Electronic Supplementary Information

Regulating electrical conductivity and Schottky nature of d^{10} metal ion based nanoarchitectonics of coordination polymers

Manik Shit,[a,b] Pubali Das,[c] Arnab Samanta,[d] Basudeb Dutta,[a] Mainak Das,[c] Sourav Roy,[e] Chittaranjan Sinha,[b] Partha Pratim Ray,*[c] and Mohammad Hedayetullah Mir*[a]

[a]*Department of Chemistry, Aliah University, New Town, Kolkata 700 160, India. Email: chmmir@gmail.com.*

[b]*Department of Chemistry, Jadavpur University, Jadavpur, Kolkata 700 032, India*

[c]*Department of Physics, Jadavpur University, Jadavpur, Kolkata 700 032, India.*

[d]*Department of Chemistry, Brainware University, Barasat, Kolkata 700 125, India.*

[e]*Solid State and Structural Chemistry Unit, Indian Institute of Science, Bangalore, 560 012 India.*

To whom correspondence should be addressed. E-mail: chmmir@gmail.com

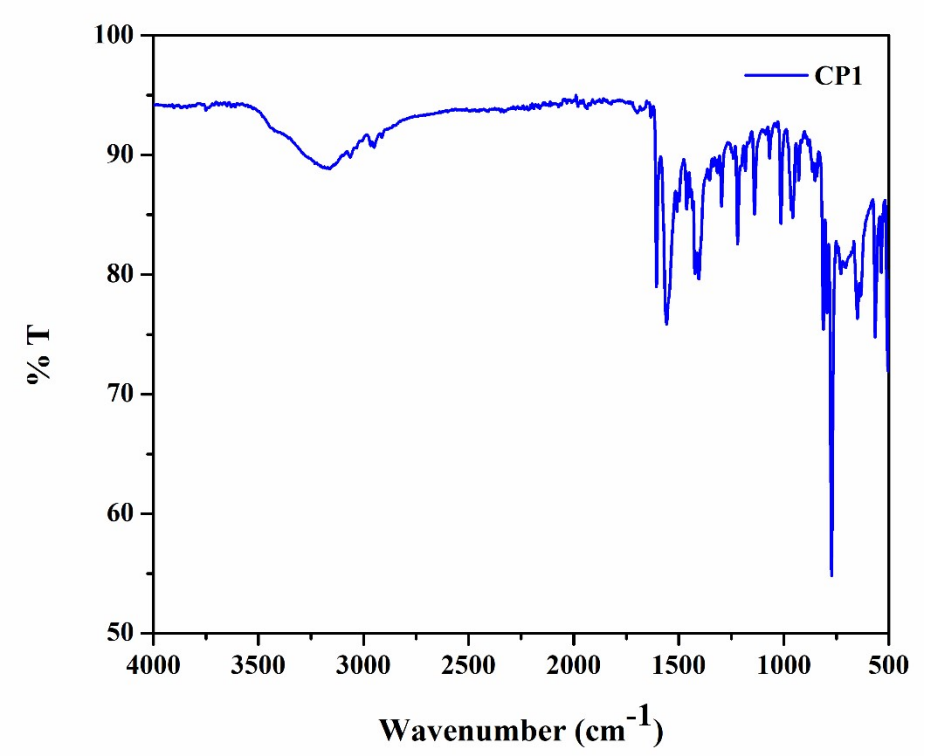

Fig. S1 IR spectroscopy of **CP1**.

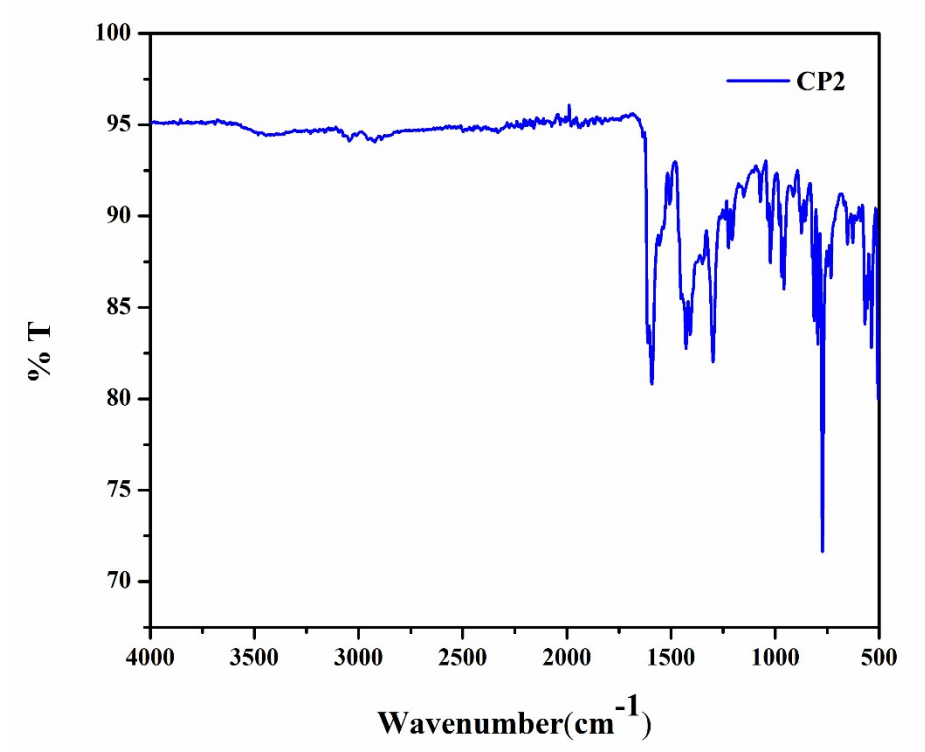

Fig. S2 IR spectroscopy of **CP2**.

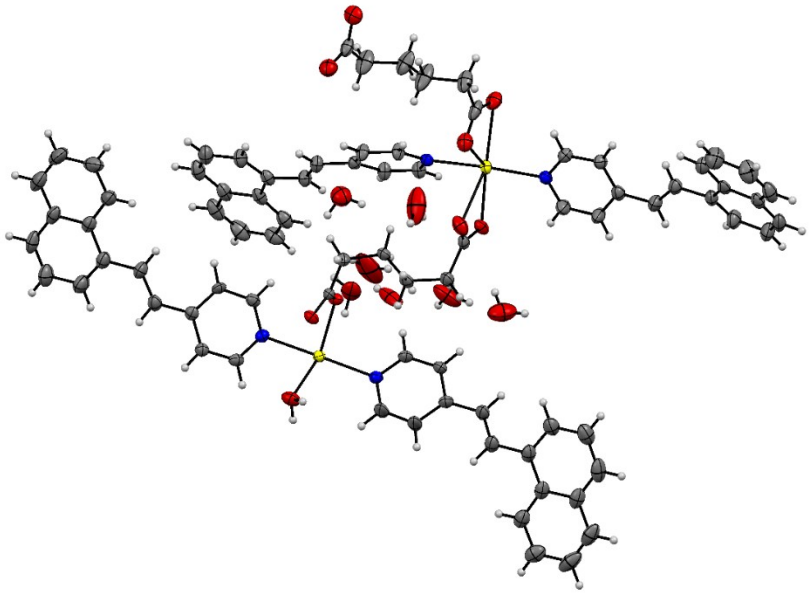

Fig. S3 Asymmetric unit of **CP1** with 30% thermal ellipsoid plot. Carbon: grey; nitrogen: blue; oxygen: red; hydrogen: white; cadmium: yellow.

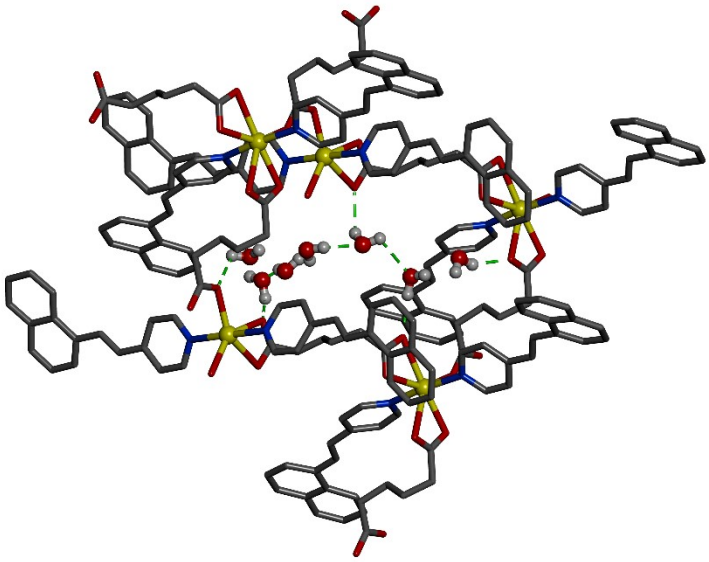

Fig. S4 Perspective view of water heptamer cluster in **CP1**.

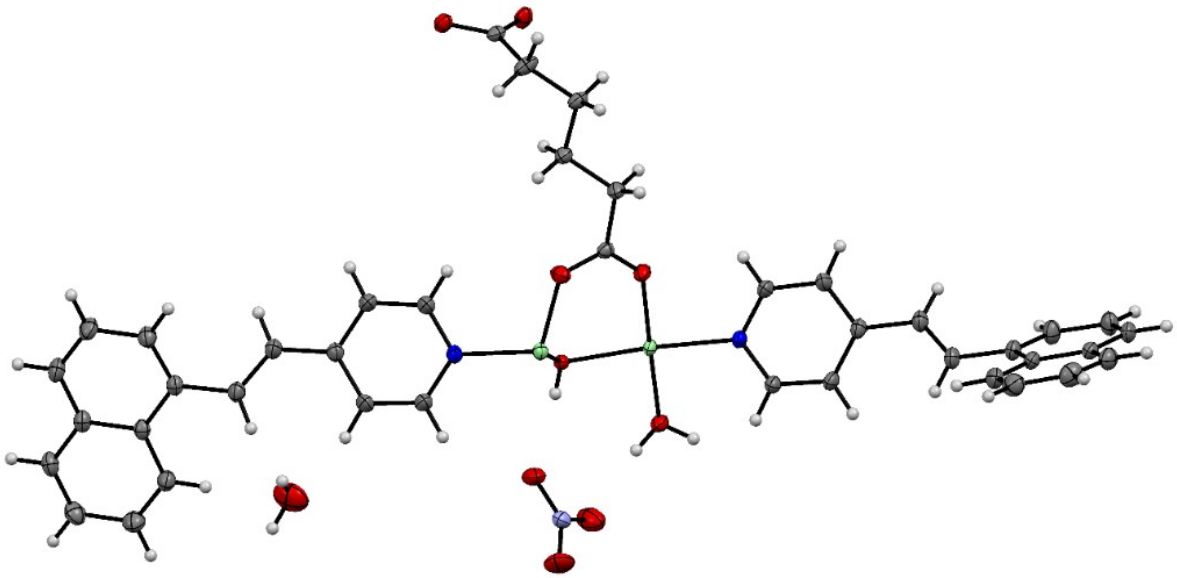

Fig. S5 Asymmetric unit of **CP2** with 30% thermal ellipsoid plot. Carbon: grey; nitrogen: blue; oxygen: red; hydrogen: white; zinc: green.

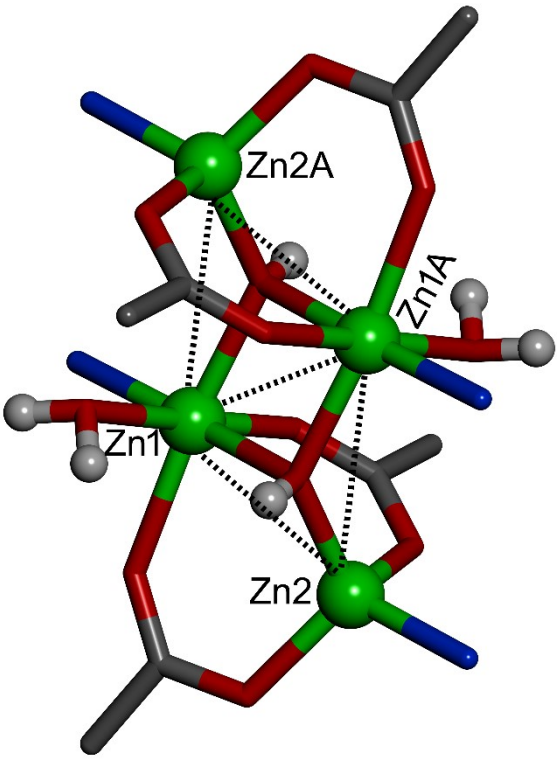

Fig. S6 The parallelogram {Zn4} SBU unit in **CP1**.

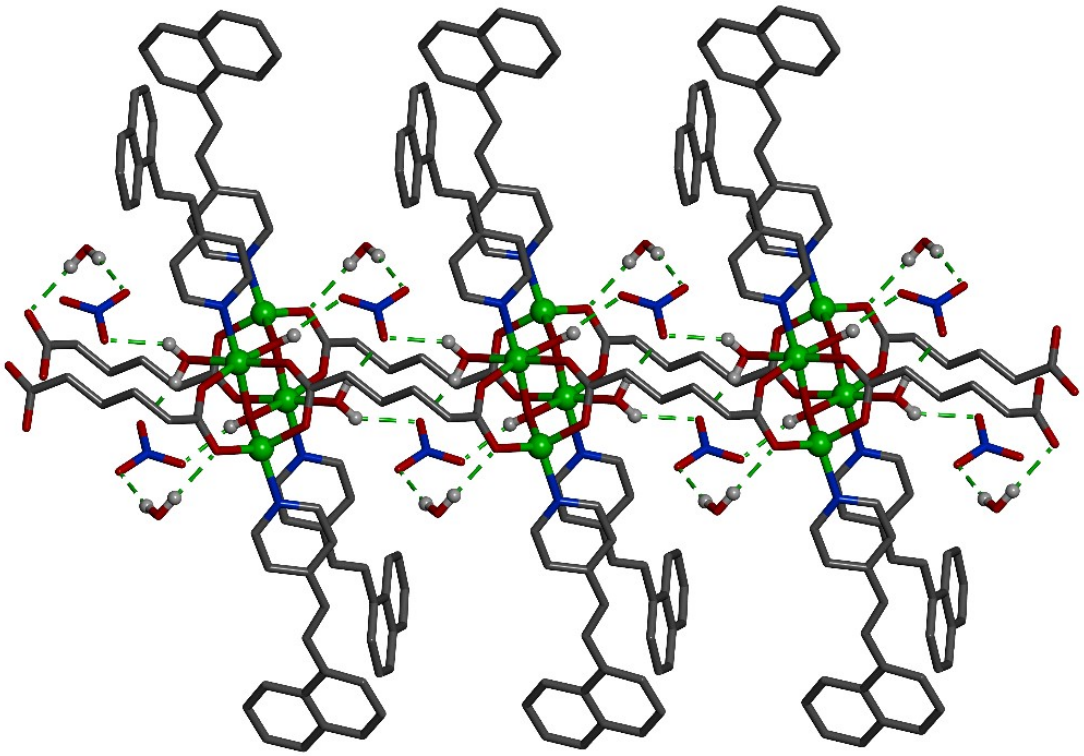

Fig. S7 A view of 1D double chain polymer of **CP2** along with extensive hydrogen bonding.

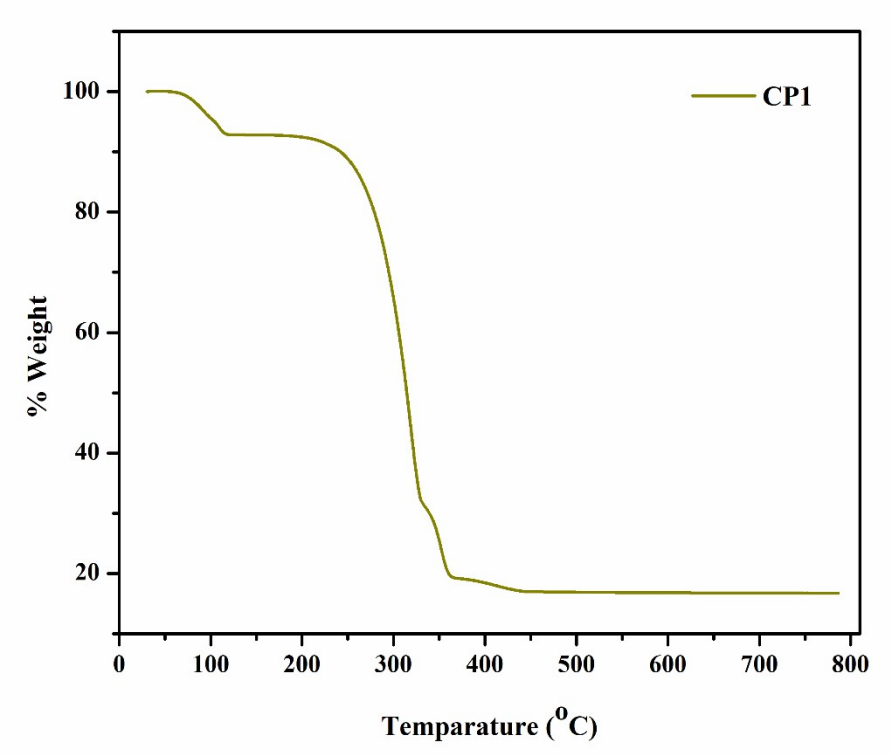

Fig. S8 TGA plot of **CP1**.

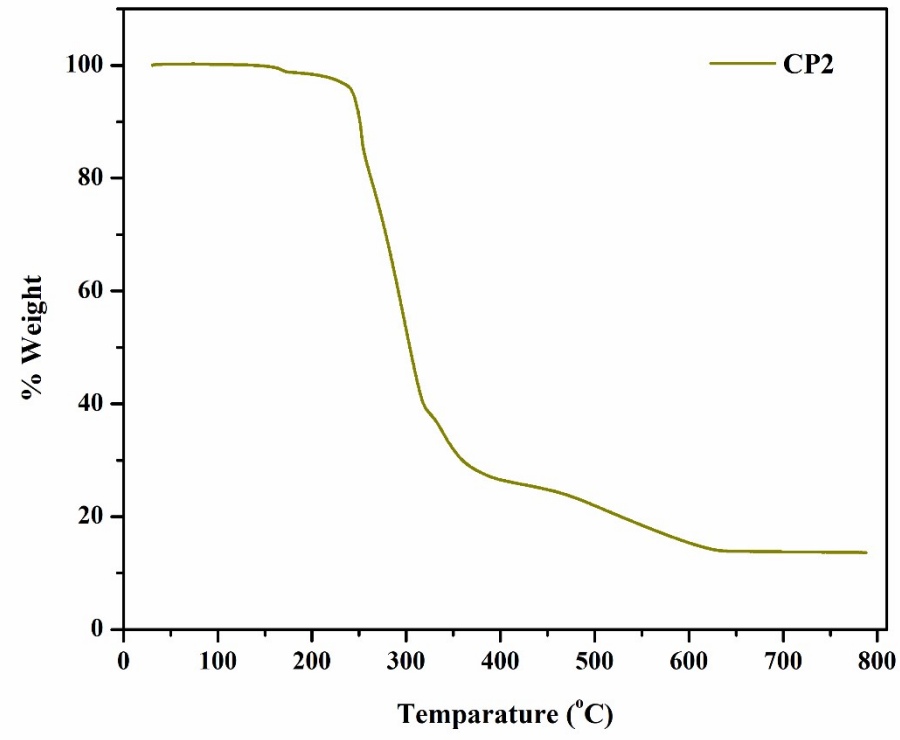

Fig. S9 TGA plot of **CP2**.

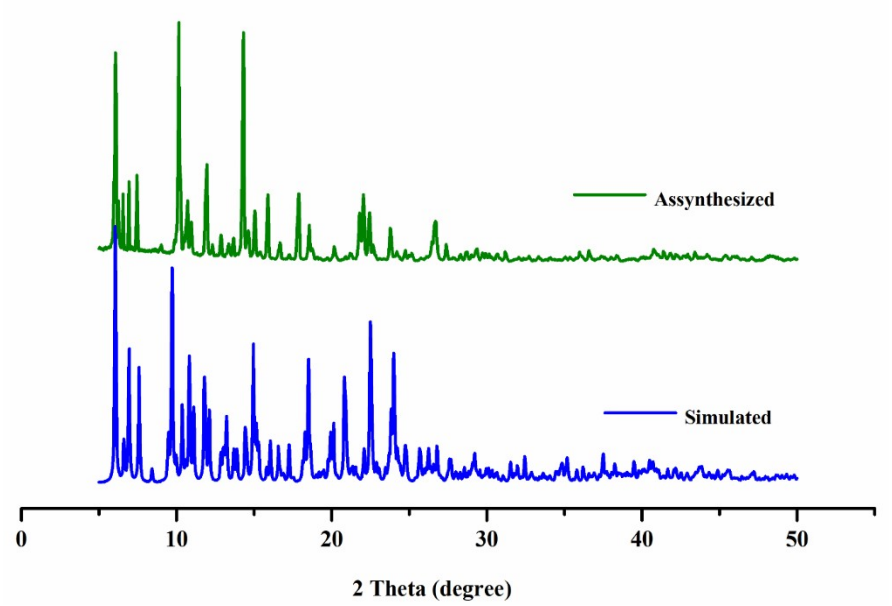

Fig. S10 PXRD patterns of simulated (blue) and as-synthesized (olive) **CP1**.

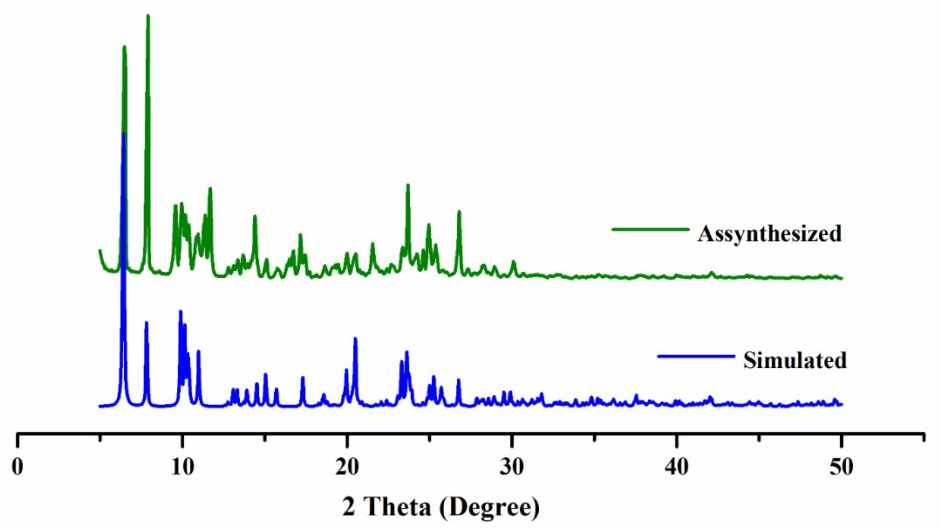

Fig. S11 PXRD patterns of simulated (blue) and as-synthesized (olive) **CP2**.

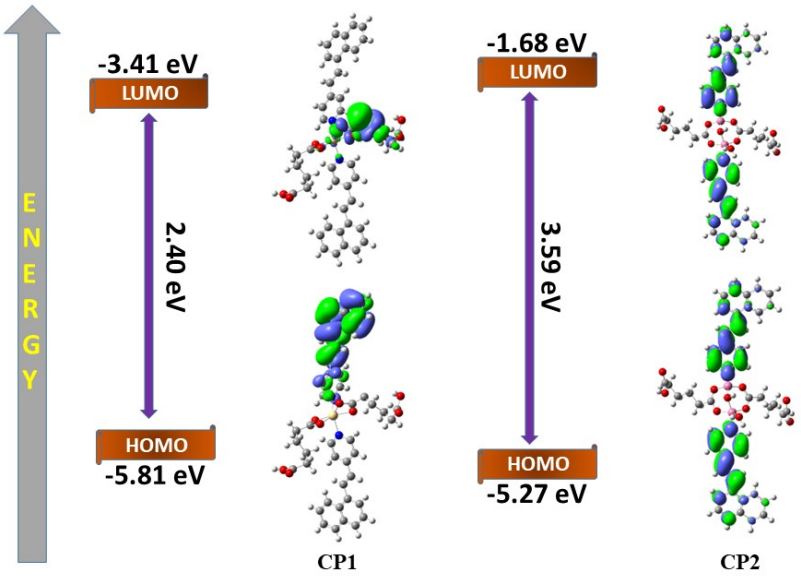

Fig. S12 DFT calculated HOMO-LUMO energy gap of **CP1** and **CP2**.

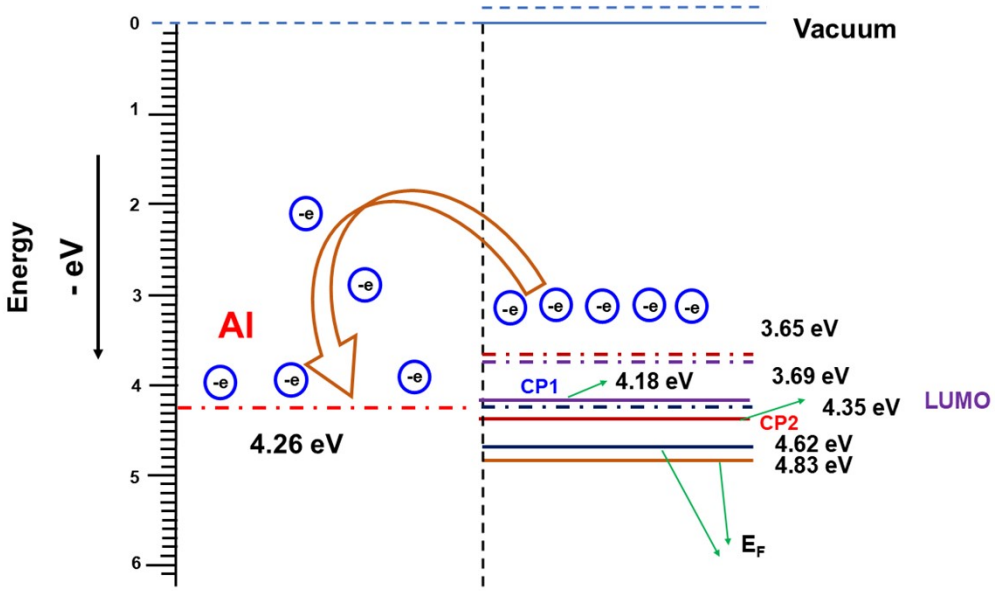

Fig. S13 Fermi level and energy band diagram of MS junction.

Table S1. Crystal data and refinement parameters for compound **CP1** and **CP2**

Compound	**CP1**	**CP2**
CCDC No.	2380875	2380876
empirical formula	$C_{80}H_{79.85}Cd_2N_4O_{14.30}$	$C_{40}H_{39}N_3O_{10}Zn_2$
formula weight	1550.95	852.52
crystal system	Triclinic	Triclinic
space group	$P\bar{1}$	$P\bar{1}$
a (Å)	9.3834(7)	9.489(3)
b (Å)	13.8555(11)	14.585(4)
c (Å)	29.438(2)	15.052(4)
α (°)	96.035(2)	72.307(13)
β (°)	92.269(2)	72.215(10)
γ (°)	103.563(2)	76.897(9)
V (Å^3)	3691.8(5)	1869.1(9)
T (K)	273K	273 K
Z	2	2
D_{calcd} (Mg/m^3)	1.395	1.515
μ (mm^{-1})	0.643	1.347
λ (Å)	0.71073	0.71073
θ range (°)	1.748-25.000	2.896-27.166
total reflections	13012	8256
refine parameters	941	505
R_1[a] [$I > 2\sigma(I)$]	0.0778 (10436)	0.0241(7437)
wR$_2$[b]	0.2014 (13012)	0.0640(8256)
goodness-of-fit	0.999	0.994

[a]$R_1 = \Sigma||F_o| \quad |F_c||/ \Sigma|F_o|$, [b]$wR_2 = [\Sigma w(F_o^2 \quad F_c^2)^2/\Sigma w(F_o^2)^2]^{1/2}$

$(0.1000P)^2+0.3347P]$, where $P= (F_o^2+2Fc^2)/3$

Table S2. Selected bond length and bond angle of **CP1**

Bond length	**Å**	**Bond angle**	**Degree (°)**
Cd1 - O9	2.359(5)	O9 - Cd1 - O10	50.74(19)
Cd1 - O10	2.617(6)	O9 - Cd1 - O11	176.98(19)
Cd1 - O11	2.574(6)	O9 - Cd1 - O12	130.1(2)
Cd1 - O12	2.322(6)	O9 - Cd1 - N3	84.79(18)
Cd1 - N3	2.324(5)	O9 - Cd1 - N4	89.8(2)
Cd1 - N4	2.290(6)	O9 - Cd1 - O8_b	80.74(17)
Cd1 - O8_b	2.387(5)	O10 - Cd1 - O11	131.9(2)
Cd2 - O1	2.258(6)	O10 - Cd1 - O12	79.5(2)
Cd2 - O7	2.248(5)	O10 - Cd1 - N3	84.92(19)
Cd2 - N1	2.335(5)	O10 - Cd1 - N4	95.46(19)
Cd2 - N2	2.340(6)	O10 - Cd1 - O8_b	131.14(19)
Cd2 - O15_d	2.390(7)	O11 - Cd1 - O12	52.7(2)

b = -1+x, y, z; d = 1+x,1+y, z

Table S3. Selected bond length and bond angle of **CP2**

Bond length	**Å**	**Bond angle**	**Degree (°)**
Zn (1) - O (1)	2.1510(15)	O (1) - Zn (1) – O (6)	178.71(5)
Zn (1) - O (6)	2.1009(15)	O (1) - Zn (1) - O (8)	86.81(5)
Zn (1) - O (8)	2.1052(12)	O (1) - Zn (1) - N (1)	88.05(5)
Zn (1) – N (1)	2.1041(15)	O (1) - Zn (1) - O (10)b	88.88(5)
Zn (1) - O (10)b	2.1779(15)	O (1) - Zn (1) - O (8)c	91.70(5)
Zn (1) - O (8)c	2.1037(13)	O (6) - Zn (1) - O (8)	94.36(5)
Zn (2) - O (7)	1.9338(14)	O (6) - Zn (1) - N (1)	90.79(5)
Zn (2) - O (8)	1.9425(13)	O (6) - Zn (1) - O (10)b	91.66(5)
Zn (2) - N (2)	2.0212(15)	O (6) - Zn (1) - O (8)c	87.92(5)
Zn (2) - O (9)b	1.9536(14)	O (8) - Zn (1) - N (1)	174.85(5)
O (6) - C (18)	1.246(2)	O (8) - Zn (1) - O (10)b	91.67(5)
O (7) - C (18)	1.2632(19)	O (8) - Zn (1) - O (8)c	81.31(4)

b = 1+x, y, z, c = 1-x,1-y,1-z

Table S4. Comparison table of electrical conductivity values of some reported Zn(II) and Cd(II) based CPs.

Sl No.	**CPs**	**Conductivity (Sm^{-1})**	**Reference**
1.	$[Zn(adc)(4\text{-}nvp)_2(H_2O)_2]_n$	9.29×10^{-4}	[1]
2.	$[Zn_2(BDC)_4(QPR)_2(H_2O)]_n$	8.07×10^{-3}	[2]
3.	$[Zn_4(bdc)_4(ppmh)_2(H_2O)]_n$	1.37×10^{-6}	[3]
4.	$[Zn(cis\text{-}1,4\text{-}chdc)(4\text{-}phpy)]_n$	1.09×10^{-3}	[4]
5.	$[Zn(adc)(4\text{-}spy)_2(H_2O)_2]_n$	5.12×10^{-4}	[5]
6.	$\{[Zn(azbpy)(HO\text{-}1,3\text{-}bdc)(H_2O)]\cdot(azbpy)\}_n$	1.1×10^{-4}	[6]
7.	$\{[Zn_3(H_2MBP)_4(H_2O)_4(SO_4)_3](H_2O)_7\}_n$	5.79×10^{-4}	[7]
8.	$Zn(OPE\text{-}C_{12})\cdot 2H_2O$ (NMOF-1)	9.6×10^{-6}	[8]
9.	$[Zn_2(DABA)_4(4,4'\text{-}BPY)]_n$	2.54×10^{-3}	[9]
10.	$\{[Cd(1,3\text{-}PDAt)(phen)]\cdot(MeOH)\cdot(H_2O)_{0.5}\}_n$,	8.87×10^{-6}	[10]
11.	$[Cd(succ)(pcih)(H_2O)]_n$	3.36×10^{-6}	[11]
12.	$[Cd(glu)_2(pbiq)_2(H_2O)]_n$	1.10×10^{-5}	[12]
13.	$\{[Cd(HAIPA)(tppz)(OH)]\cdot 3H_2O\}_n$	7.42×10^{-5}	[13]
14.	$\{[Cd_2(5\text{-}nip)_2(pdiq)_2(H_2O)_2(CH_3OH)]\cdot H_2O\}_n$	1.12×10^{-3}	[14]
15.	**$[Cd_2(adp)_2(4\text{-}nvp)_4(H_2O)]\cdot(H_2O)_7$**	**2.94×10^{-3}**	**This work**
16.	**$[Zn_2(adp)(4\text{-}nvp)_2(H_2O)(\mu_3\text{-}OH)]\cdot(H_2O)\cdot(NO_3)$**	**3.64×10^{-4}**	**This work**

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