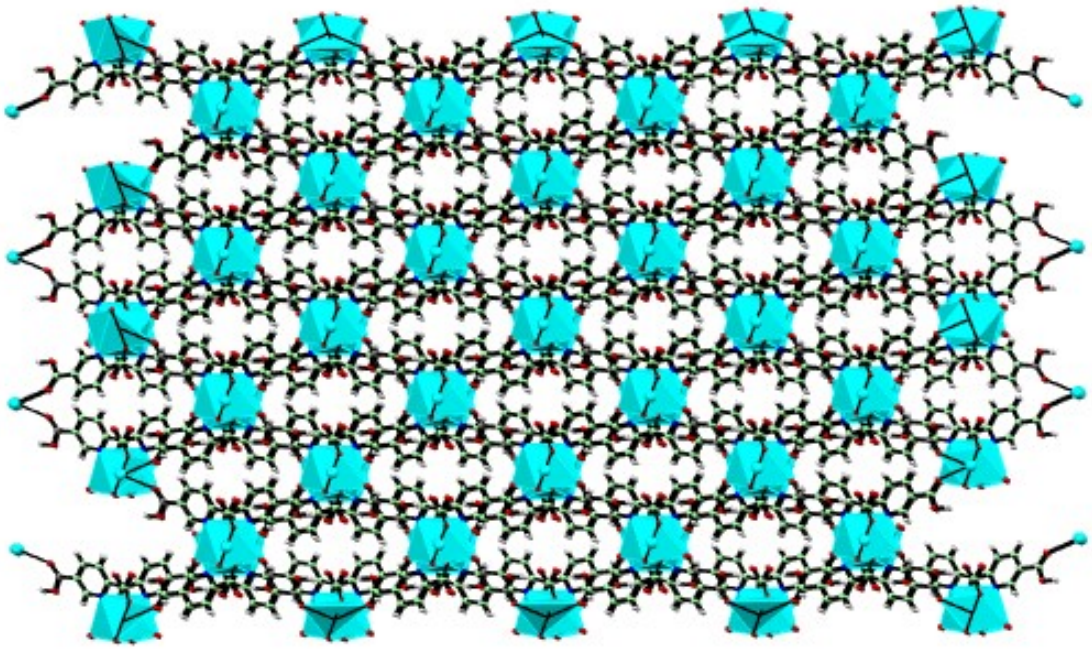

Fig. S4. Polyhedral view of YK-2.

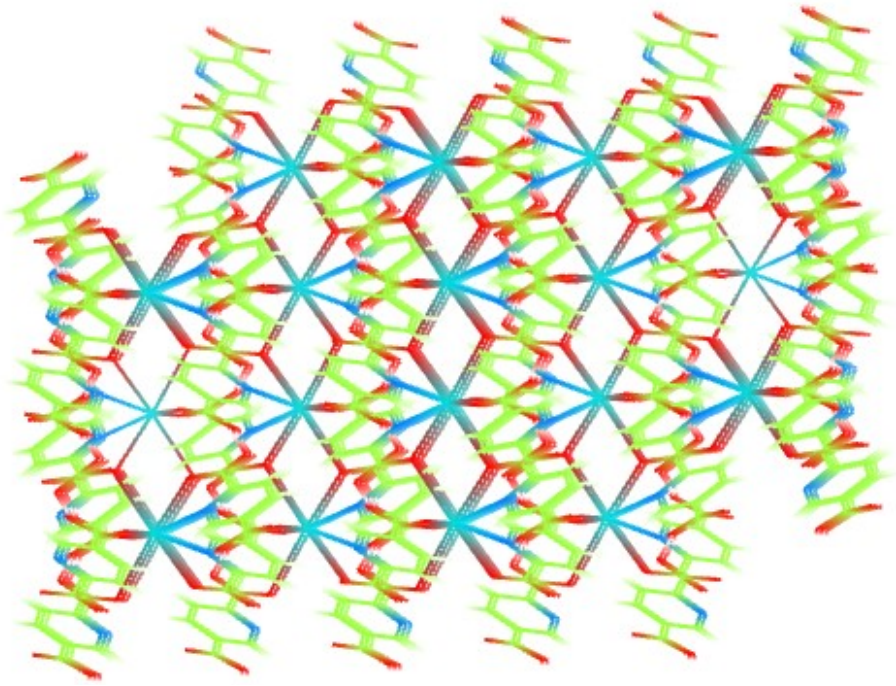

Fig. S5. Capped stick model showing interconnected atoms within the framework.

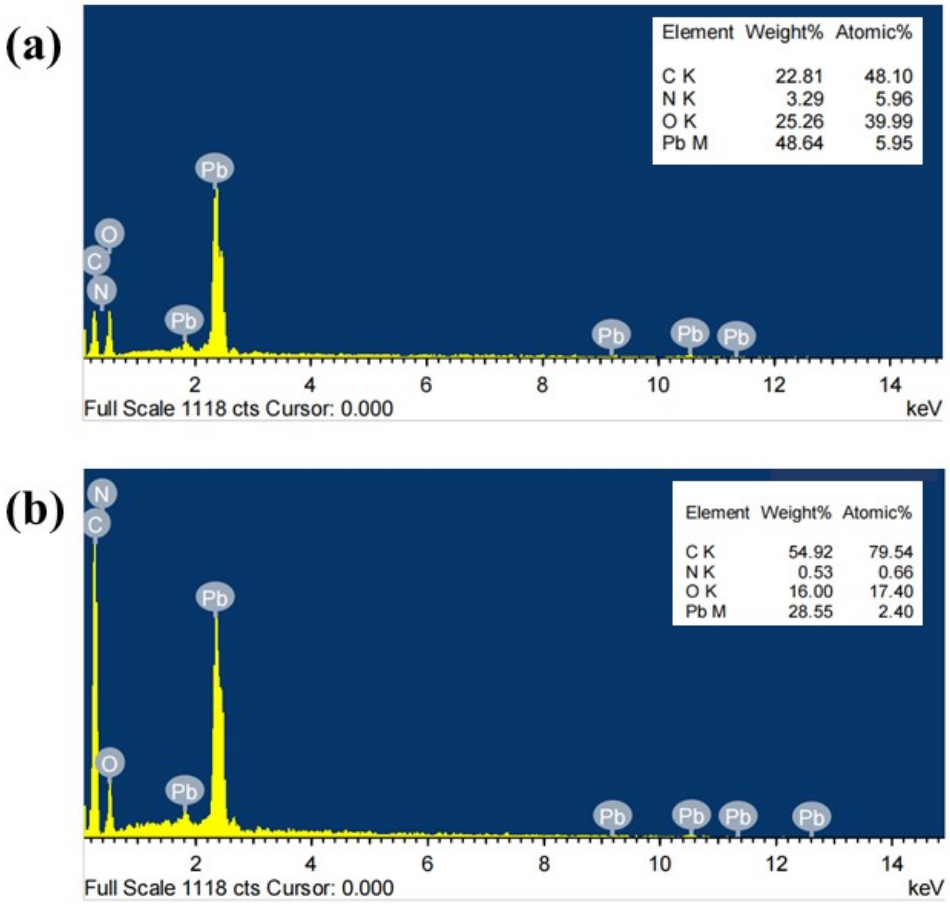

Fig. S6. EDX spectrum of (a) YK-2 and (b) YK-2@FCNT(10).