Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

A Series of Interdigitated Cd(II) Coordination Polymers based on 4,6-dibenzoylisophthalic acid and Flexible triazole ligands

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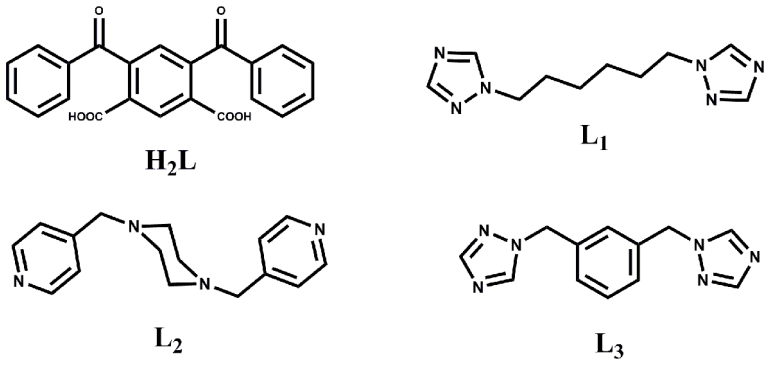
Materials and general methods

All reagents and solvents were purchased from commercial sources and used without further purification. Powder X-ray diffraction (PXRD) patterns were collected on a Rigaku D_{max} 2000 X-ray diffractometer with graphite monochromatized Cu $K\alpha$ radiation (λ = 0.154 nm). The FI-IR spectra were measured in KBr pellets in the range 4000–400 cm^{-1} on a Mattson Alpha-Centauri spectrometer. Elemental analysis (EA) for C, H and N was performed on a Perkin-Elmer 2400 Elemental Analyzer. Thermogravimetric analysis (TGA) was performed on a Perkin-Elmer Thermal Analyzer under nitrogen atmosphere at a heating rate of 10 °C min^{-1}. The fluorescent property was measured on a FLS920 Edinburgh Luminescence Spectrometer at room temperature with a light source of Xe lamp.

Single-crystal X-ray crystallography

Colorless block shape single crystal was mounted on a glass fiber for X-ray diffraction analysis. Data was performed at 293(2) K on an Oxford Diffraction Gemini R CCD for **1** and on a Rigaku AFC7R diffractometer for **2** and **3** with graphite-monochromated Mo-$K\alpha$ radiation (λ = 0.71073 Å). The structure was solved by Direct Method of SHELXS-97 and refined by full-matrix least-squares techniques using the SHELXL-97 program. [1] All non-hydrogen atoms were refined with anisotropic temperature parameters. All Hydrogen atoms were placed in geometrically idealized position as a riding mode. CCDC 975867 (1), 890982 (2) and 975868 (3) contain the supplementary X-ray crystallographic files in CIF format can be obtained free of charge from The Cambridge Crystallographic Data Centre via http://www.ccdc.cam.ac.uk/conts/retrieving.html. The crystallographic data for **1-3** is shown in Table S2.



Scheme S1 Schematic representation of ligands used in this work.

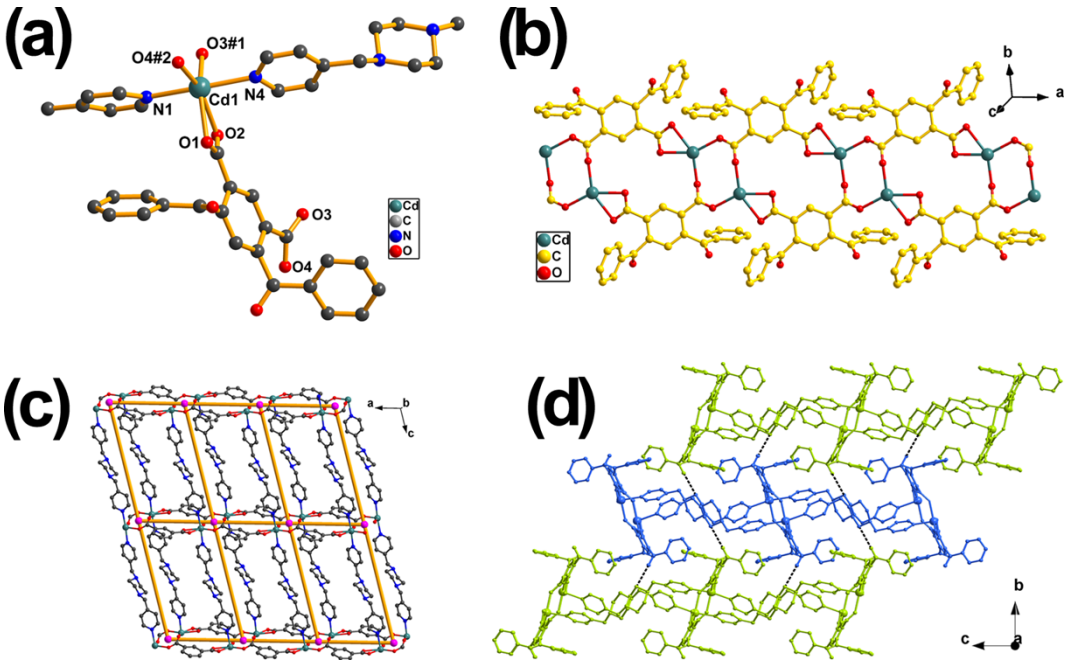


Figure S1 (a) Coordination environment of Cd ion of **2**. Symmetry codes: #1, $x + 1$, y, z; #2, $-x + 1$, $-y + 1$, $-z + 1$. (b) View of 1D $\{Cd(L)\}_n$ chain of **2**. (c) Schematic description of 4^4-**sql** layer of **2**. (d) The 3D supramolecular structure of **2** contains a feature of 2D→3D interdigitation. The C31–H31a···O6 hydrogen-bonding interactions are showing in dashed black lines.

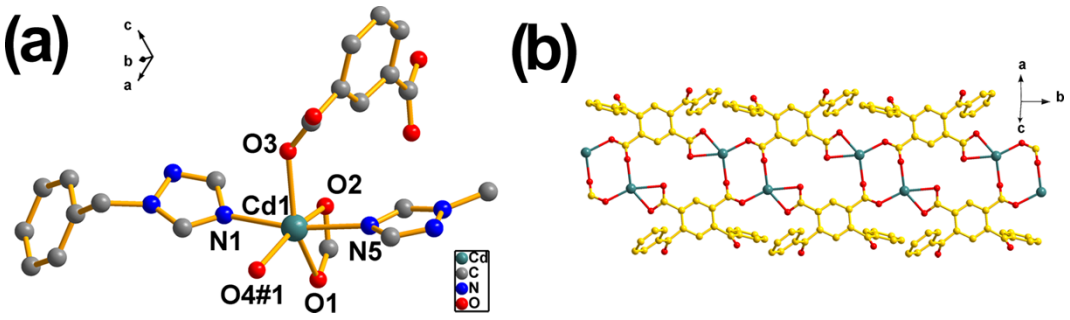


Figure S2 (a) Coordination environment of Cd ion of **3**. Symmetry codes: #1, 1−*x*, 2−*y*, 1−*z*. (b) View of 1D $\{Cd(L)\}_n$ chain of **3**.

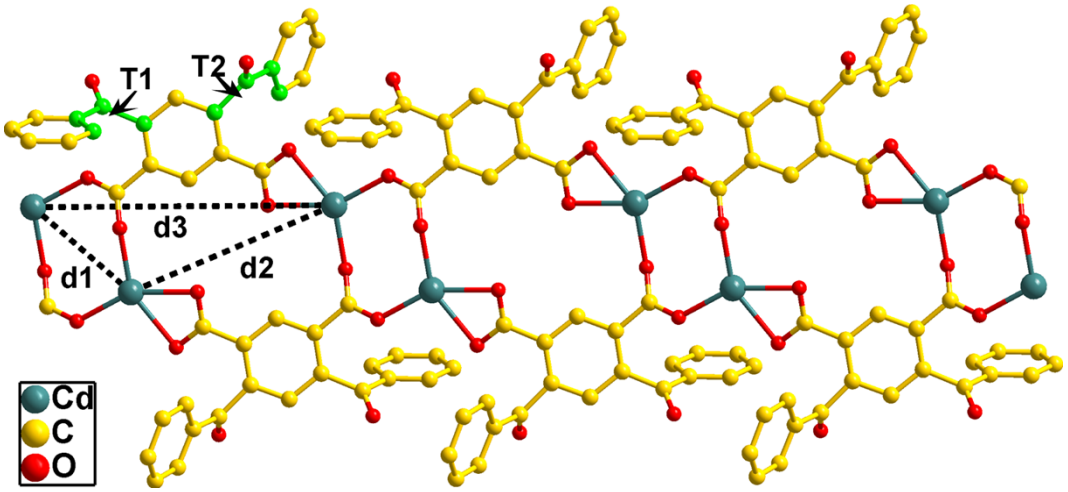


Figure S3 View of the distance and the torsion angels between the selected atoms. As shown in table S1, only slight difference of the 1D $\{Cd(L)\}_n$ chains can be found in the three title compounds. That is, the distances of d_3 gradually increase while the torsion angels of T_1 and T_2 gradually decreases (except for T_2 of compound **2**) as the flexibility of the N-donor ligands reduced from L_1 to L_3.

Table S1 Distances of Cd···Cd and torsion angels of the selected atoms.[a]

	d_1 (Å)	d_2 (Å)	d_3 (Å)	T_1 (°)[b]	T_2 (°)[c]
Compound **1**	4.439	7.329	10.385	26.396(5)	10.654(5)
Compound **2**	4.497	7.563	10.430	25.517(6)	-24.300(7)
Compound **3**	4.454	7.613	10.522	21.013(9)	5.091(9)

[a] d = distance of the selected atoms; T = Torsion angels of the selected atoms.

[b] C3-C8-C9-C14 for **1**, C6-C9-C10-C11 for **2** and C6-C9-C10-C11 for **3**, respectively.

[c] C5-C16-C17-C22 for **1**, C8-C16-C17-C22 for **2** and C8-C16-C17-C18 for **3**, respectively.

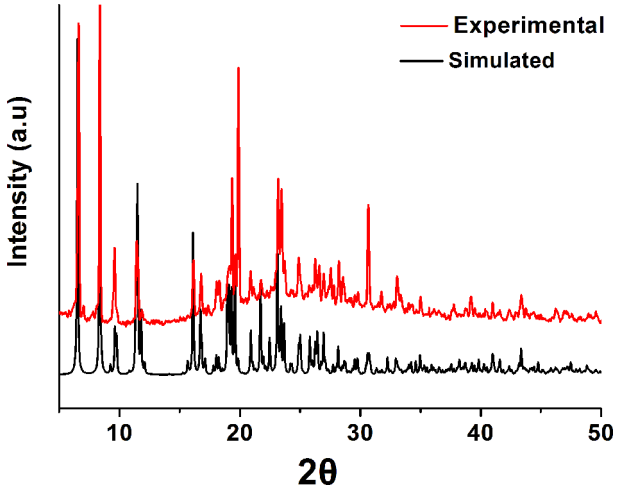


Figure S4 The PXRD patterns of **1**.

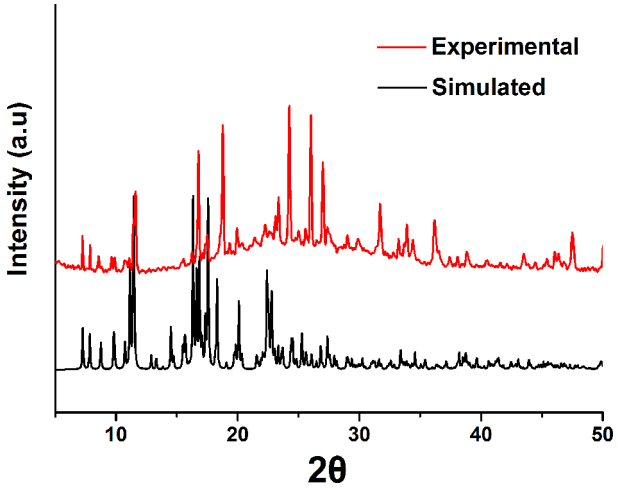


Figure S5 The PXRD patterns of **2**.

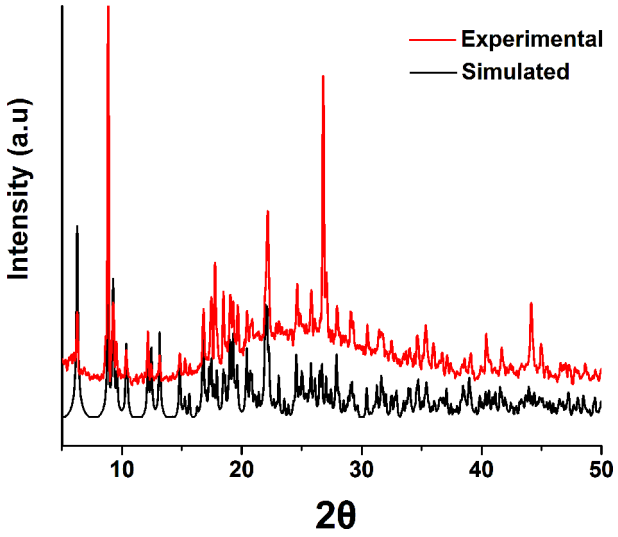


Figure S6 The PXRD patterns of **3**.

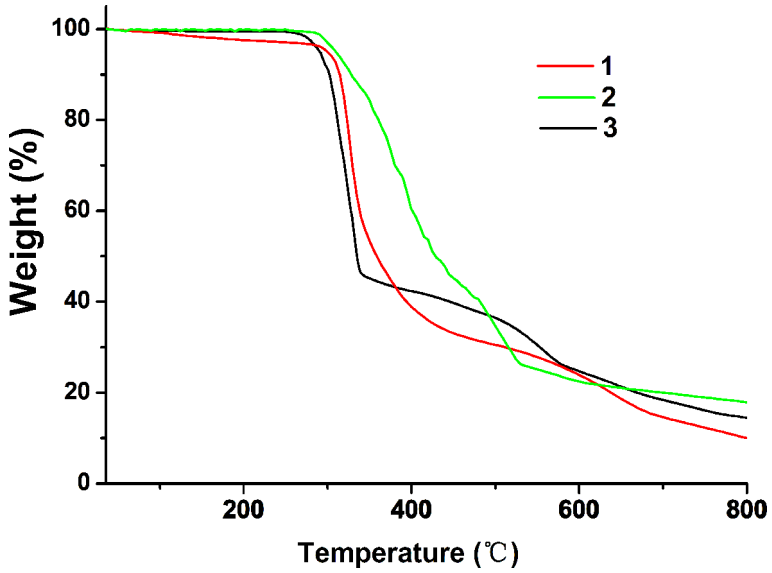


Figure S7 Thermogravimetric analysis curves of **1**-**3**.

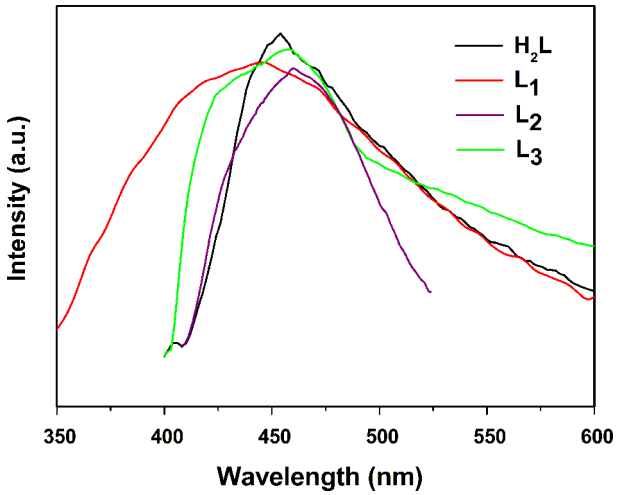


Figure S8 Emission spectra of free ligands.

Table S2 Crystal data and structure refinement parameters for compounds **1**–**3**.

Complex	**1**	**2**	**3**
Formula	$C_{32}H_{28}CdN_6O_6$	$C_{38}H_{32}CdN_4O_6$	$C_{34}H_{24}CdN_6O_6$
Formula weight	705.00	753.08	725.00
Crystal system	Triclinic	Monoclinic	Monoclinic
Space group	*P*-1	$P2_1/c$	$P2_1/c$
a/Å	10.3849(5)	10.430(5)	15.402(5)
b/Å	11.6302(3)	20.209(8)	10.522(3)
c/Å	13.8223(6)	16.880(7)	20.877(5)
α/°	99.133(3)	90	90.00
β/°	91.357(4)	104.816(7)	114.070(17)
γ/°	112.426(4)	90	90.00

V/Å^3	1517.11(11)	3440(3)	3089.1(15)
Z	2	4	4
D_c /g cm^{-3}	1.543	1.454	1.559
μ/mm^{-1}	0.775	0.687	0.764
F(000)	716	1536	1464
R_{int}	0.0272	0.0591	0.0678
GOF	1.029	1.183	1.068
R_1, wR_2[a] [$I>2\sigma(I)$]	0.0375, 0.0911	0.0583, 0.1382	0.0596, 0.1498
R_1, wR_2[a] (all data)	0.0439, 0.0954	0.0753, 0.1562	0.0949, 0.1902

[a] $R_1 = \sum||F_0| - |Fc||/\sum|F_0|$. w$R_2 = \sum[w(F_0^2 - Fc^2)^2]/\sum[w(F_0^2)^2]^{1/2}$

Table S3 Selected bond lengths (Å) and Angles (°) of **1-3**. [a]

1			
Cd(1)-O(1)	2.220(2)	Cd(1)-O2#1	2.339(2)
Cd(1)-N(1)	2.285(3)	Cd(1)-O(3)	2.493(2)
Cd(1)-N(4)	2.295(3)	Cd(1)-C(15)	2.727(3)
Cd(1)-O(4)	2.317(2)		
O(1)-Cd(1)-N(1)	109.40(10)	N(4)-Cd(1)-O(2)#1	79.87(10)
O(1)-Cd(1)-N(4)	89.76(10)	O(4)-Cd(1)-O(2)#1	153.07(8)
N(1)-Cd(1)-N(4)	158.79(12)	O(1)-Cd(1)-O(3)	149.57(8)
O(1)-Cd(1)-O(4)	97.72(8)	N(1)-Cd(1)-O(3)	86.03(10)
N(1)-Cd(1)-O(4)	92.18(10)	N(4)-Cd(1)-O(3)	81.32(10)
N(4)-Cd(1)-O(4)	94.20(10)	O(4)-Cd(1)-O(3)	54.46(8)
O(1)-Cd(1)-O(2)#1	108.43(8)	O(2)-Cd(1)-O(3)#1	98.61(8)
N(1)-Cd(1)-O(2)#1	85.31(10)		
2			
Cd(1)-O(4)#1	2.227(3)	Cd(1)-N(1)	2.330(4)
Cd(1)-O(3)#2	2.291(3)	Cd(1)-O(2)	2.400(3)
Cd(1)-N(4)	2.311(4)	Cd(1)-O(1)	2.408(3)
O(3)#2-Cd(1)-O(2)	92.66(11)	N(4)-Cd(1)-O(2)	86.32(13)
O(4)#1-Cd(1)-O(3)#2	112.76(12)	N(1)-Cd(1)-O(2)	87.93(13)
O(4)#1-Cd(1)-N(4)	100.73(13)	O(4)#1-Cd(1)-O(1)	99.38(11)
O(3)#2-Cd(1)-N(4)	87.65(13)	O(3)#2-Cd(1)-O(1)	147.62(12)
O(4)#1-Cd(1)-N(1)	89.10(13)	N(4)-Cd(1)-O(1)	90.21(14)
O(3)#2-Cd(1)-N(1)	81.95(14)	N(1)-Cd(1)-O(1)	95.22(14)
N(4)-Cd(1)-N(1)	167.86(14)	O(2)-Cd(1)-O(1)	54.96(11)
O(4)#1-Cd(1)-O(2)	153.71(11)		
3			
Cd1-O4#1	2.213(4)	Cd1-O3	2.314(4)

Cd1-N1	2.298(5)	Cd1-O1	2.321(4)
Cd1-N5	2.302(5)	Cd1-O2	2.509(4)
O4-Cd1-N1#1	86.47(17)	O3-Cd1-O1	145.91(14)
O4-Cd1-N5#1	105.47(17)	O4-Cd1-O2#1	156.70(13)
N1-Cd1-N5	166.97(19)	N1-Cd1-O2	83.56(16)
O4-Cd1-O3#1	108.26(15)	N5-Cd1-O2	87.08(17)
N1-Cd1-O3	83.19(18)	O3-Cd1-O2	91.42(13)
N5-Cd1-O3	88.02(17)	O1-Cd1-O2	54.55(13)
O4-Cd1-O1#1	105.39(14)	N5-Cd1-O1	88.26(17)
N1-Cd1-O1	93.64(17)		

[a] Symmetry transformations used to generate equivalent atoms: For **1**: #1, 1−*x*, 1−*y*, 1−*z*. For **2**: #1, *x* + 1, *y*, *z*; #2, −*x* + 1, −*y* + 1, −*z* + 1. For **3**: #1, 1−*x*, 2−*y*, 1−*z*.

Table S4 Hydrogen-bonding geometry parameters for **1**.

D−H···A	d(D−H) (Å)	d(H···A) (Å)	d(D···A) (Å)	<(DHA) (°)
C20–H20···O6	0.93	2.56	3.487(6)	176

Table S5 Hydrogen-bonding geometry parameters for **2**.

D−H···A	d(D−H) (Å)	d(H···A) (Å)	d(D···A) (Å)	<(DHA) (°)
C31–H31a···O6	0.97	2.38	3.333(8)	166

Table S6 Hydrogen-bonding geometry parameters for **3**.

D−H···A	d(D−H) (Å)	d(H···A) (Å)	d(D···A) (Å)	<(DHA) (°)
C25–H25a···O6	0.97	2.647	3.487(6)	145

References:

[1] (a) G. M. Sheldrick, *SHELXS-97: Programs for X-ray Crystal Structure Solution*; University of Göttingen: Göttingen, Germany, 1997;
(b) G. M. Sheldrick, *SHELXL-97: Programs for X-ray Crystal Structure Refinement*; University of Göttingen: Göttingen, Germany, 1997.