Supporting Information for the Manuscript:

A series of d^{10} metal coordination polymers based on a flexible bis(2-methylbenzimidazole) ligand and different carboxylates: synthesis, structures, photoluminescence and catalytic properties

Jin-ming Hao[a], Bao-yi Yu[b], Kristof Van Hecke[b], Guang-hua Cui[a,*]

a College of Chemical Engineering, Hebei United University, 46 West Xinhua Road, Tangshan, 063009, Hebei, PR China
b Department of Inorganic and Physical Chemistry, Ghent University, Krijgslaan 281 S3, 9000 Ghent, Belgium

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*Corresponding author. Fax: +86-0315-2592170. Tel: +86-0315-2592169.

*Corresponding author. E-mail: tscghua@126.com.

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Table S1. Crystallographic data and structure refinement details for complexes 1−6

	1	**2**	**3**	**4**	**5**	**6**
Formula	$C_{31}H_{26}Ag_2N_4O_4$	$C_{27}H_{22}Br_4N_4O_5Zn$	$C_{27}H_{22}Br_4CdN_4O_5$	$C_{29}H_{24}N_4O_9Zn_2$	$C_{40}H_{35}N_4O_8Zn_2$	$C_{27}H_{25}CdN_5O_7$
fw	734.30	867.48	914.53	703.26	830.46	643.92
Cryst syst	Monoclinic	Monoclinic	Triclinic	Triclinic	Monoclinic	Triclinic
Space group	$P2_1/n$	$P2/n$	$P\bar{1}$	$P\bar{1}$	$P2_1/n$	$P\bar{1}$
a, Å	16.7454(9)	11.7886(5)	9.5556(4)	9.3237(4)	13.8342(9)	10.931(2)
b, Å	8.1590(5)	9.8051(4)	12.1747(2)	11.4454(5)	20.8728(13)	11.727(2)
c, Å	20.5264(11)	12.5957(8)	12.9664(3)	13.6744(6)	14.2205(9)	11.928(2)
α, deg			84.089(2)	66.862(4)		98.983(3)
β, deg	96.7490(10)	93.596(5)	89.206(2)	78.859(4)	112.7790(1)	101.005(2)
γ, deg			88.552(2)	85.704(4)		115.316(3)
V, Å^3	2785.0(3)	1453.05(13)	1499.87(8)	1316.57(10)	3786.0(4)	1307.1(4)
Z	4	2	2	2	4	2
D_{calc}, g/m^3	1.751	1.983	2.025	1.774	1.457	1.636
μ, mm^{-1}	1.451	6.390	6.100	1.890	1.325	0.892
F(000)	1464	844	880	716	1708	652
Crystal size, mm	0.24 x 0.22 x 0.21	0.26 x 0.25 x 0.22	0.23 x 0.22 x 0.22	0.25 x 0.24 x 0.19	0.28 x 0.26 x 0.22	0.20 x 0.19 x 0.19
Total reflections	20513	14532	28646	24848	34662	7790
Unique reflections	4910	2553	5299	4630	8675	5588
R_{int}	0.0230	0.0538	0.0491	0.0404	0.0456	0.0457
GOF	1.027	1.045	1.127	1.035	1.003	0.974
R_1 ($I >$ 2σ(I))	0.0265	0.0321	0.0541	0.0260	0.0387	0.0624
wR_2 ($I >$ 2σ(I))	0.0661	0.0716	0.1431	0.0614	0.0874	0.1268
$\Delta\rho$max, eÅ^{-3}	1.253	0.805	3.569	0.345	0.371	0.632
$\Delta\rho$min, eÅ^{-3}	-0.872	-0.637	-1.277	-0.418	-0.314	-0.767

Table S2. Selected bond lengths (Å) and angles (°) for complexes 1-6

Compound **1**			
Ag(1)-N(3)A	2.221(2)	Ag(1)-O(2)	2.309(2)
Ag(1)-O(3)B	2.3155(19)	Ag(1)-O(1)C	2.503(2)
Ag(2)-N(1)	2.175(2)	Ag(2)-O(3)D	2.2425(19)
Ag(2)-O(1)C	2.4863(19)	N(3)A-Ag(1)-O(2)	111.52(8)
N(3)A-Ag(1)-O(3)B	125.13(8)	O(2)-Ag(1)-O(3)B	111.88(7)
N(3)A-Ag(1)-O(1)C	122.51(8)	O(2)-Ag(1)-O(1)C	92.78(7)
O(3)B-Ag(1)-O(1)C	86.86(7)	N(1)-Ag(2)-O(3)D	141.75(8)
N(1)-Ag(2)-O(1)C	107.48(8)		
Symmetry code: A -*x*+1/2,*y*+1/2,-*z*+3/2; B *x*-1/2,-*y*+5/2,*z*-1/2; C -*x*,-*y*+2,-*z*+2; D -*x*+1/2,*y*-1/2,-*z*+5/2			
Compound **2**			
Zn(1)-N(1)	1.993(3)	Zn(1)-O(2)	1.978(3)
O(2)A-Zn(1)-O(2)	93.74(16)	O(2)-Zn(1)-N(1)	114.16(12)
O(2)A-Zn(1)-N(1)	100.40(12)	N(1)A-Zn(1)-N(1)	128.89(18)
Compound **3**			
Cd(1)-N(3)A	2.182(7)	Cd(1)-N(1)	2.185(7)
Cd(1)-O(3)	2.201(6)	Cd(1)-O(1)	2.213(6)
N(3)A-Cd(1)-N(1)	132.9(3)	N(3)A-Cd(1)-O(3)	100.2(2)
N(1)-Cd(1)-O(3)	111.9(3)	N(1)-Cd(1)-O(1)	99.1(3)
N(3)A-Cd(1)-O(1)	117.2(3)	O(3)-Cd(1)-O(1)	85.8(3)
Symmetry code: A *x*,*y*-1,*z*			
Compound **4**			
Zn(1)-O(8)A	1.9283(16)	Zn(1)-O(1W)	1.9599(18)
Zn(1)-N(3)B	1.979(2)	Zn(2)-N(1)	1.9666(19)
Zn(1)-O(6)	1.9808(16)	Zn(2)-O(4)C	1.9710(16)
Zn(2)-O(2)B	1.9500(17)	Zn(2)-O(5)	2.0365(16)
O(8)A-Zn(1)-O(1W)	107.71(8)	O(8)A-Zn(1)-N(3)B	118.32(7)
O(1W)-Zn(1)-N(3)B	113.10(8)	N(1)-Zn(2)-O(4)C	113.49(8)
O(8)A-Zn(1)-O(6)	96.87(7)	O(2)B-Zn(2)-O(5)	93.80(7)
O(1W)-Zn(1)-O(6)	101.97(8)	N(1)-Zn(2)-O(5)	109.98(7)
N(3)B-Zn(1)-O(6)	116.62(7)	O(4)C-Zn(2)-O(5)	90.72(7)
O(2)B-Zn(2)-N(1)	133.07(8)	O(2)B-Zn(2)-O(4)C	105.73(7)
Symmetry code: A -*x*+2,-*y*+2,-*z*-1; B -*x*+2,-*y*+2,-*z*; C *x*+1,*y*,*z*			
Compound **5**			
Zn(1)-O(4)	1.9204(19)	Zn(1)-O(7)	1.9307(17)
Zn(1)-O(1)	1.9594(17)	Zn(1)-N(3)	1.988(2)
Zn(2)-O(7)	1.9177(17)	Zn(2)-O(5)A	1.9681(16)
Zn(2)-N(1)B	2.013(2)	Zn(2)-O(2)	2.0187(17)
O(4)-Zn(1)-O(7)	104.69(8)	O(4)-Zn(1)-O(1)	111.58(9)
O(7)-Zn(1)-O(1)	101.30(7)	O(4)-Zn(1)-N(3)	107.15(9)
O(7)-Zn(1)-N(3)	119.67(8)	O(1)-Zn(1)-N(3)	112.20(8)

O(7)-Zn(2)-O(5)A	124.88(7)	O(7)-Zn(2)-O(2)	98.59(7)
O(7)-Zn(2)-N(1)B	119.13(9)	O(5)A-Zn(2)-O(2)	98.69(7)
O(5)A-Zn(2)-N(1)B	109.16(9)	N(1)B-Zn(2)-O(2)	98.86(8)

Symmetry code: A -*x*+1,-*y*+1,-*z*+2; B *x*+1,*y*,*z*

Compound 6

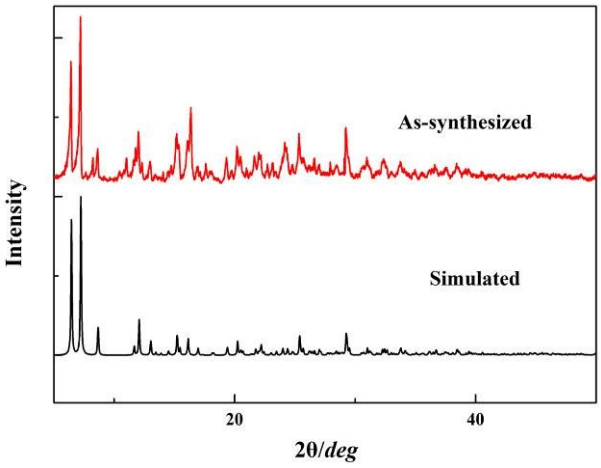
Cd(1)-O(6)A	2.271(5)	Cd(1)-N(2)	2.282(5)
Cd(1)-N(4)B	2.333(5)	Cd(1)-O(1W)	2.384(5)
Cd(1)-O(2)	2.366(5)	Cd(1)-O(1)	2.516(5)
O(6)A-Cd(1)-N(2)	99.23(19)	O(6)A-Cd(1)-N(4)B	101.29(19)
N(2)-Cd(1)-N(4)B	105.79(19)	N(4)B-Cd(1)-O(1W)	168.53(19)
O(6)A-Cd(1)-O(2)	111.79(18)	O(2)-Cd(1)-O(1W)	80.58(17)
N(2)-Cd(1)-O(2)	142.12(18)	O(6)A-Cd(1)-O(1)	155.42(17)
N(4)B-Cd(1)-O(2)	89.37(17)	N(2)-Cd(1)-O(1)	88.47(18)
O(6)A-Cd(1)-O(1W)	77.62(18)	N(4)b-Cd(1)-O(1)	98.94(18)
N(2)-Cd(1)-O(1W)	85.61(19)	O(1W)-Cd(1)-O(1)	79.77(18)
O(2)-Cd(1)-O(1)	54.50(16)		

Symmetry code: A -*x*,-*y*+1,-*z*+2; B -*x*,-*y*,-*z*+1

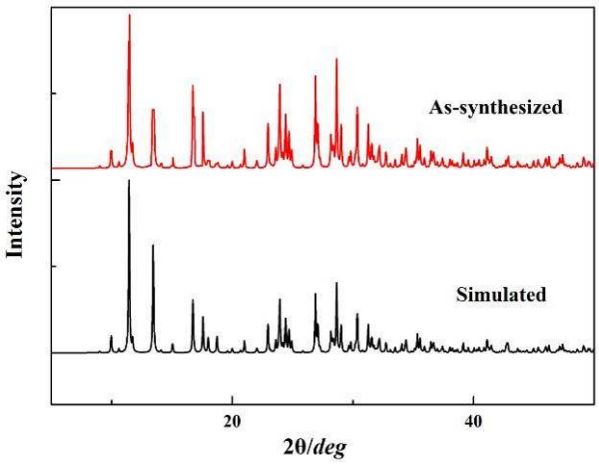
Table S3. the mineralization degrees and degradation efficiency reached after 120 min for the methyl orange solution without catalyst at each pH and with persulfate.

pH	1.0	3.0	5.0	7.0	9.0
Mineralization degrees	13.0%	15.2%	13.6%	11.2%	10.6%

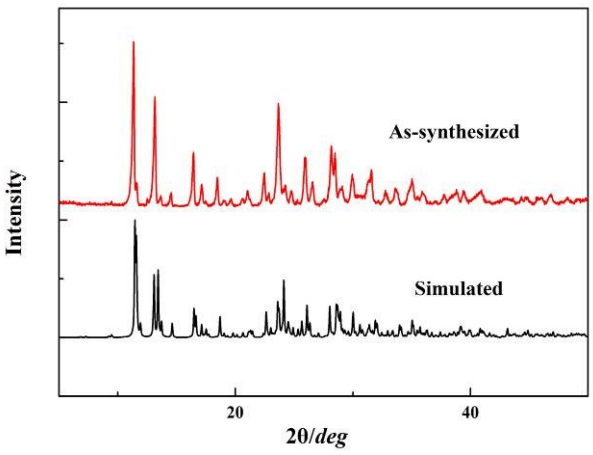
(a)


As-synthesized
Simulated
Intensity
20
40
2θ/deg

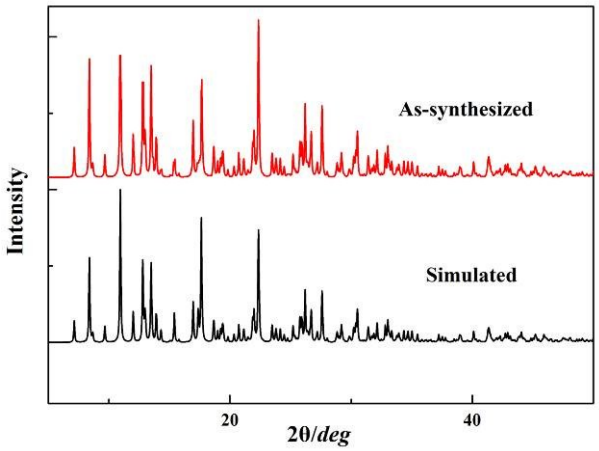
(b)


As-synthesized
Simulated
Intensity
20
40
2θ/deg

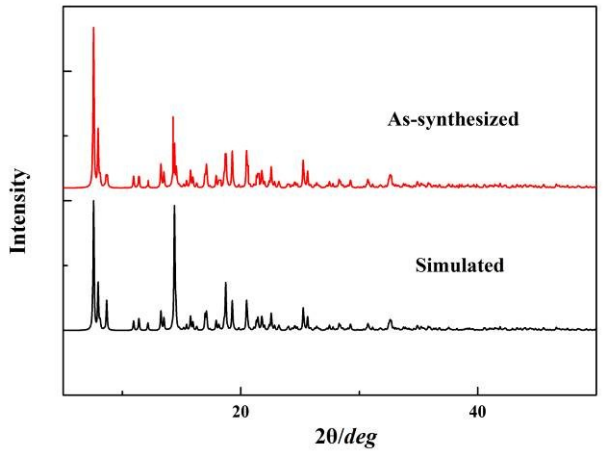
(c)


As-synthesized
Simulated
Intensity
20
40
2θ/deg

(d)



(e)



(f)

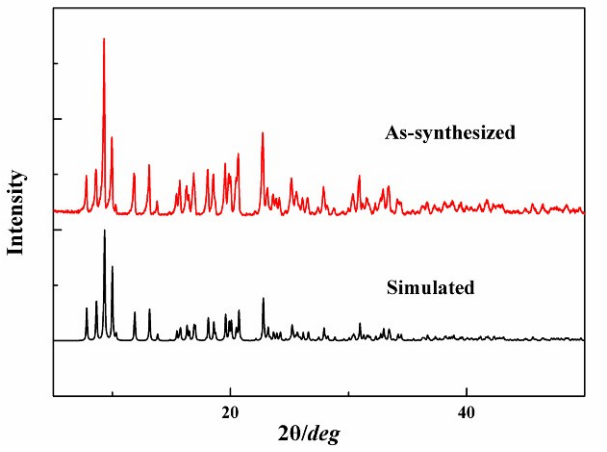


Fig. S1. The simulated (black) and experimental (red) PXRD patterns for compounds 1-6.

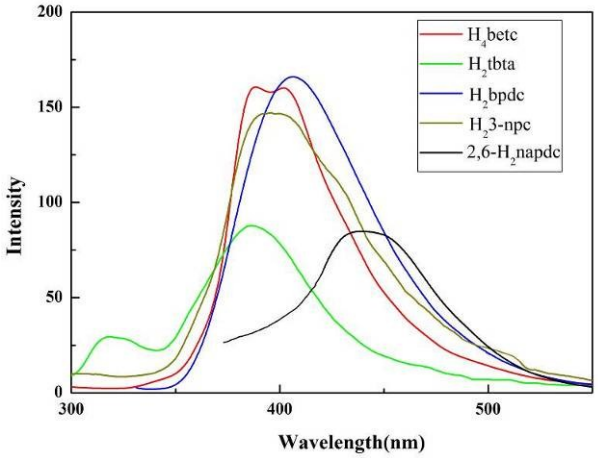


Fig. S2. Solid-state photoluminescent spectra of free carboxylic acids.

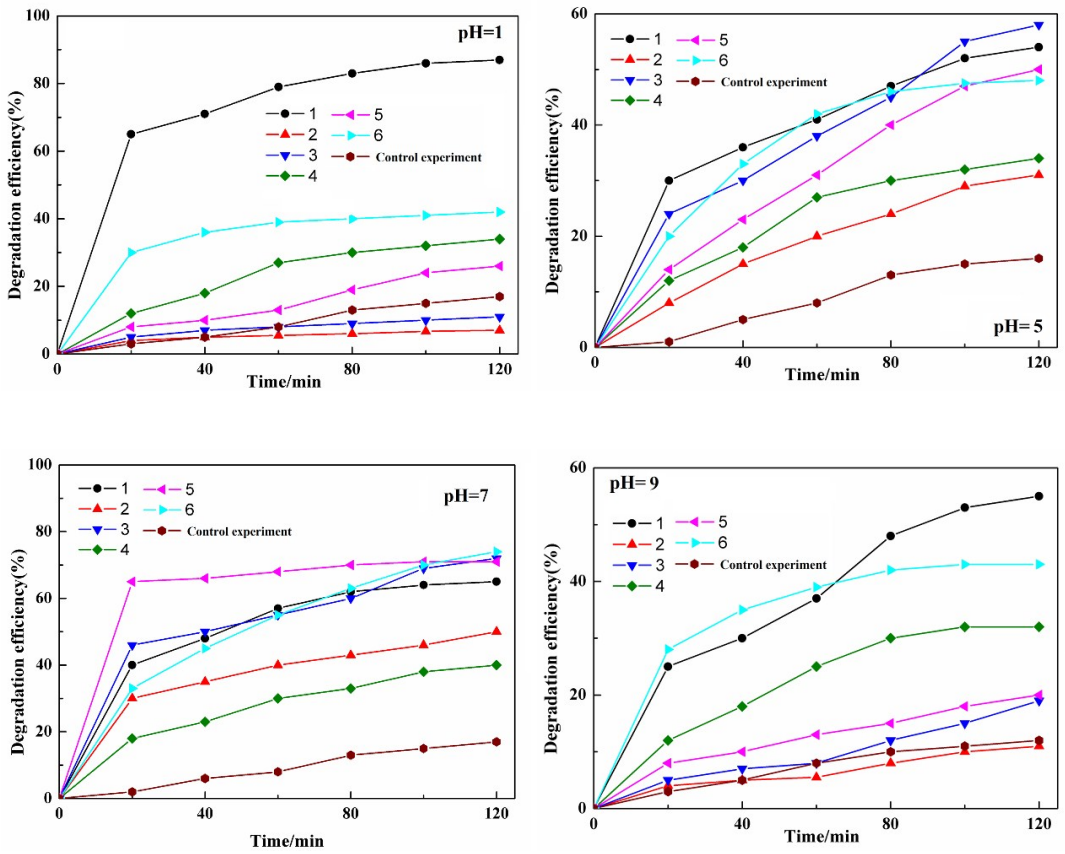
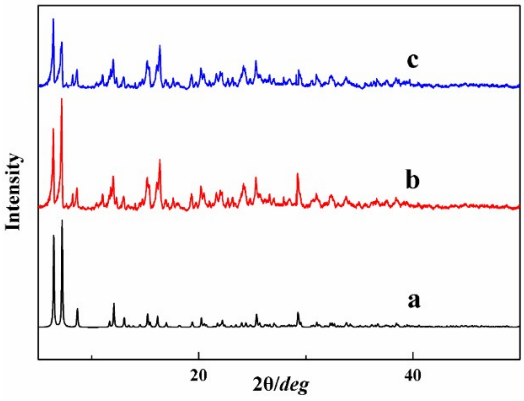
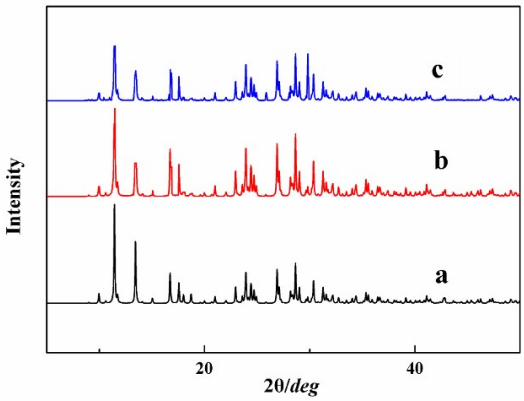


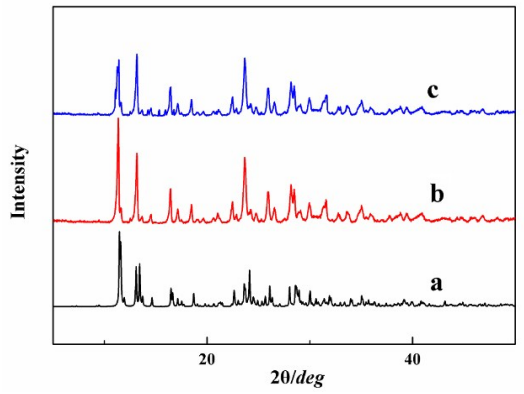
Fig. S3. The experiment results of the photocatalytic degradation of methyl orange in different pH values.


c
b
a
Intensity
20
40
2θ/deg

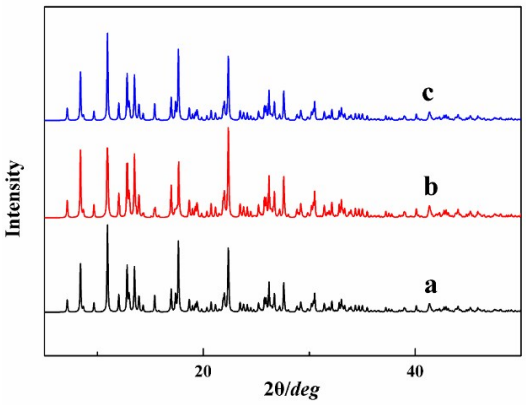
(a)


c
b
a
Intensity
20
40
2θ/deg

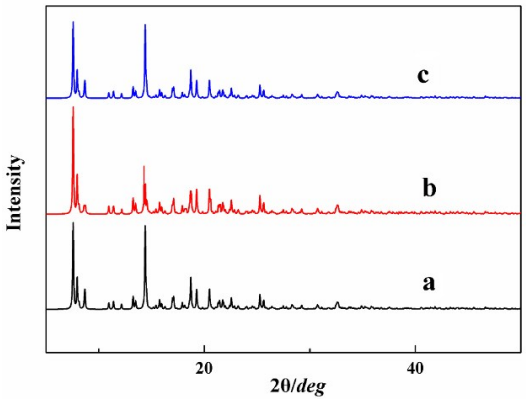
(b)


c
b
a
Intensity
20
40
2θ/deg

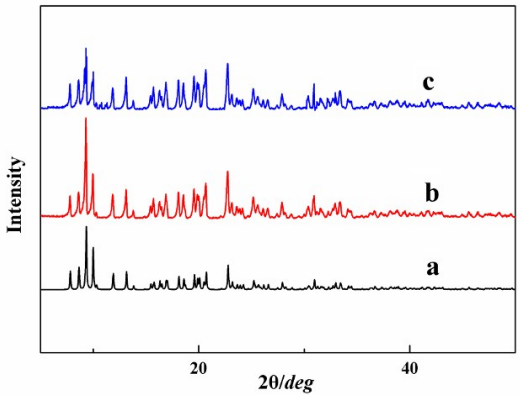
(c)



(d)



(e)



(f)

Fig. S4. The XRPD patterns for compounds **1-6**, **a**: simulated, **b**: experimental, and **c**: samples after catalytic experiments.