Synthesis of a Zn(II)-based 1D zigzag coordination polymer for the fabrication of optoelectronic device with remarkably high photosensitivity

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Supporting Information

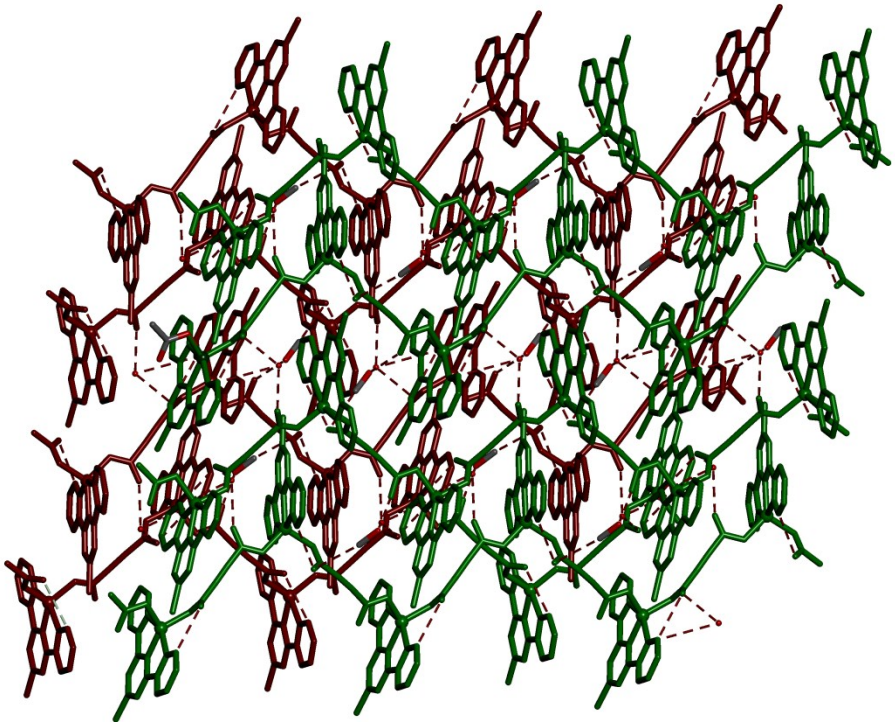


Fig. S1 3D supramolecular architecture of compound **1**.

Table S1 Crystal data and refinement parameters of compound **1**

Formula	$C_{77}H_{49}Cl_4N_{12}O_{19}Zn_4$
fw	1849.64
cryst syst	monoclinic
space group	$P2_1/c$
a (Å)	14.6802(6)
b (Å)	16.8579(9)
c (Å)	16.1761(7)
α(deg)	90
β(deg)	96.378(3)
γ (deg)	90
V (Å^3)	3978.4(3)
Z	2
D_{calcd}(g/cm^3)	1.544
μ(mm^{-1})	1.404
λ(Å)	0.71073
data[$I > 2\sigma(I)$]/params	6835/539
GOF on F^2	1.028
final R indices[$I > 2\sigma(I)$][a,b]	$R1 = 0.0357$ $wR2 = 0.0962$

[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 **1**

Zn1 O1	1.985(2)	N2 Zn1 N3	74.36(9)
Zn1 O5	2.006(2)	N1 Zn1 N3	150.58(9)
Zn1 N2	2.085(2)	O3 Zn2 O7	104.10(10)
Zn1 N1	2.147(2)	O3 Zn2 N5	134.32(10)
Zn1 N3	2.211(3)	O7 Zn2 N5	120.83(9)
Zn2 O3	1.957(2)	O3 Zn2 N6	101.95(10)
Zn2 O7	1.971(2)	O7 Zn2 N6	104.43(10)
Zn2 N5	2.079(2)	N5 Zn2 N6	75.90(9)
Zn2 N6	2.160(2)	O3 Zn2 N4	99.15(10)
Zn2 N4	2.197(3)	O7 Zn2 N4	89.87(9)
O1 Zn1 O5	99.63(9)	N5 Zn2 N4	74.72(9)
O1 Zn1 N2	127.38(9)	N6 Zn2 N4	150.60(9)
O5 Zn1 N2	130.85(9)	C40 O1 Zn1	119.80(19)
O1 Zn1 N1	110.91(10)	C8 O5 Zn1	107.33(19)
O5 Zn1 N1	102.06(9)	C29 N2 Zn1	120.66(17)
N2 Zn1 N1	76.22(9)	C33 N2 Zn1	118.22(18)
O1 Zn1 N3	87.24(9)	C5 O7 Zn2	122.9(2)
O5 Zn1 N3	97.19(9)	C1 O3 Zn2	120.4(2)
C14 N5 Zn2	120.12(19)	C23 N6 Zn2	125.7(2)
C19 N6 Zn2	115.4(2)	C38 N1 Zn1	125.3(2)
C34 N1 Zn1	115.56(18)	C24 N3 Zn1	126.3(2)
C28 N3 Zn1	116.08(18)	C13 N4 Zn2	116.01(19)
C41 N5 Zn2	118.83(19)	C9 N4 Zn2	125.5(2)

Table S3 π···π distances in **1**

Cg →Cg	Cg-Cg(Å)
Cg(1)→Cg(7)	3.8906(17)
Cg(4)→Cg(9)	3.6680(17)
Cg(2)→Cg(7)	3.8906(17)
Cg(3)→Cg(1)	2.6599(15)
Cg(3)→Cg(2)	2.6599(15)
Cg(4)→Cg(1)	2.7536(16)
Cg(4)→Cg(2)	2.7536(16)
Cg(8)→Cg(9)	3.6680(19)

Table S4 X–H···π distances in **1**

X–H→Cg	H···Cg (Å)	X···Cg (Å)	< X–H···Cg (°)
O(9)–H(9A) →Cg(4)	2.92	3.624(6)	145
O(9)–H(9A) →Cg(8)	2.65	3.436(6)	160

π rings are:

Cg(3) = Zn(1)/N(1)/C(34)/C(33)/N(2)
Cg(4) = Zn(1)/N(2)/C(29)/C(28)/N(3)
Cg(5) = Zn(2)/N(4)/C(13)/C(14)/N(5)
Cg(6) = Zn(2)/N(5)/C(41)/C(19)/N(6)
Cg(7) = N(1)/C(34)/C(35)/C(36)/C(37)/C(38)
Cg(8) = N(2)/C(29)/C(30)/C(31)/C(32)/C(33)
Cg(9) = N(3)/C(24)/C(25)/C(26)/C(27)/C(28)
Cg(10) = N(4)/C(9)/C(10)/C(11)/C(12)/C(13)
Cg(11) = N(5)/C(14)/C(15)/C(16)/C(17)/C(41)
Cg(12) = N(6)/C(19)/C(20)/C(21)/C(22)/C(23)

Table S5 Hydrogen bonding distances and angles in **1**

Donor (D)–H···Acceptor (A)	D–H (Å)	H···A (Å)	D···A (Å)	< D–H···A (°)
O(9)–H(9A)···O(6)	0.82	2.42	2.680(6)	100
O(11)–H(11A)···O(4)	0.86(4)	2.05(3)	2.827(4)	150(5)
O(11)–H(11B)···O(2)	0.87(5)	2.12(5)	2.925(4)	156(5)
C(12)–H(12)···O(7)	0.93	2.59	3.182(4)	122
C(17)–H(17)···O(8)	0.93	2.50	3.125(4)	125

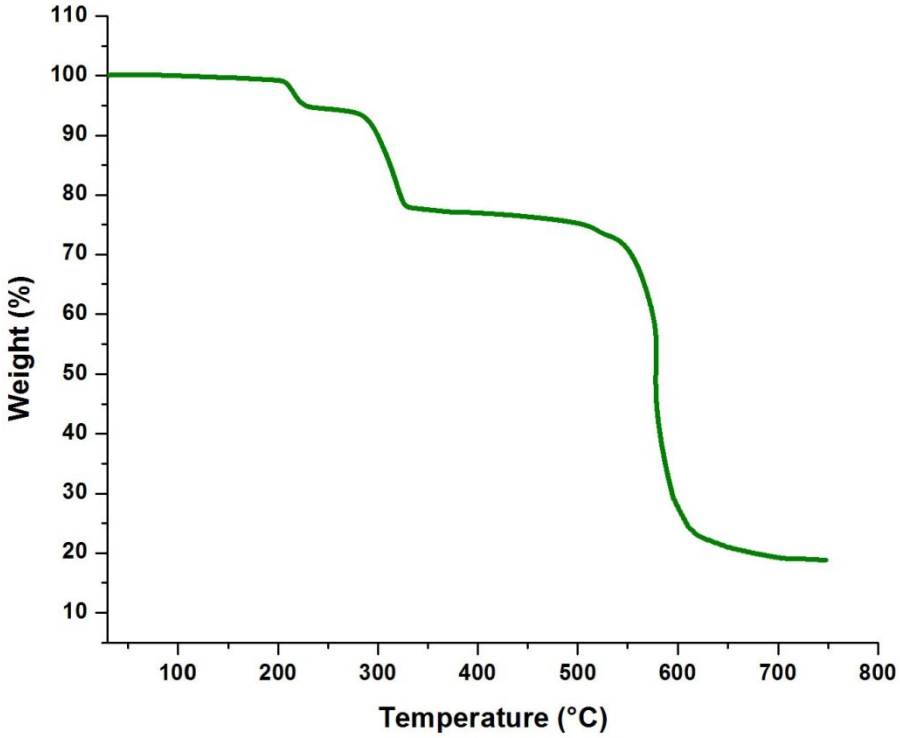


Fig. S2 TGA plot of **1**.

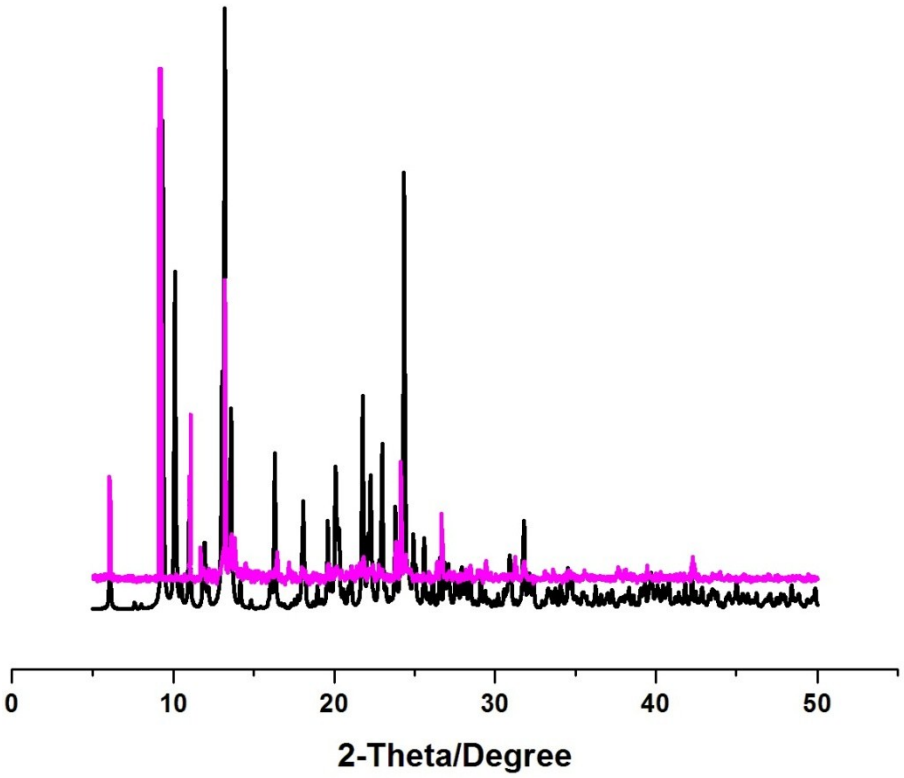
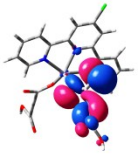
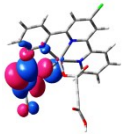
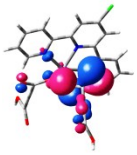
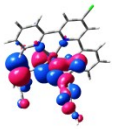
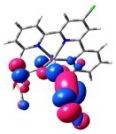
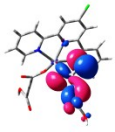
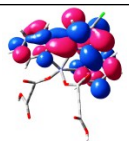
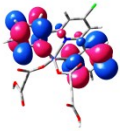
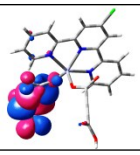


Fig. S3 PXRD patterns of simulated **1** (black) and as-synthesized **1** (pink).

Table S6 DFT table of the compound **1**

				
LUMO -3.11 eV	LUMO+1 -3.01 eV	LUMO+2 -1.97 eV	LUMO+3 -1.82 eV	LUMO+4 -1.67 eV
				
HOMO -6.8 eV	HOMO-1 -7.0 eV	HOMO-2 -7.32 eV	HOMO-3 -7.52 eV	HOMO-4 -7.65 eV

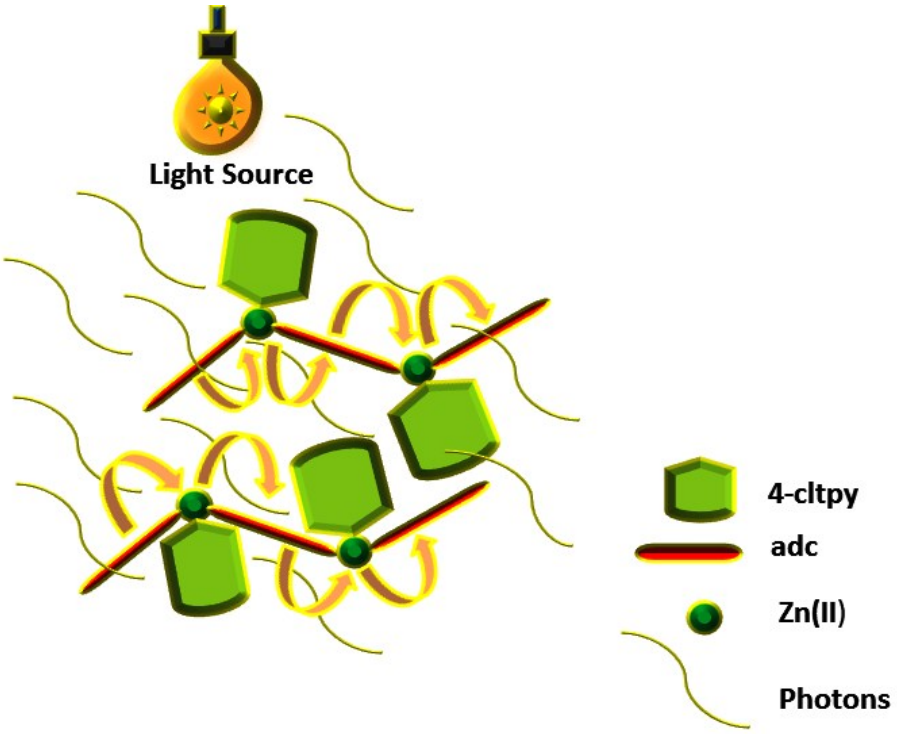


Fig. S4 Schematic diagram of possible mechanism for the charge transport in **1**.

Table S7 Table for comparative data on the performance of materials

Compound	Condition	Ideality factor	Barrier height, Φb (eV)	Transit time, τ (s)	Photo sensitivity	References
$[Zn(adc)(4\text{-}nvp)_2(H_2O)_2]_n$	Dark light	1.93 1.43	0.45 0.38	1.03×10^{-3} 3.04×10^{-4}	2.73	1
$[Cu_2(muco)_2(py)_4]\cdot 4H_2O\cdot 2EtOH$	Dark light	- -	- -	- -	1.65	2
$C_{40}H_{34}Cu_2N_6O_{18}$	Dark light	2.78 1.85	0.47 0.43	1.01×10^{-1} 5.29×10^{-2}	2.27	3
$C_{20}H_{18}CuN_2O_{10}$	Dark light	2.08 1.13	0.44 0.41	1.33×10^{-1} 4.59×10^{-2}	3.77	3
$[Cd(4\text{-}bpd)(SCN)_2]_n$	Dark light	5.52 3.54	0.367 0.337	1.02×10^{-5} 5.39×10^{-6}	- -	4
$[(NCS)Pb(H_2O)\text{-}LNi(NCS)]_n$	Dark light	0.52 0.79	0.71 0.55	0.35×10^{-6} 0.11×10^{-6}	5.76	5
$[\{CuLNa\}_2(m\text{-}1,1,3\text{-}NCS)HgCl_2(m\text{-}1,3\text{-}NCS)]_n$	Dark light	0.35 0.58	0.71 0.62	0.135 0.074	57	6
$[Zn(INH)(succ)]_n$	Dark light	1.43	0.368	1.7×10^{-3}		7
$\{[Zn(adc)(4\text{-}spy)_2(H_2O)_2]\}_n$	Dark light	2.89 2.08	0.43 0.39	$3.82 \times 10{-}5$ $3.04 \times 10{-}5$	1.96	8
$[Zn_4(adc)_4(4\text{-}cltpy)_4]\cdot CH_3OH\cdot 2H_2O$	Dark light	3.21 3.06	0.41 0.27	1.02×10^{-6} 1.25×10^{-9}	1134	This Work

References:

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