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Exploration of semiconducting properties of Zn(II) and Cd(II) based coordination polymers with dicarboxylate of chair-type backbone

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Supporting Information

Table S1. Crystal data and refinement parameters for CP **1**

Formula	$C_{40}H_{42}Cd_2N_4O_{13}$
Fw	1011.60
crystsyst	Triclinic
space group	$P\bar{1}$
a (Å)	11.7888(4)
b (Å)	13.2584(4)
c (Å)	14.3334(5)
α(deg)	88.695(1)
β(deg)	66.249(1)
γ (deg)	89.327(1)
V (Å^3)	2050.03(12)
Z	2
D_{calcd}(g/cm^3)	1.639
μ(mm^{-1})	1.107
λ(Å)	0.0713
GOF on F^2	1.112
data[$I>2\sigma(I)$]/params	3506/226
final *R* indices [$I>2\sigma(I)$][a,b]	$R1$ = 0.0361 $wR2$ = 0.1238

[a] $R1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$, [b] $wR2 = [\Sigma w(F_o^2 - F_c^2)^2/\Sigma w(F_o^2)^2]^{1/2}$

Table S2. Selected bond lengths and bond angles in CP **1**

Bond lengths (Å)		Bond angles (°)			
Cd(01)-O(3)	2.298(3)	O(3)-Cd(01)-O(4)	54.32(9)	O(1)-Cd(02)-O(2)	53.00(11)
Cd(01)-O(4)	2.473(3)	O(3)-Cd(01)-O(8)	110.57(11)	O(1)-Cd(02)-N(3)	139.38(13)
Cd(01)-O(8)	2.330(3)	O(3)-Cd(01)-N(1)	163.64(13)	O(1)-Cd(02)-N(4)	98.68(12)
Cd(01)-N(1)	2.355(4)	O(3)-Cd(01)-N(2)	94.67(13)	O(1)-Cd(02)-O(1)a	71.40(10)
Cd(01)-N(2)	2.346(4)	O(3)-Cd(01)-C(33)	27.13(11)	O(1)-Cd(02)-O(5)c	87.66(10)
Cd(01)-O(7)b	2.524(3)	O(3)-Cd(01)-O(7)b	88.22(9)	O(1)-Cd(02)-O(6)c	123.42(12)
Cd(01)-O(8)b	2.361(3)	O(3)-Cd(01)-C(8)b	86.19(10)	O(1)-Cd(02)-C(30)c	106.28(11)
Cd(02)-O(1)	2.335(3)	O(4)-Cd(01)-O(8)	84.29(11)	O(2)-Cd(02)-N(3)	86.89(12)
Cd(02)-O(2)	2.532(3)	O(4)-Cd(01)-N(1)	129.16(11)	O(2)-Cd(02)-N(4)	88.27(12)
Cd(02)-N(3)	2.363(4)	O(4)-Cd(01)-N(2)	85.95(13)	O(1)a-Cd(02)-O(2)	121.78(9)
Cd(02)-N(4)	2.340(3)	O(4)-Cd(01)-C(33)	27.20(11)	O(2)-Cd(02)-O(5)c	84.36(10)
Cd(02)-O(1)a	2.380(3)	O(4)-Cd(01)-O(7)b	141.79(10)	O(2)-Cd(02)-O(6)c	138.08(9)
Cd(02)-O(5)c	2.335(3)	O(4)-Cd(01)-C(08)b	122.69(10)	O(2)-Cd(02)-C(30)c	111.40(11)
Cd(02)-O(6)c	2.423(3)	O(8)-Cd(01)-N(1)	85.73(12)	N(3)-Cd(02)-N(4)	70.83(11)
		O(8)-Cd(01)-N(2)	139.72(12)	O(1)a-Cd(02)-N(3)	141.48(11)
		O(8)-Cd(01)-C(33)	97.86(12)	O(5)c-Cd(02)-N(3)	95.23(11)
		O(7)b-Cd(01)-O(8)	120.17(11)	O(6)c-Cd(02)-N(3)	89.49(12)
		O(8)-Cd(01)-O(8)b	72.01(9)	N(3)-Cd(02)-C(30)c	93.19(11)
		N(1)-Cd(01)-N(2)	70.80(14)	O(1)a-Cd(02)-N(4)	83.89(11)
		N(1)-Cd(01)-C(33)	153.62(13)	O(5)c-Cd(02)-N(4)	164.61(12)
		O(7)b-Cd(01)-N(1)	84.53(11)	O(6)c-Cd(02)-N(4)	129.46(12)
		O(8)b-Cd(01)-N(1)	100.81(12)	N(4)-Cd(02)-C(30)c	154.35(12)
		N(2)-Cd(01)-C(33)	90.68(14)	O(1)a-Cd(02)-O(5)c	111.47(12)
		O(7)b-Cd(01)-N(2)	90.43(13)	O(1)a-Cd(02)-O(6)c	84.61(10)
		O(8)b-Cd(01)-N(2)	142.91(12)	O(1)a-Cd(02)-C(30)c	98.31(11)
		O(7)b-Cd(01)-C(33)	115.11(11)	O(5)c-Cd(02)-O(6)c	54.41(9)
		O(8)b-Cd(01)-C(33)	105.17(11)	O(5)c-Cd(02)-C(30)c	27.24(11)
		O(7)b-Cd(01)-O(8)b	52.50(10)	O(6)c-Cd(02)-C(30)c	27.18(11)

Symmetry transformations: a = 1-x,1-y,2-z; b = 2-x,-y,1-z; c = 2-x,1-y,1-z

Table S3. Hydrogen bonding in CP **1**

D—H···A	Distance (Å) D—H	Distance (Å) H···A	Distance (Å) D··A	Angle (°) ∠D—H···A	Symmetry
O10—H10A···O9	0.8500	1.9300	2.711(10)	152.00	-
O10—H10B···O11	0.8500	2.0000	2.787(8)	154.00	-
O12—H12A···O4	0.86(3)	1.97(4)	2.799(5)	161(7)	-
O12—H12B···O5	0.85(8)	2.36(7)	2.794(5)	113(6)	c= 2-x,1-y,1-z
O13—H13A···O3	0.8500	1.9500	2.729(6)	152.00	v = x,1+y,z
O13—H13B···O6	0.8500	1.9200	2.763(6)	171.00	c= 2-x,1-y,1-z

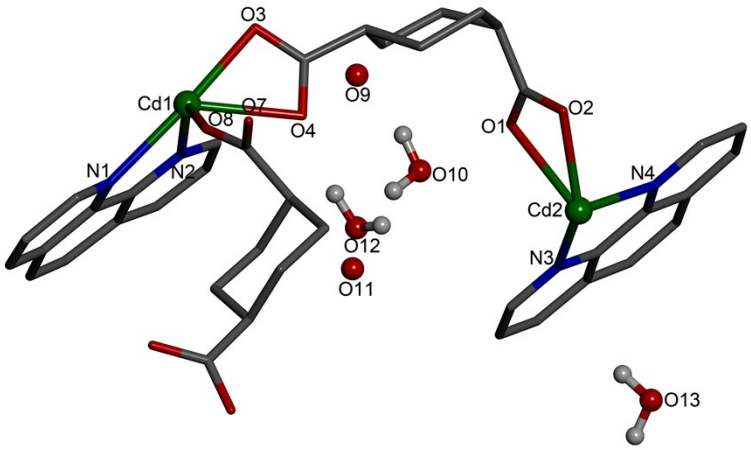


Fig. S1 Asymmetric unit of compound **1**.

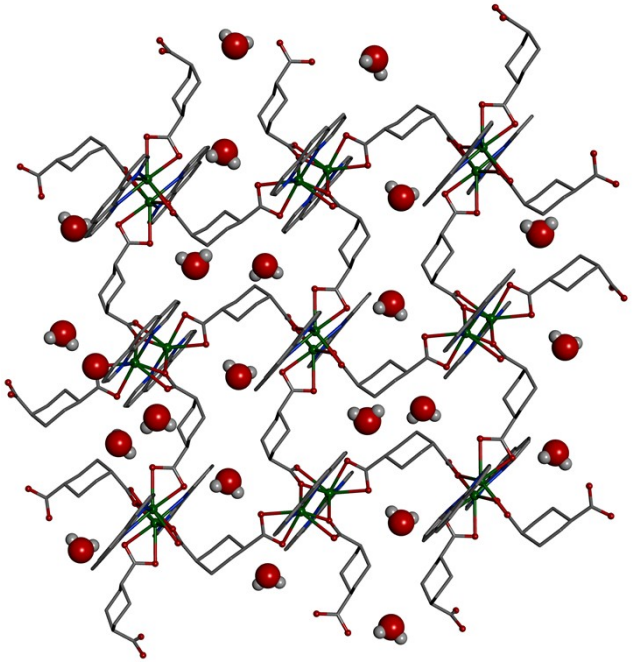


Fig. S2 2D sheet formed in CP **1** showing water molecules in the cavity.

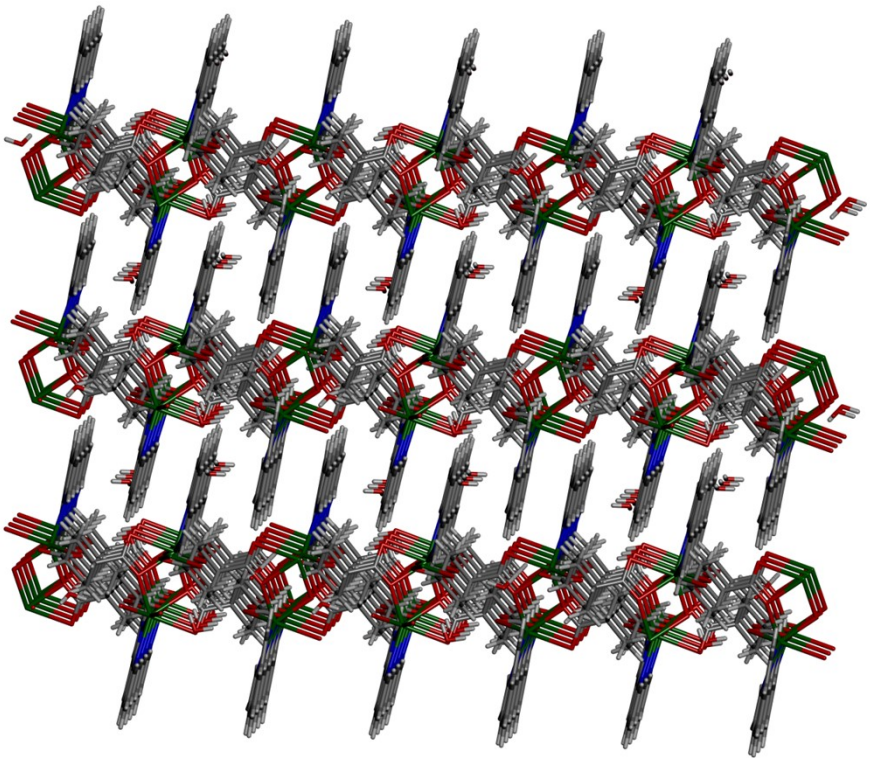


Fig. S3 Intermolecular hydrogen bonding leading to 3D network formation in **1**.

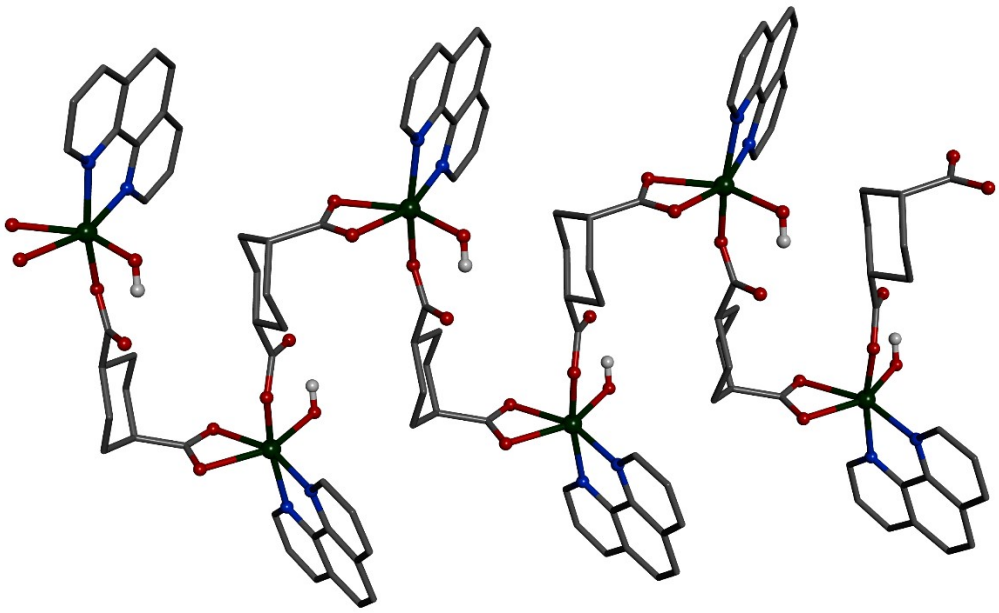


Fig. S4 Formation of 1D chain in **2**.

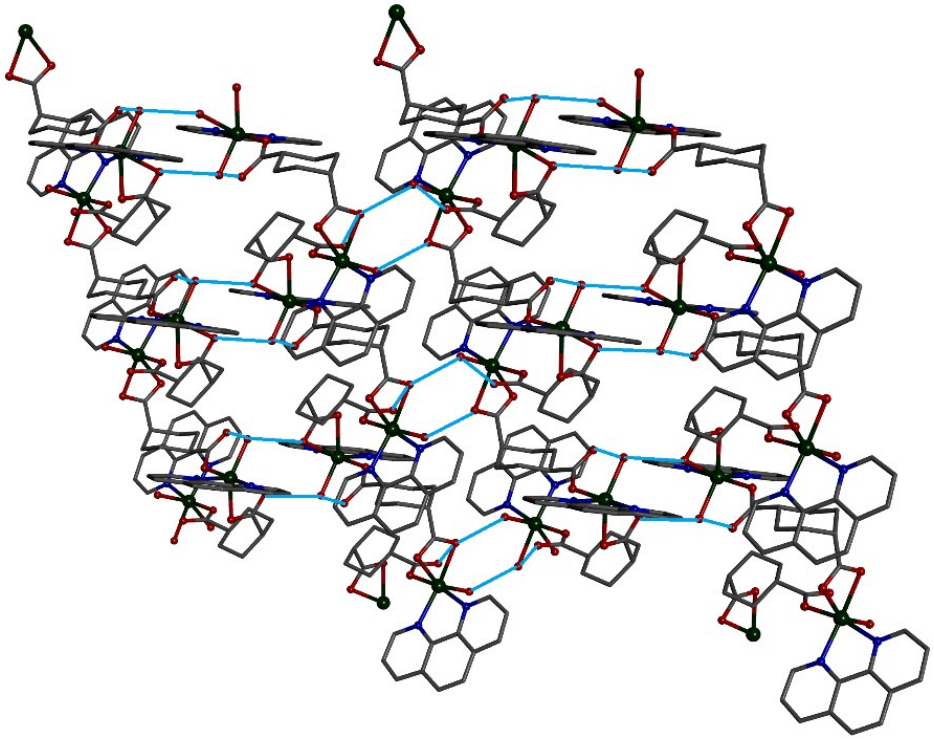


Fig. S5 Intermolecular hydrogen bonding leading to 2D sheet formation in **2**.

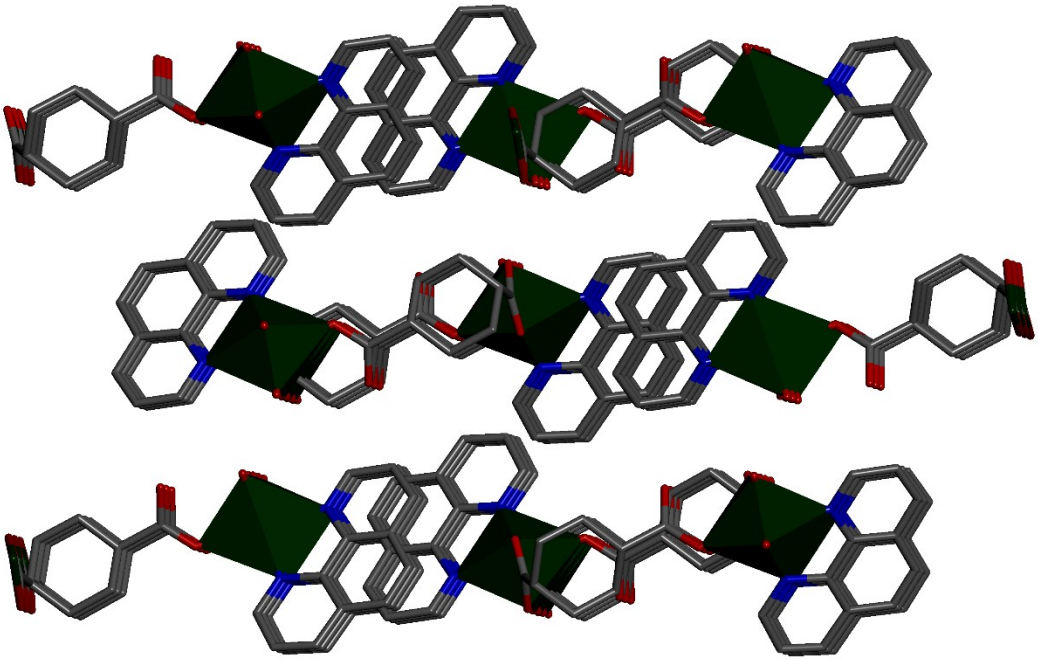
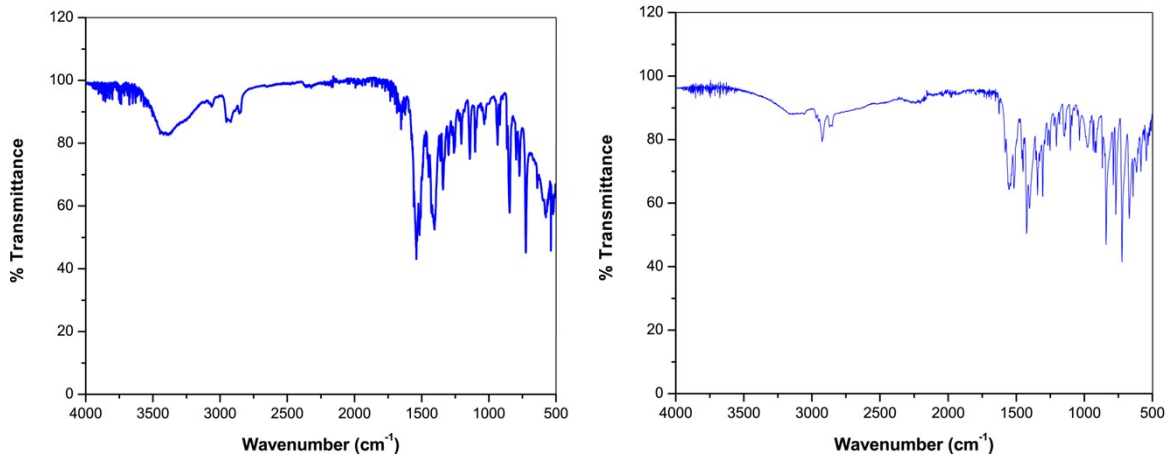


Fig. S6 Formation of 3D network CP **2**.



(a) (b)

Fig. S7 IR spectrum of (a) CP **1** and (b) CP **2**.

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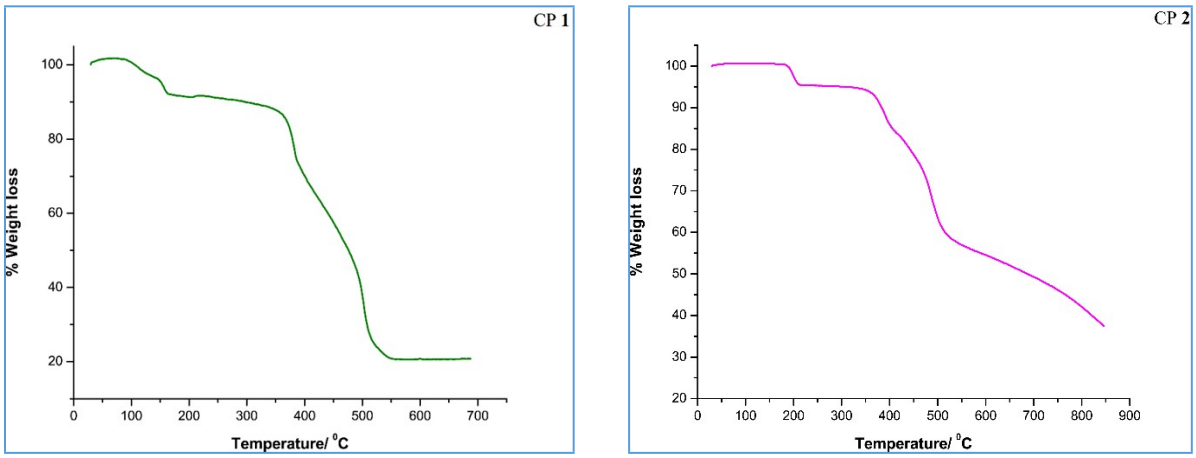

Fig. S8 TGA of CP **1** (left) and CP **2** (right).

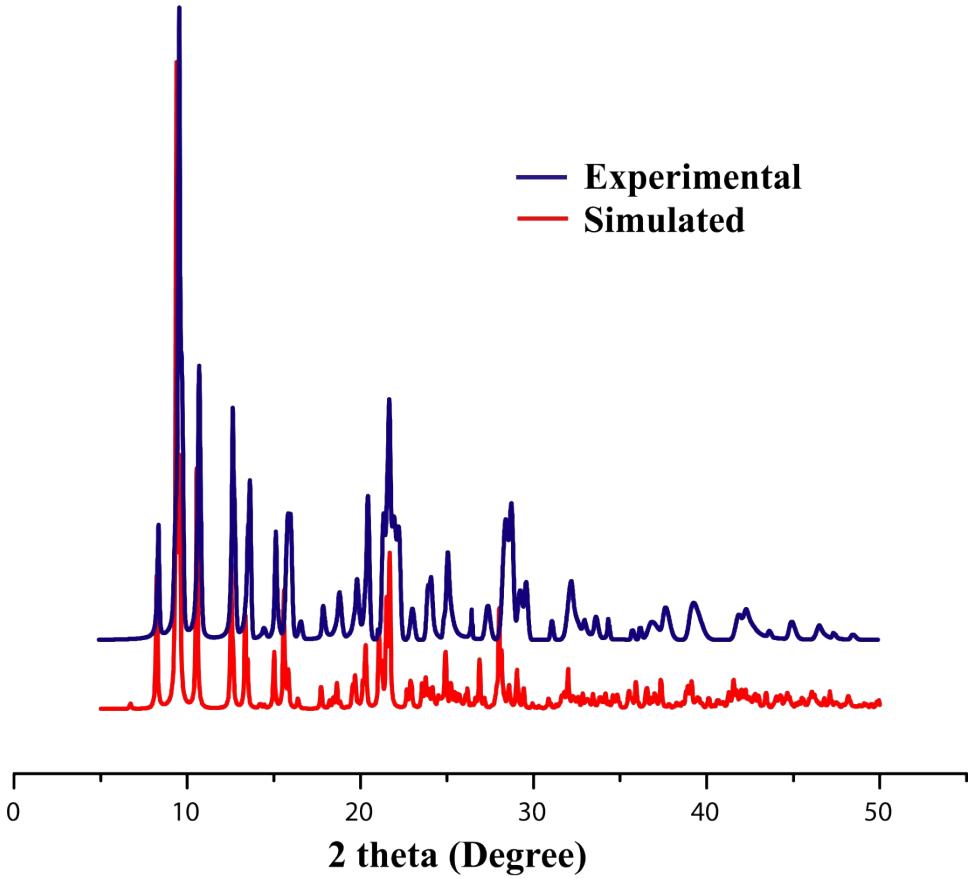

Fig. 9 PXRD patterns of CP **1**.

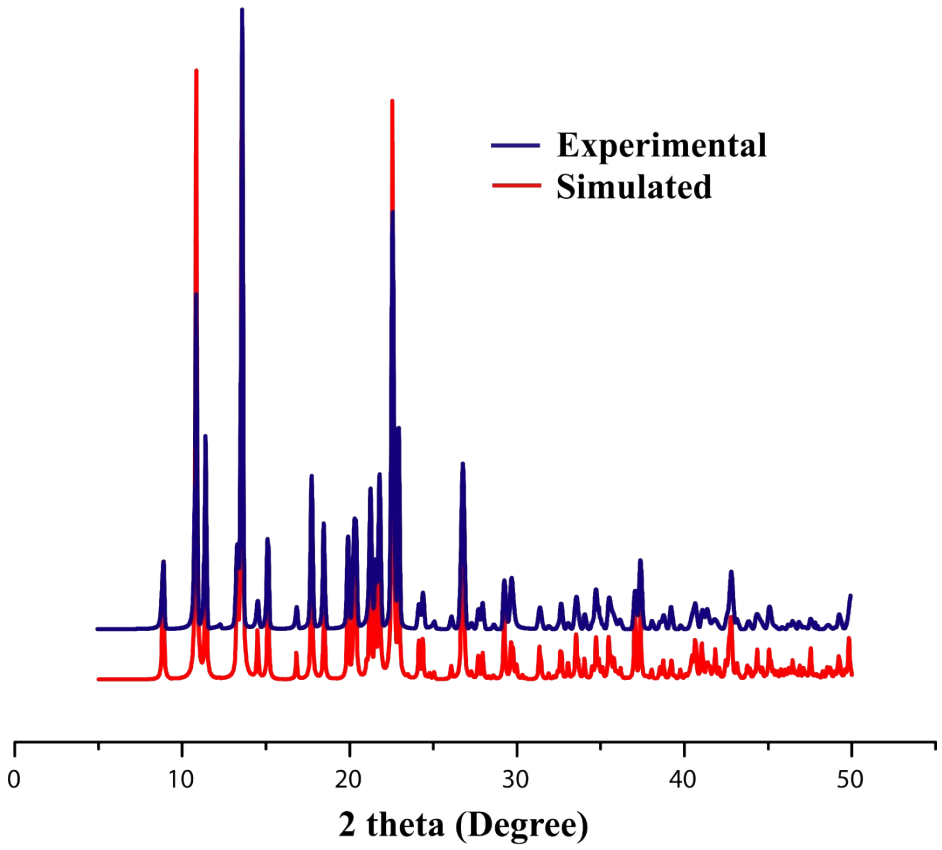

Fig. 10 PXRD patterns of CP **2**.

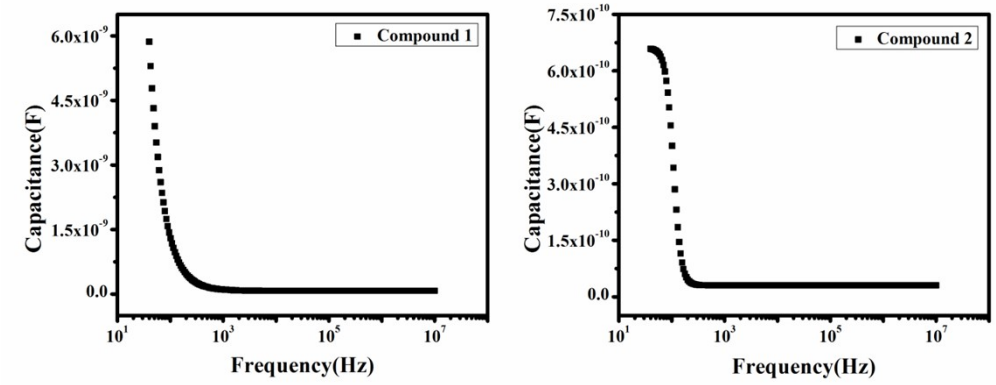

Fig. S11 Capacitance *versus* frequency plot of (a) CP **1** and (b) CP **2**.