

Four 2D Metal–Organic Networks Incorporating Cd–Cluster SUBs: Hydrothermal Synthesis, Structures and Photoluminescent Properties

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Elemental analyses were performed on a Perkin-Elmer 240C elemental analyzer. The IR spectra were obtained as KBr pellets on a VECTOR 22 spectrometer. Thermal analyses were performed on a TGA V5.1A Dupont 2100 instrument from room temperature to 750°C with a heating rate of 10°C/min in a nitrogen atmosphere. Luminescence spectra for the solid samples were recorded with a Hitachi 850 fluorescence spectrophotometer.

Table S1. Hydrogen bond distances (\AA) and angles ($^\circ$) for **2**, **3**, **4** and **5**. (D, donor atom; A, acceptor atom).

D-H	d(D-H)	d(H \cdots A)	\angle DHA	d(D \cdots A)	A
compound 2 ^{#1}					
O(18)-H(18A)	0.98	2.21	137	3.004	O(9)
O(21)-H(21C)	0.85	2.06	159	2.868	O(4)
O(26)-H(26D)	0.85	2.36	112	2.793	O(1)
O(18)-H(18A)	0.98	2.19	138	2.999	O(13) ^a
O(19)-H(19C)	0.85	2.27	138	2.957	O(13) ^a
O(25)-H(25C)	0.96	1.98	150	2.850	O(11) ^a
O(22)-H(22B)	0.96	1.77	158	2.682	O(2) ^b
O(23)-H(23C)	0.96	1.75	151	2.636	O(10) ^b
O(20)-H(20B)	0.85	2.39	112	2.823	O(17) ^c
O(21)-H(21A)	0.85	1.93	173	2.772	O(17) ^d
O(22)-H(22C)	0.96	2.40	156	3.297	O(17) ^d
O(24)-H(24A)	0.96	2.06	133	2.812	O(12) ^d
O(24)-H(24B)	0.96	1.85	156	2.757	O(14) ^e
O(25)-H(25B)	0.96	1.97	128	2.671	O(26) ^f
O(26)-H(26E)	0.85	2.27	138	2.964	O(8) ^g
compound 3 ^{#2}					
O(9)-H(9B)	0.85	1.94	165.6	2.772	O(3) ^a
O(10)-H(10B)	0.85	1.96	141.9	2.677	O(1) ^b
O(10)-H(10A)	0.85	1.78	166.9	2.617	O(5) ^b
O(9)-H(9A)	0.85	2.14	146.2	2.889	O(10) ^c
compound 4 ^{#3}					
O(18)-H(18A)	0.85	2.25	171	3.090	O(15)
O(20)-H(20B)	0.85	2.21	150	2.978	O(10)
O(17)-H(17B)	0.85	2.34	134	2.998	O(12) ^a
O(17)-H(17B)	0.85	2.42	170	3.258	O(11) ^a
O(17)-H(17A)	0.85	2.46	147	3.205	O(3) ^a
O(19)-H(19C)	0.85	2.48	157	3.276	O(17) ^a
O(18)-H(18B)	0.85	2.27	142	2.986	O(9) ^b
N(2)-H2	0.86	1.70	173.7	2.553	O(16) ^c
compound 5 ^{#4}					
O(9)-H(9B)	0.85	2.18	149.4	2.947	O(3) ^a
O(9)-H(9B)	0.85	2.45	126.1	3.026	O(3)
O(9)-H(9C)	0.85	2.19	156.3	2.991	O(8) ^b

^{#1} Symmetry codes: ^a-x, -y+1, -z+1; ^b-x+1, -y+2, -z; ^c-x+1, -y+1, -z+1; ^dx, y, z-1; ^ex+1, y, z-1; ^fx-1, y, z; ^g-x+2, -y+2, -z. ^{#2} Symmetry codes: ^a-x + 1, -y + 1, -z + 1; ^b-x + 2, -y + 1, -z + 1; ^cx - 1, y,

$z; ^d -x+1, -y+1, -z.$ ^{#3} Symmetry codes: $^a -x+1, -y, -z+1;$ $^b x+1, y, z;$ $^b -x+1, -y+1, -z+2.$ ^{#4}
Symmetry codes: $^a -x, -y+1, -z;$ $^b -x+1, -y+1, -z.$

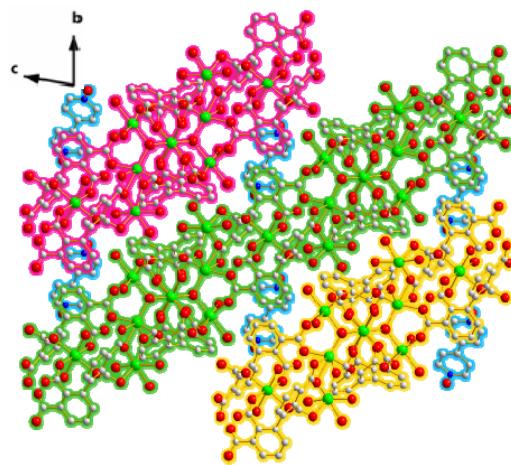


Fig. S1. 3D supramolecular structure of **2**. Three adjacent metal-organic layers are marked as red, green and yellow, whereas the “template” bpydo molecules are highlighted as blue color.

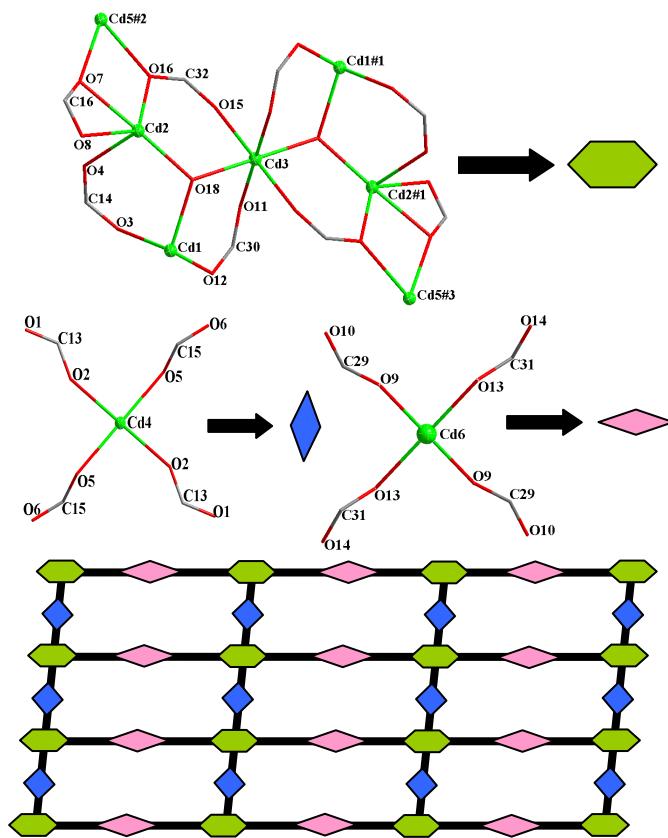


Fig. S2. Topology structure of **2**. Cd_7 cluster can be simplified as four connected net, whereas Cd_4 and Cd_6 atoms can be regarded as two connected nets.

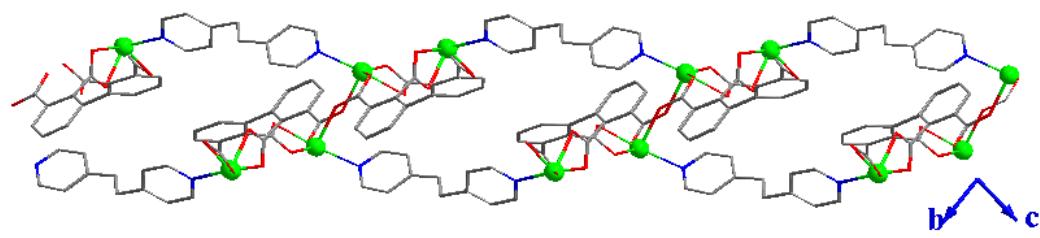


Fig. S3. 2D metal–organic double layer structure of **3**. Hydrogen atoms are omitted for clarity.

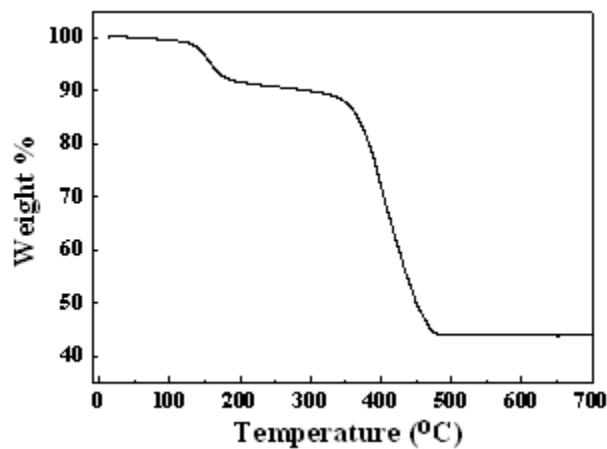


Fig. S4. TG curve of **2**.

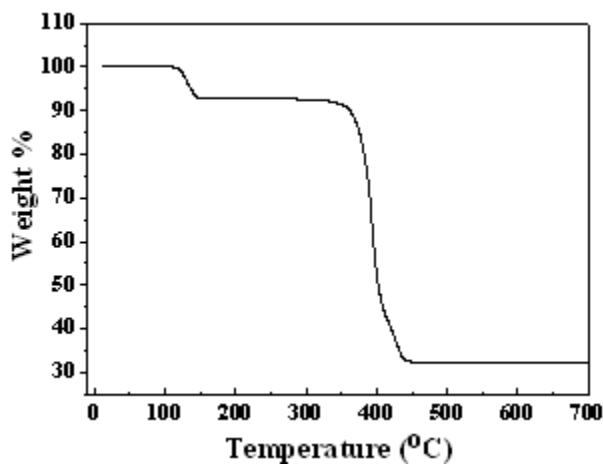


Fig. S5. TG curve of **3**.

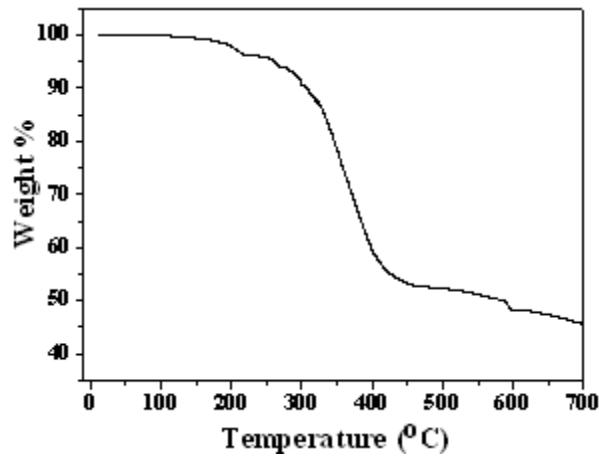


Fig. S6. TG curve of 4.

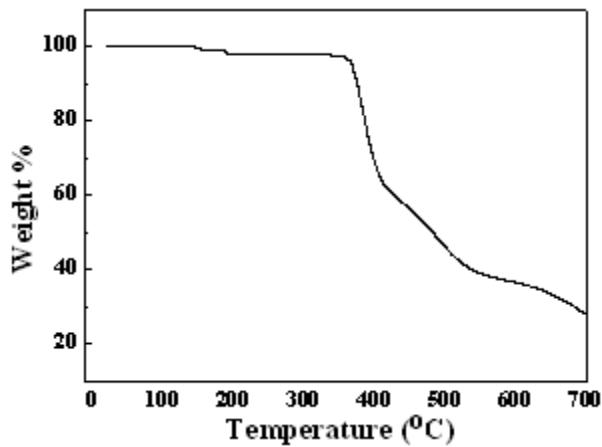


Fig. S7. TG curve of 5.

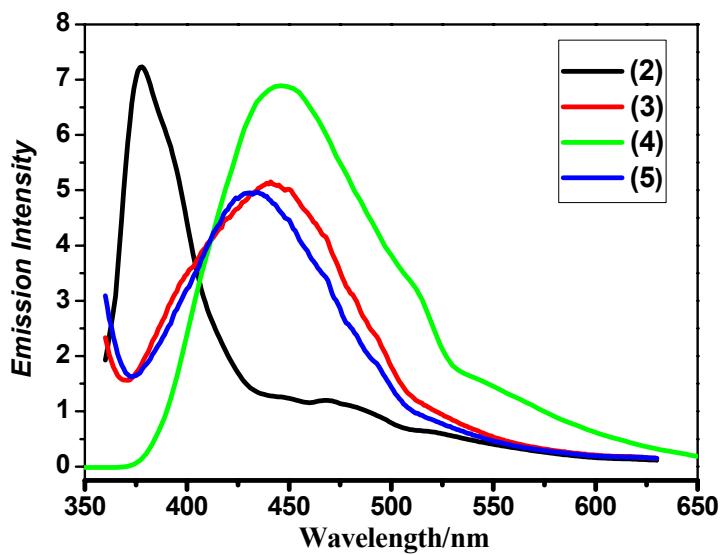


Fig. S8. Fluorescent emission spectra of 2, 3, 4 and 5 in solid state at room temperature.