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Electronic Supplementary Information

Synthesis and structural characterization of Cu(II)-based 1D coordination polymer and its application in Schottky device

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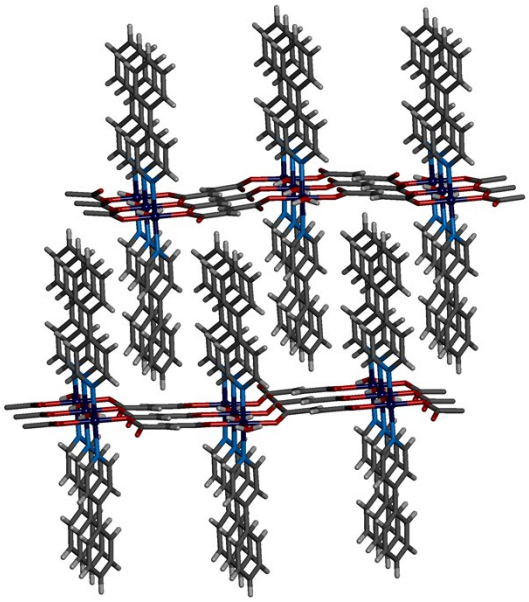

Fig. S1 A view of 3D supramolecular aggregate of compound **1**.

Table S1 Crystal data and refinement parameters for compounds **1**

Formula	$C_{26}H_{22}CuN_2O_5$
Fw	505.99
cryst syst	Orthorhombic
space group	$P2_12_12_1$
a (Å)	5.4915(2)
b (Å)	17.4030(5)
c (Å)	24.2402(7)
α (deg)	90
β (deg)	90
γ (deg)	90
V (Å^3)	2316.60(13)
Z	4
D_{calcd} (g/cm^3)	1.451
μ (mm^{-1})	0.983
λ (Å)	0.71073
data [$I > 2\sigma(I)$]/params	5726/315
GOF on F^2	1.159
final R indices [$I > 2\sigma(I)$][a,b]	R1 = 0.0417
	wR2 = 0.0998

[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**

Cu(1)-O(1)	1.916(2)	Cu(1)-N(1)	2.042(3)
Cu(1)-O(4)a	1.9253(19)	Cu(1)-N(2)	2.039(3)
Cu(1)-O(3)	2.204(3)		
O(1)-Cu(1)-O(3)	89.11(12)	O(1)-Cu(1)-N(1)	89.68(11)
O(1)-Cu(1)-N(2)	90.43(11)	O(1)-Cu(1)-O(4)a	179.32(14)
O(3)-Cu(1)-N(1)	95.96(15)	O(3)-Cu(1)- N(2)	91.35(14)
O(3)-Cu(1)-O(4)a	90.22(12)	N(1)-Cu(1)-N(2)	172.69(15)
N(1)-Cu(1)-O(4)a	90.33(11)	N(2)-Cu(1)-O(4)a	89.64(11)

Symmetry Code: a = 1-x,-1/2+y,3/2-z

Table S3 Intermolecular hydrogen bonding interactions in **1**

D-H···A	D-H (Å)	H···A (Å)	D···A (Å)	<D-H···A (°)	Symmetry
O(3)-H(3A)···O(2)	0.80(5)	1.95(5)	2.693(4)	156(4)	-1+x,y,z
O(3)-H(3B)···O(5)	0.79(5)	1.90(5)	2.683(4)	169(6)	-x,-1/2+y,3/2-z

Table S4 MO composition of compound **1**

	Energy (eV)	H_2O	Cu	Fum	4-PhPy
LUMO+2	-1.95	00	00	00	100
LUMO+1	-2.5	00	89	00	11
LUMO	-2.67	01	38	40	21
HOMO	-5.27	01	04	86	09
HOMO-1	-5.61	12	07	77	04
HOMO-2	-6.06	00	56	44	00
Key Transitions: HOMO-2→LUMO+1					

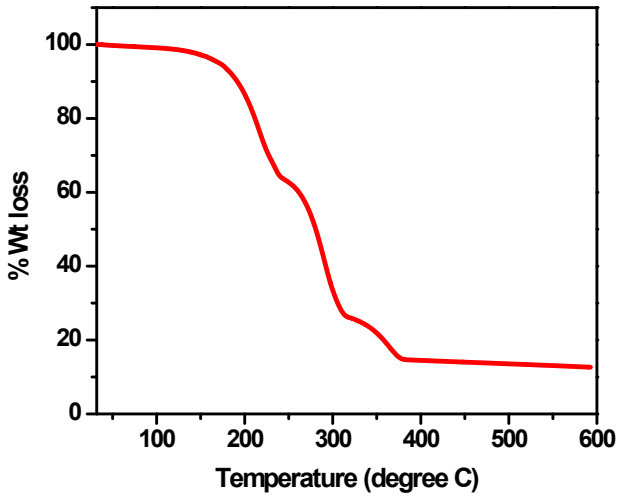

Fig. S2 TGA plots of compounds **1** under N_2 atmosphere.

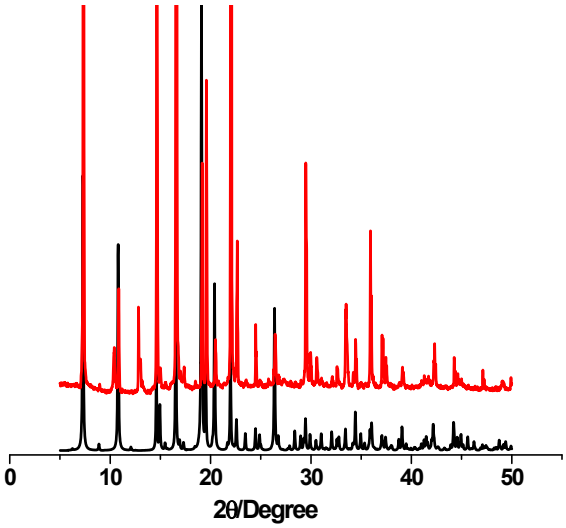

Fig. S3 Powder X-ray diffraction patterns of simulated **1** (black) and as-synthesized **1** (red).

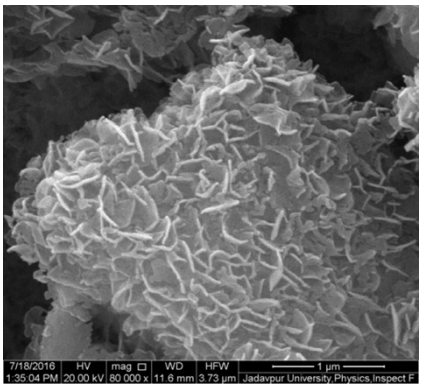

Fig. S4 FESEM image of compound **1**.