Supporting Information

Photochromic Naphthalenediimide Cd-MOFs based on Different Second Dicarboxylic Acid Ligands

Ziyin Li,[a] Junzhi Guo,[a] Fahui Xiang,[a] Quanjie Lin,[a] Yingxiang Ye,[a] Jindan Zhang,[a] Shimin Chen,[a] Zhangjing Zhang,[*ab] and Shengchang Xiang[*ab]

[a]*Fujian Provincial Key Laboratory of Polymer Materials, College of Chemistry and Materials Science, Fujian Normal University, 32 Shangsan Road, Fuzhou 350007, PR China*

[b]*State Key Laboratory of Structural Chemistry, Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, Fuzhou, Fujian 350002, PR China*

E-mail: zzhang@fjnu.edu.cn; scxiang@fjnu.edu.cn

Contents

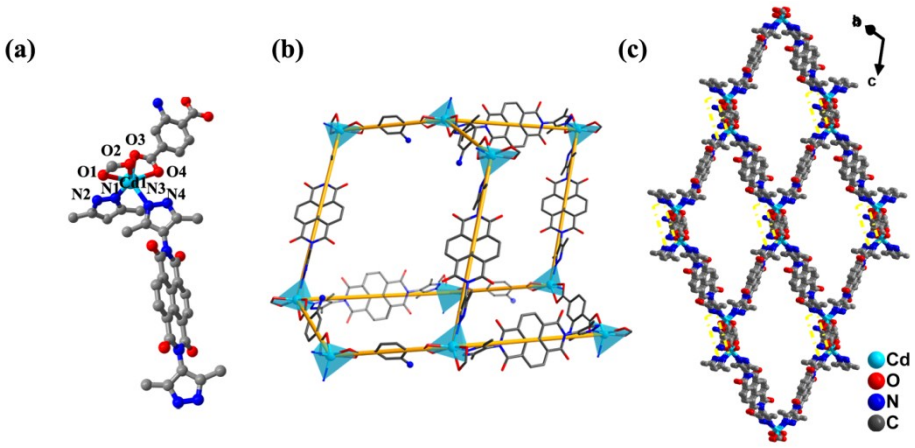

Figure S1. (a) Local coordination environment of Cd(II) atoms in **FJU-68**; (b) the perspective view of a single *dia* unit cage and (c) a 3D single *dia* framework in **FJU-68**.

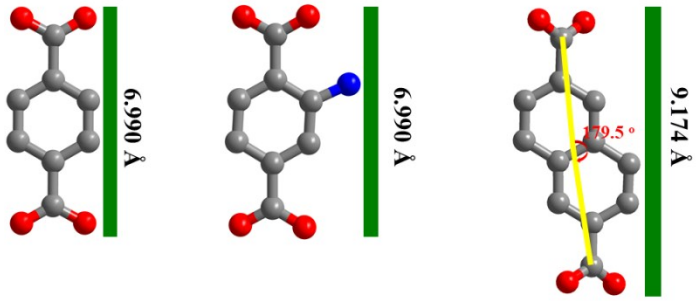

Figure S2. Three second dicarboxylic acid ligands (H_2BDC, NH_2-H_2BDC, and H_2NDC).

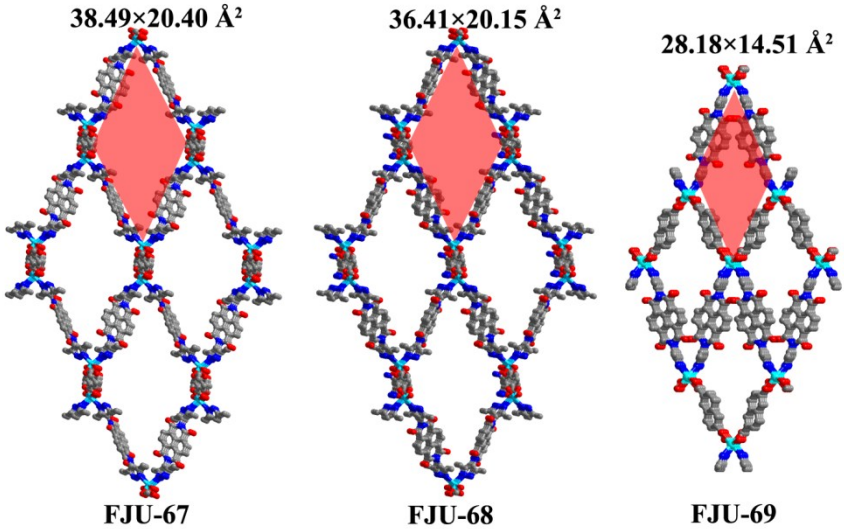

Figure S3. Schematic diagram for the evolution of the rhombic 1D channel in the single *dia* frameworks for three Cd-MOFs with the participation of the different second dicarboxylic acid ligands.

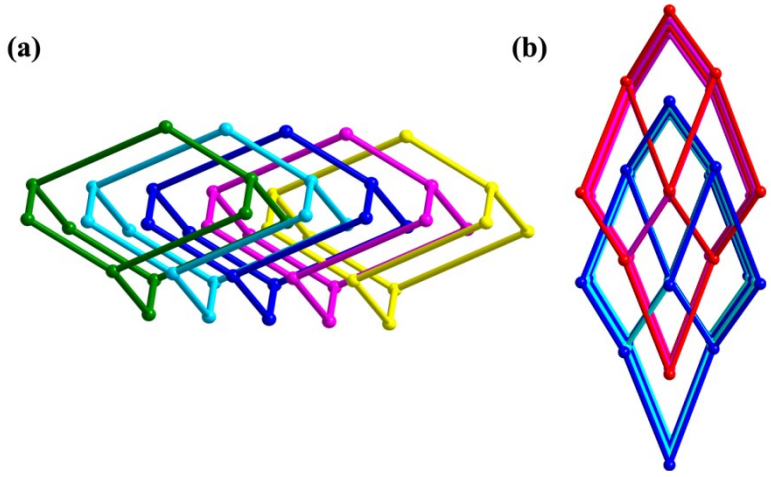

Figure S4. The *dia* net topologies for **FJU-67**, **FJU-68** (a) and **FJU-69** (b).

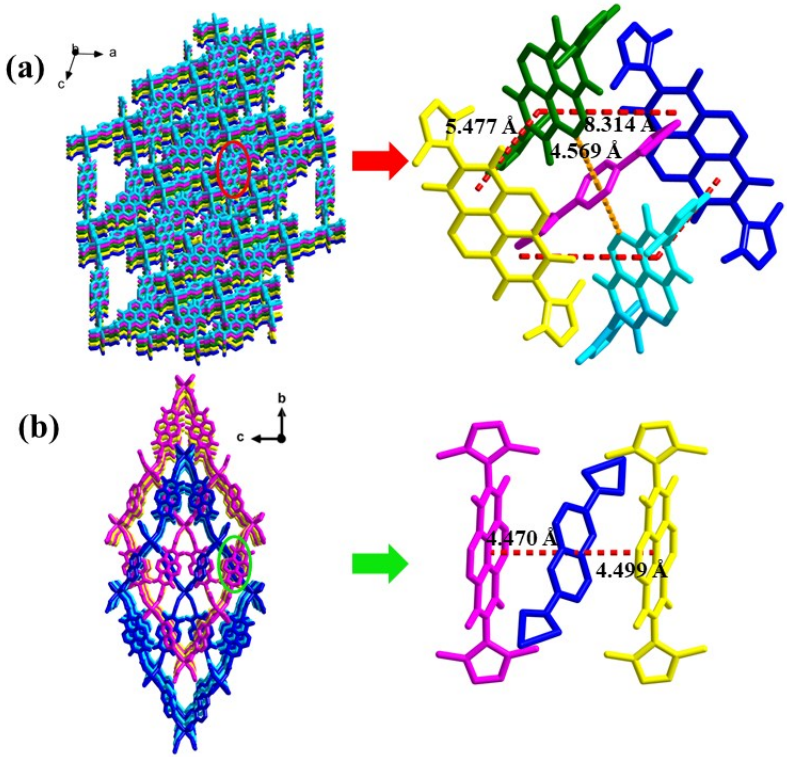

Figure S5. The π-π stacking distances in **FJU-67** (a) and **FJU-69** (b) between adjacent H_2NDI ligands accompany with the alternative H_2NDI and H_2NDC ligands.

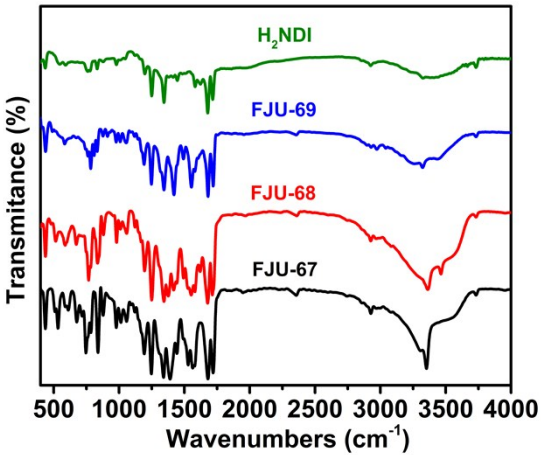

Figure S6. IR spectrum of **FJU-67**, **FJU-68** and **FJU-69**.

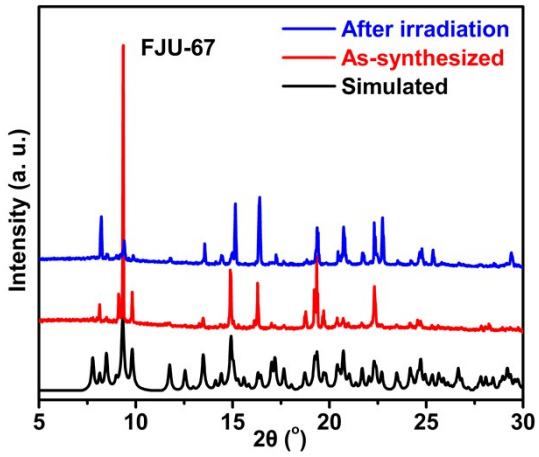

Figure S7. PXRD patterns of the simulated, as-synthesized **FJU-67**.

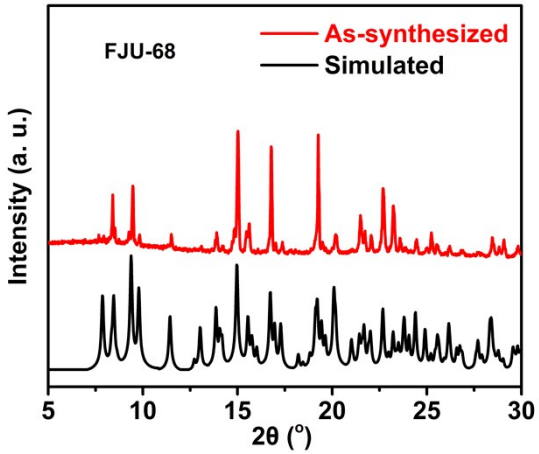

Figure S8. PXRD patterns of the simulated, as-synthesized **FJU-68**.

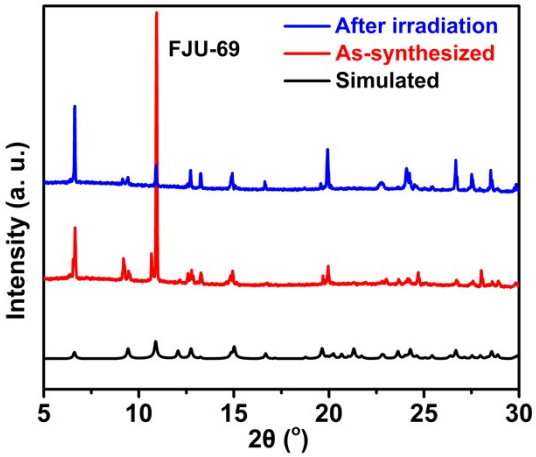

Figure S9. PXRD patterns of the simulated, as-synthesized **FJU-69**.

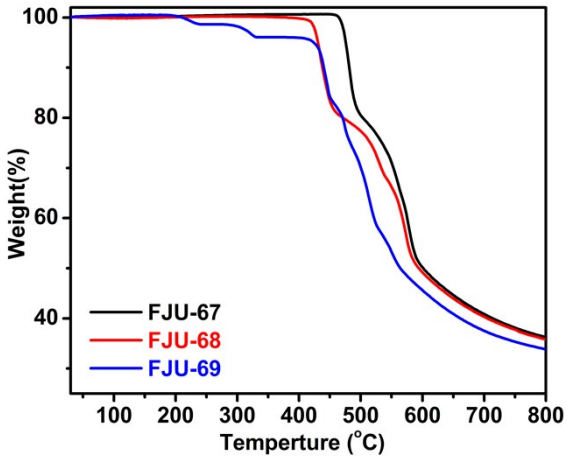

Figure S10. TGA of **FJU-67**, **FJU-68** and **FJU-69**.

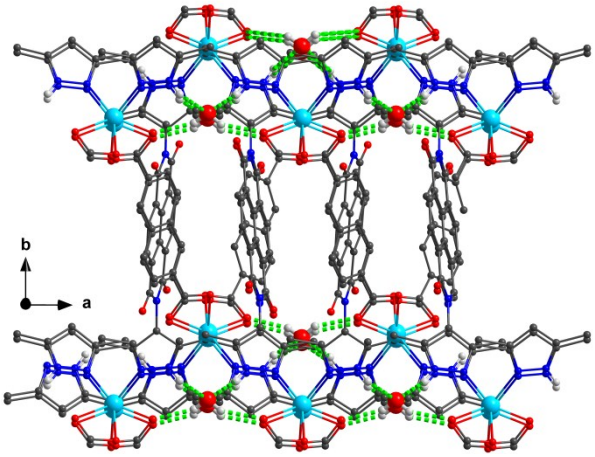

Figure S11. Hydrogen-bonded water molecules inside the channel of **FJU-69** along the *c* axis.

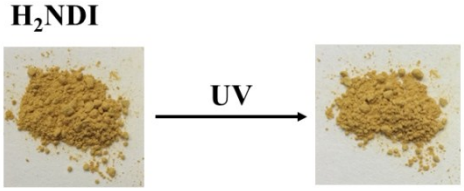

Figure S12. The photographic images of the H_2NDI before and after UV irradiation, showing there is no photochromic behavior in only ligand of H_2NDI.

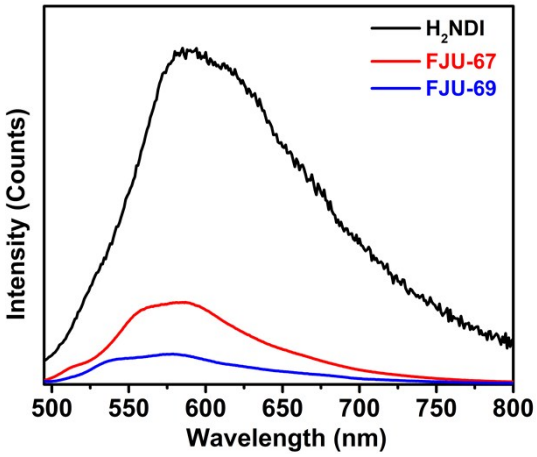

Figure S13. The fluorescence emission spectra for H_2NDI, **FJU-67**, and **FJU-69**.

Table S1 Crystal Data and refinement results for the **FJU-67**, **FJU-68**, **FJU-69**.

	FJU-67	**FJU-68**	**FJU-69**
CCDC	1851265	1851266	1851267
empirical formula	$C_{32}H_{22}CdN_6O_8$	$C_{32}H_{20}CdN_7O_8$	$C_{36}H_{26}CdN_6O_9$
formula weight	730.95	742.95	799.03
Temperature	293 K	293 K	293 K
Radiation	CuKα (λ = 1.54184 Å)	CuKα (λ = 1.54184 Å)	CuKα (λ = 1.54184 Å)
crystal system	triclinic	triclinic	monoclinic
space group	*P-1*	*P-1*	*Pn*
Dimensions	3D	3D	3D
a(Å)	10.9477(5)	11.2419(4)	8.9688(2)
b (Å)	12.6996(5)	12.4720(4)	13.3571(3)
c (Å)	12.7984(4)	12.7658(4)	13.4352(3)
α	110.328(3)°	112.810(3)°	90°
β	100.145(3)°	98.524(3)°	102.071(2)°
γ	108.530(4)°	107.333(3)°	90°
Volume (Å^3)	1497.63(10)	1502.58(9)	1573.91(6)
Z	2	2	2
Density (calcd)	1.621 g/cm^3	1.642 g/cm^3	1.686 g/cm^3
Absorption	6.392 mm^{-1}	0.793 mm^{-1}	6.166 mm^{-1}
Goodness-of-fit on F^2	1.045	1.092	1.060
F(000)	736.0	746.0	808.0
*R*1, *wR*2 [$I>2\sigma(I)$][a]	0.0232, 0.0589	0.0277, 0.0737	0.0257, 0.0644
*R*1, *wR*2 (all data)[a]	0.0267, 0.0610	0.0298, 0.0754	0.0295, 0.0677

(a) $R_1 = \sum \left| |F_O| - |F_C| \right| / \sum |F_O|$; $wR_2 = \left[\sum w\left(|F_O|^2 - |F_C|^2\right)^2 / \sum w\left(F_O{}^2\right)^2 \right]^{1/2}$

Table S2 Selected bond lengths [Å] for **FJU-67**, **FJU-68** and **FJU-69**.

FJU-67		**FJU-68**		**FJU-69**	
Atom-Atom	bond lengths [Å]	Atom-Atom	bond lengths [Å]	Atom-Atom	bond lengths [Å]
Cd1-O2	2.3231(17)	Cd1-O2	2.3711(17)	Cd1-O2	2.289(9)
Cd1-O3	2.4156(16)	Cd1-O3	2.308(2)	Cd1-O3	2.296(8)
Cd1-O1	2.3158(18)	Cd1-O4	2.317(2)	Cd1-O4	2.450(8)
Cd1-O4	2.3170(17)	Cd1-O1	2.349(19)	Cd1-O1	2.472(9)
Cd1-N3	2.3155(17)	Cd1-N1	2.310(2)	Cd1-N3	2.278(9)
Cd1-N2	2.2541(17)	Cd1-N3	2.252(2)	Cd1-N1	2.296(9)

Table S2 Selected bond angles [°] for **FJU-67**, **FJU-68** and **FJU-69**.

FJU-67		**FJU-68**		**FJU-69**	
Atom-Atom-Atom	Angle/°	Atom-Atom-Atom	Angle/°	Atom-Atom-Atom	Angle/°
O2-Cd1-O3	96.22(6)	O3-Cd1-O2	96.43(7)	O2-Cd1-O3	80.61(15)
O1-Cd1-O2	56.26(6)	O3-Cd1-O4	56.39(7)	O2-Cd1-O4	97.7(3)
O1-Cd1-O3	106.06(7)	O3-Cd1-O1	102.98(8)	O2-Cd1-O1	55.1(3)
O1-Cd1-O4	152.68(7)	O3-Cd1-N1	99.60(8)	O2-Cd1-N1	148.5(3)
O4-Cd1-O2	102.84(7)	O4-Cd1-O2	106.21(8)	O3-Cd1-O4	54.0(3)
O4-Cd1-O3	55.02(5)	O4-Cd1-O1	153.01(8)	O3-Cd1-O1	99.0(3)
N3-Cd1-O2	102.51(6)	O1-Cd1-O2	55.16(6)	O3-Cd1-N1	101.7(3)
N3-Cd1-O3	133.71(6)	N1-Cd1-O2	134.79(7)	O4-Cd1-O1	146.93(9)
N3-Cd1-O1	119.61(7)	N1-Cd1-O4	117.90(8)	N3-Cd1-O2	102.0(4)
N3-Cd1-O4	79.52(6)	N1-Cd1-O1	80.05(7)	N3-Cd1-O3	148.3(3)
N2-Cd1-O2	144.85(7)	N3-Cd1-O2	97.86(8)	N3-Cd1-O4	94.6(3)
N2-Cd1-O3	96.49(7)	N3-Cd1-O3	146.58(8)	N3-Cd1-O1	108.3(3)
N2-Cd1-O1	88.71(6)	N3-Cd1-O4	90.56(8)	N3-Cd1-N1	92.18(11)
N2-Cd1-O4	111.30(7)	N3-Cd1-O1	109.99(9)	N1-Cd1-O4	109.1(3)
N2-Cd1-N3	91.90(6)	N3-Cd1-N1	91.40(8)	N1-Cd1-O1	93.9(3)