Supporting Information

Fluorescent Coordination-Polymer Single Crystals with Tunable Elastic-Plastic Transformations

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Experimental section

Crystal Synthesis:

$[Cd_2Cl_4(Im)_2]_n$ (**1**): $CdCl_2$ (1.5 mmol), Imidazole (3mmol) and 10 mL Distilled water were added in a 20 mL Teflon-sealed autoclave. The mixture was stirred for approximately 24 hours and then filtered to obtain a clear solution. Needle-like crystals of compound **1** after the system was gradually cooled to room temperature, formed the high-quality needle-shaped single crystals. The yield was ca.61.26%. Anal. $C_3H_4CdCl_2N_2$ (251.37); calcd C 14.33%, H 1.60%, N 11.41%; found C 14.47%, H1.76%, N 11.00%.

$[Cd_2Cl_4(MeIm)_2]_n$ (**2**): $CdCl_2$ (1.5 mmol), 1-methylimidazole (3mmol) and 10 mL Distilled water were added in a 20 mL Teflon-sealed autoclave. The mixture was stirred for approximately 24 hours and then filtered to obtain a clear solution. Needle-like crystals of compound **2** after the system was gradually cooled to room temperature, formed the high-quality needle-shaped single crystals. The yield was ca.56.46%. Anal. $C_4H_6CdCl_2N_2$ (265.40); calcd C 18.10%, H 2.28%, N 10.55%; found C 18.09%, H 2.03%, N 10.50%.

$[Cd_2Cl_4(EtIm)_2]_n$ (**3**): $CdCl_2$ (1.5 mmol), 1-ethylimidazole (3mmol) and 10 mL Distilled water were added in a 20 mL Teflon-sealed autoclave. The mixture was stirred for approximately 24 hours and then filtered to obtain a clear solution. Needle-like crystals of compound **3** after the system was gradually cooled to room temperature, formed the high-quality needle-shaped single crystals. The yield was ca.47.73%. Anal.

$C_5H_8CdCl_2N_2$ (279.43); calcd C 21.49%, H 2.88%, N 10.02%; found C 21.21%, H 2.68%, N 9.88%.

Single-crystal X-ray diffraction (SC-XRD): The single-crystal X-ray diffraction data were collected using a Rigaku Oxford XtaLAB PRO diffractometer equipped with a Mo-Kα radiation source. The diffraction data were collected at 298 K. The structures at different phases were solved using direct methods and refined by full matrix least-squares techniques on F2 with the SHELX program implemented in the Olex2 program.

Photoluminescence (PL) spectra: The data were obtained with an FLS1000 fluorescence spectrophotometer (Edinburgh Instruments) featuring a continuous xenon lamp and visible/NIR photomultiplier tube (PMT) detectors (Hamamatsu P9289P and R5509).

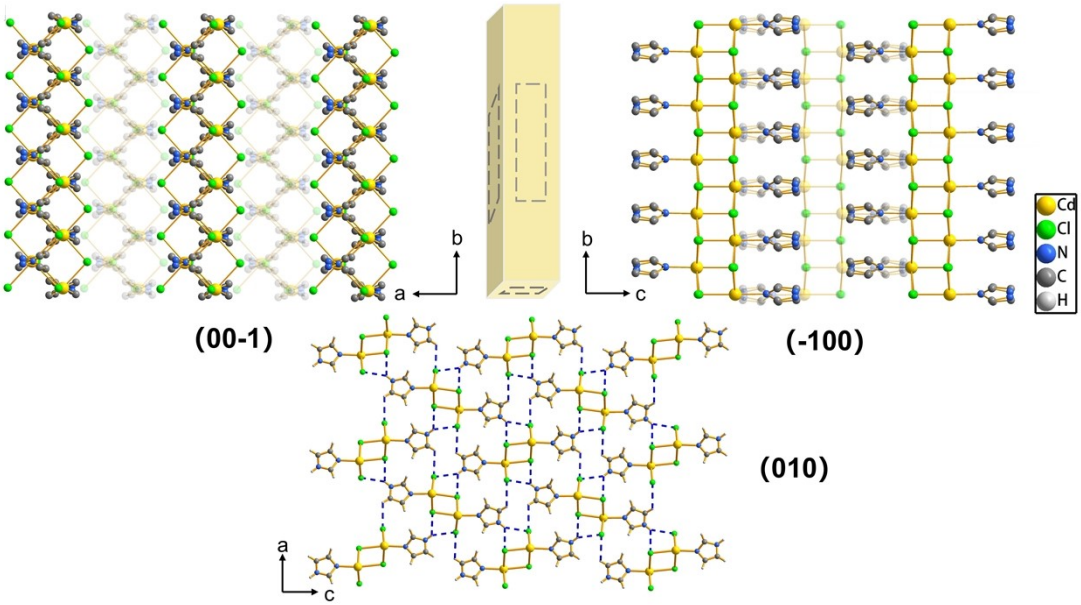

Figure S1. Stacking structure of compound **1**.

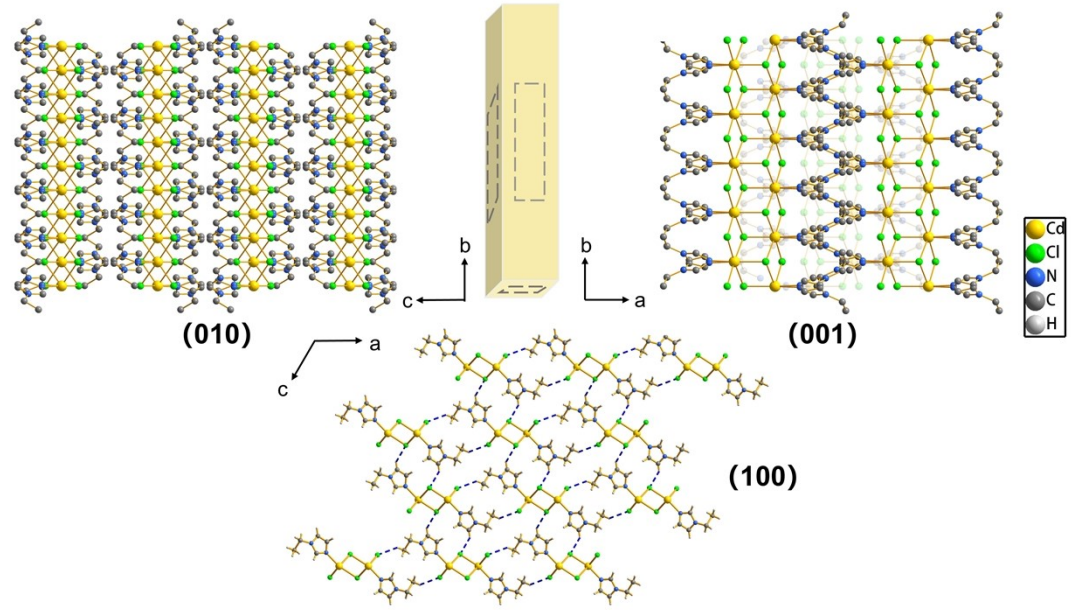

Figure S2. Stacking structure of compound **3**.

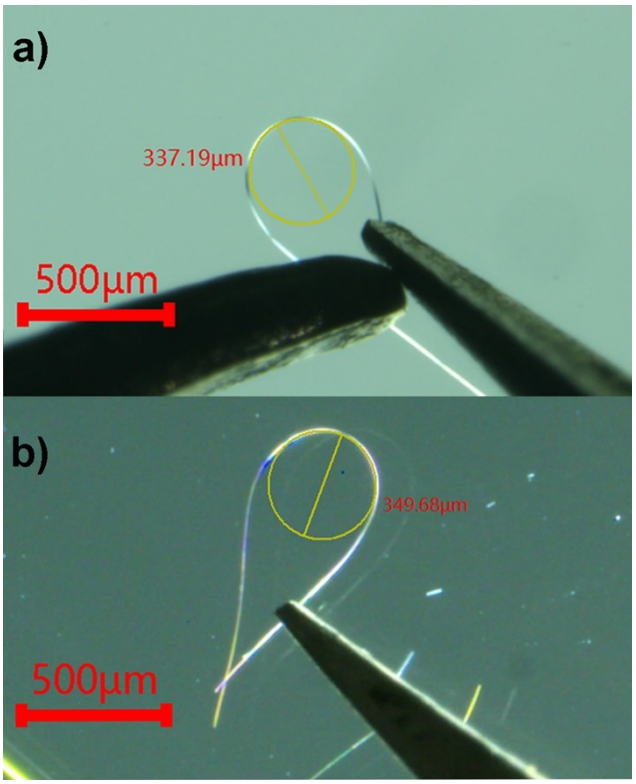

Figure S3. Measurement of the maximum bending strain. a) crystal **1**. b) crystal **2**.

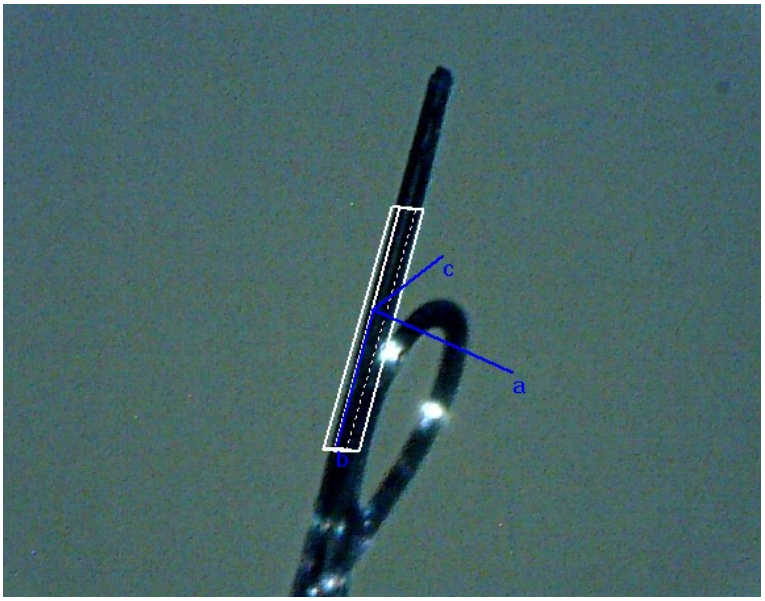

Figure S4. Crystal morphology with the face indices of compound **1**.

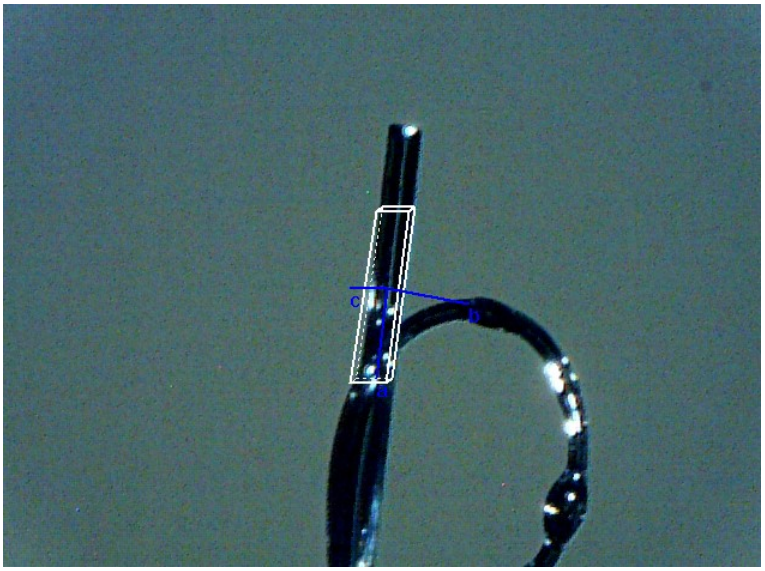

Figure S5. Crystal morphology with the face indices of compound **2**.

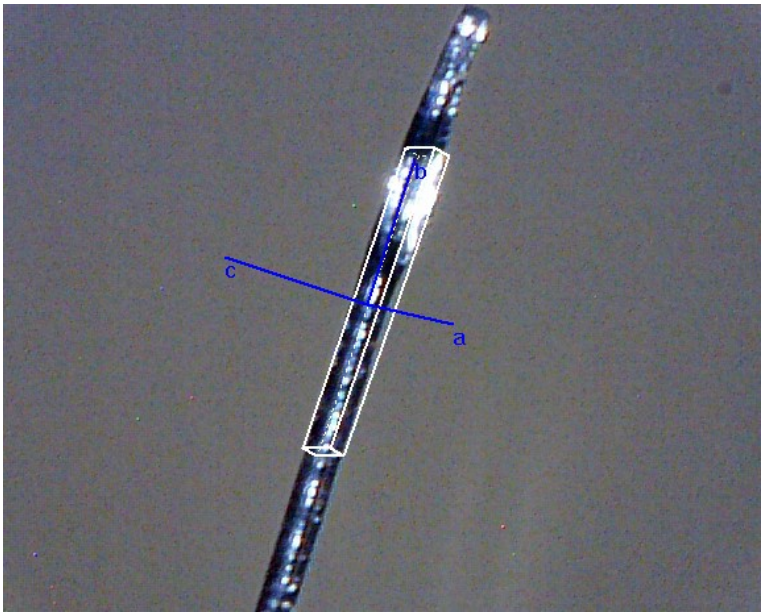

Figure S6. Crystal morphology with the face indices of compound **3**.

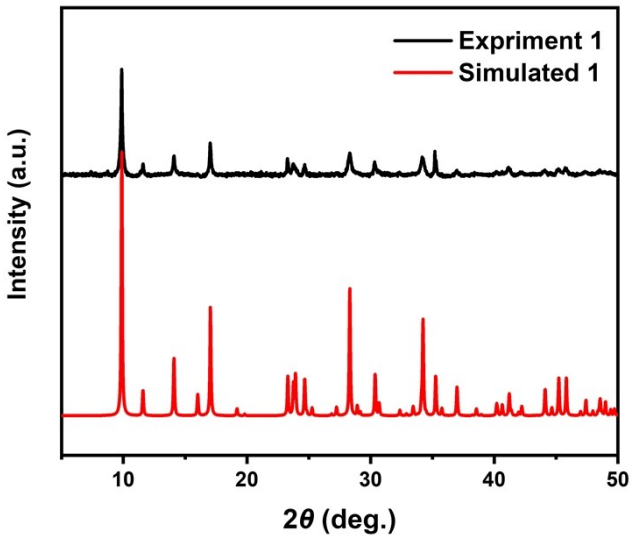

Figure S7. Experimental and simulated PXRD patterns of compound **1** at room temperature.

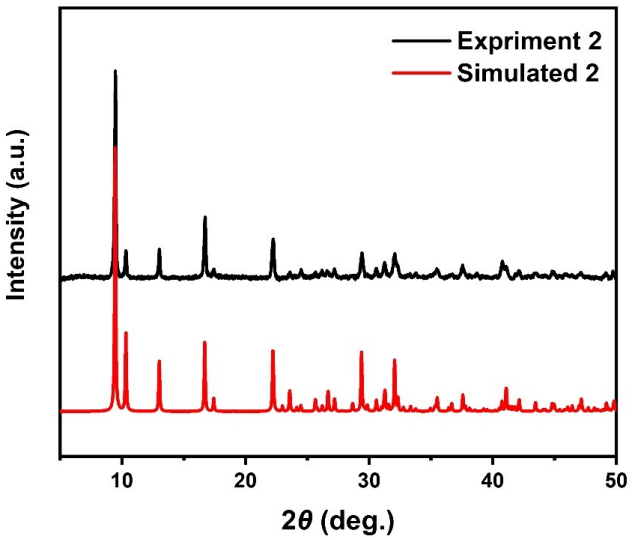

Figure S8. Experimental and simulated PXRD patterns of compound **2** at room temperature.

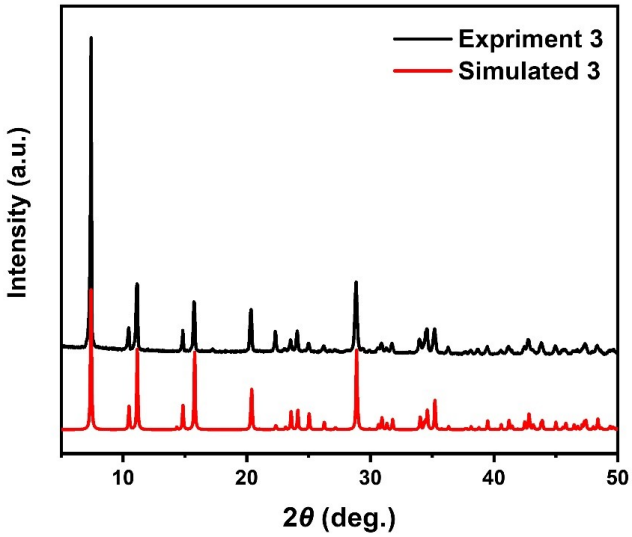

Figure S9. Experimental and simulated PXRD patterns of compound **3** at room temperature.

Table S1. Types and distances of weak intermolecular interactions between 1D chains.

Style	1	2	3
$d_{C-H\cdots Cl}$(Å)	2.887 2.994 3.044	2.897 3.047 3.082 3.163	2.919 2.989 3.111
$d_{N-H\cdots Cl}$(Å)	2.5502 2.8867		

Table S2. Cd···Cd distance along the direction of the one-dimensional chain.

Samples	Distance (Cd···Cd)/ Å
1	3.8319
2	3.8859
3	3.9649

Table S3. Changes in the framework angle.

Samples	$\angle Cl_1CdCl_1$/°	$\angle Cl_2CdCl_2$/°	$\angle CdCl_1Cd$/°	$\angle CdCl_2Cd$/°
1	87.36		95.08	89.68
2	86.17	86.73	96.60	90.30
3	85.47		97.72	91.16

Table S4. Crystal data and structure refinement for compound **1-3**.

Identification code	**1**	**2**	**3**
Empirical formula	$C_3H_4CdCl_2N_2$	$C_4H_6CdCl_2N_2$	$C_5H_8CdCl_2N_2$
Formula weight	251.37	265.40	279.43
Temperature/K	293(2)	293(2)	293(2)
Crystal system	orthorhombic	monoclinic	monoclinic
Space group	*Pnma*	$P2_1/c$	$I2/m$
a/Å	11.0566(10)	3.8859(4)	13.164(3)
b/Å	3.8319(3)	17.1403(15)	3.9649(6)
c/Å	15.2570(10)	11.2169(9)	16.918(3)
α/°	90	90	90
β/°	90	95.796(8)	110.14(2)
γ/°	90	90	90
Volume/Å^3	646.41(9)	743.29(12)	829.0(3)
Z	1.333333	4	4
$\rho_{calc.}$g/cm^3	2.583	2.372	2.239
μ/mm^{-1}	4.092	3.565	3.203
F(000)	472.0	504.0	536.0
Radiation	Mo Kα (λ = 0.71073)	Mo Kα (λ = 0.71073)	Mo Kα (λ = 0.71073)
2Θ range /°	7.84 to 58.218	7.68 to 59.394	7.254 to 58.38
Index ranges	$-11 \le h \le 15$, $-4 \le k \le 4$, $-18 \le l \le 20$	$-5 \le h \le 5$, $-23 \le k \le 23$, $-15 \le l \le 15$	$-17 \le h \le 16$, $-4 \le k \le 5$, $-20 \le l \le 23$
Reflections collected	3651	7873	3382
Independent reflections	870 [R_{int} = 0.0335, R_{sigma} = 0.0291]	870 [R_{int} = 0.0335, R_{sigma} = 0.0291]	1090 [R_{int} = 0.1408, R_{sigma} = 0.1230]
Data/restraints/parameters	870/9/64	1860/0/83	1090/42/83
Goodness-of-fit on F^2	1.255	0.990	0.952
Final R indexes [I>=2σ (I)]	R_1 = 0.0285, wR_2 = 0.0704	R_1 = 0.0323, wR_2 = 0.0645	R_1 = 0.0532, wR_2 = 0.1064
Final R indexes [all data]	R_1 = 0.0340, wR_2 = 0.0720	R_1 = 0.0500, wR_2 = 0.0732	R_1 = 0.0671, wR_2 = 0.1122

Largest diff. peak/hole / e Å^{-3}	0.72/-0.61	1.13/-1.16	1.12/-1.31
CCDC	2486224	2486226	2486225

Table S5. Summary and comparison of reported work on 1D CPs.

Compounds	**Distance (Cd···Cd)/ Å**	**Ɛ (%)**
$[CdCl_2(3\text{-}Clpy)_2]_n$	3.812	0.71
$[CdCl_2(3\text{-}Brpy)_2]_n$	3.854	0.47
$[CdBr_2(3\text{-}Brpy)_2]_n$ [1]	No found	0.59
$[CdCl_2(I\text{-}pz)_2]_n$	3.9399	0.573
$[CdBr_2(I\text{-}pz)_2]_n$	4.0317	0.505
$[CdI_2(I\text{-}pz)_2]_n$	4.2080	0.473
$[CdCl_2(Br\text{-}pz)_2]_n$	3.846	0.757
$[CdBr_2(Br\text{-}pz)_2]_n$	3.9125	1.162
$[CdCl_2(Cl\text{-}pz)_2]_n$	3.7369	1.134
$[CdBr_2(Cl\text{-}pz)_2]_n$ [2]	3.8547	1.244
$[CdI_2(3\text{-}CNpy)_2]_n$	No found	1.09
$[CdCl_2(3\text{-}CNpy)_2]_n$	3.795	1.09
$[CdCl_2(4\text{-}CNpy)_2]_n$ [3]	3.781	1.07
$[Pb(SCN)_2(3F\text{-}spy)_2]_n$ [4]	4.175	1.3
$[Pb(SCN)_2(2F\text{-}spy)_2]_n$ [5]	No found	0.8
$[CdCl_2(3\text{-}Ipy)_2]_n$	3.95	0.28
$[CdI_2(3\text{-}Ipy)_2]_n$ [6]	No found	0.4
$[CdCl_2$(1-Methyl-2-pyridone)$]_n$ [7]	3.840	2.24
$[Pb_2Br_4(DMA)_2]_n$	4.379	1.36
$[Pb_2Br_4(DMF)_2]_n$ [8]	4.343	0.34
Crystal of this work **1**	3.8319	4.98
Crystal of this work **2**	3.8859	4.45

py = pyridine; pz = pyrazine; spy = 3-fluoro-4'-styrylpyridine; DMF = *N, N*-dimethylformamide; DMA = *N, N*-dimethylacetamide

Reference

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