Electronic Supplementary Information

Electrically conductive Cu(II)-based 1D coordination polymer with theoretical insight

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

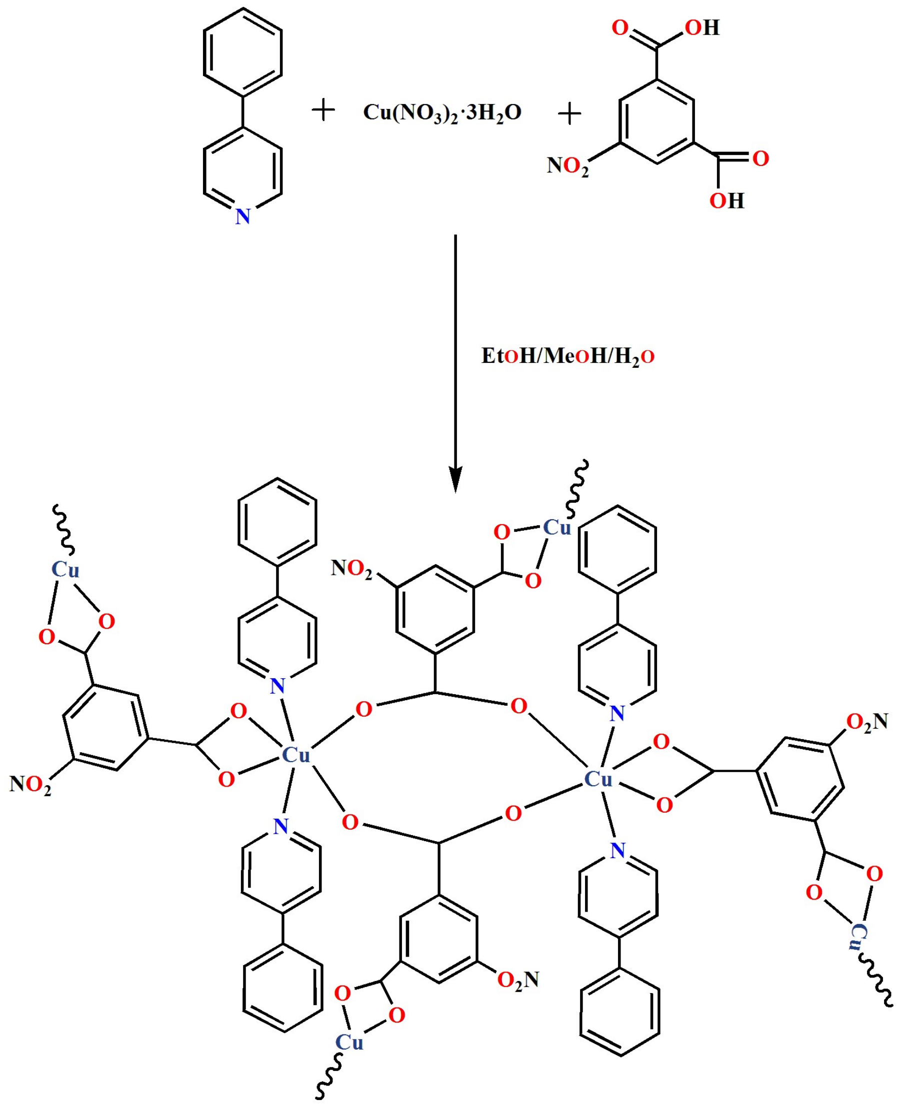
Formula	$C_{30}H_{21}CuN_3O_6$
fw	583.05
cryst syst	monoclinic
space group	*P 2/c'*
a (Å)	25.8018
b (Å)	10.0911(3)
c (Å)	20.3821(7)
α(deg)	90
β(deg)	92.472(2)
γ (deg)	90
V ($Å^3$)	5301.9(3)
Z	8
D_{calcd}(g/cm^3)	1.461
μ(mm^{-1})	0.874
λ(Å)	0.71073
GOF on F^2	1.061
final *R* indices $[I > 2\sigma(I)]^{a,b}$	$R1 = 0.0467$ $wR2 = 0.1133$

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

Table S2 Selected bond lengths and bond angles of the Compound 1

Cu(1)-O(1)	1.951(3)	N(1)-Cu(1)-N(2)	173.30(15)
Cu(1)-O(4)a	2.710(3)	N(1)-Cu(1)-O(2)c	89.96(13)
Cu(1)-N(1)	2.033(3)	N(2) -Cu(1)-O(2)c	96.60(13)
Cu(1)-O(2)c	2.268(3)	O(4)a-Cu(1)-O(2)c	141.56(11)
Cu(1)-N(2)	2.012(3)	O(3)a-Cu(1)-O(4)a	53.72(12)
Cu(1)-O(3)a	1.981(3)	O(1)-Cu(1)-N(2)	89.35(16)
O(1)-Cu(1)-N(1)	86.99(16)	O(1)-Cu(1)-O(2)c	111.29(13)
O(1)-Cu(1)-O(4)a	105.73(13)	N(1)-Cu(1)-O(4)a	81.84(13)
N(1)-Cu(1)-O(3)a	88.37(16)	N(2)-Cu(1)-O(4)a	93.77(13)
N(2)-Cu(1)-O(3)a	93.12(16)	O(3)a -Cu(1)-O(2)c	88.75(13)
O(1)-Cu(1)-O(3)a	159.41(15)		

Symmetry transformations used to generate equivalent atoms: a = -1+x,y,z ; c= 1-x,-1-y,1-z



Scheme S1. Synthetic route to compound **1**.

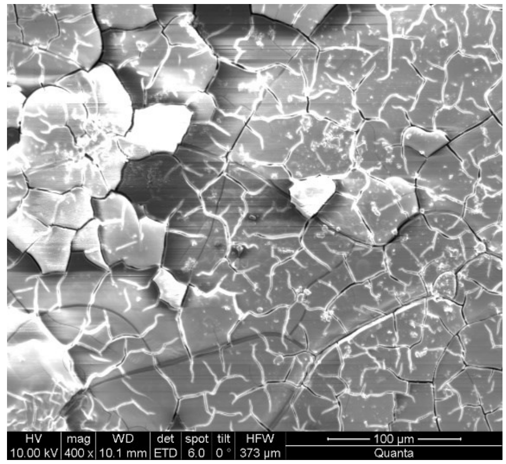


Fig. S1 FESEM image of the film of **1**.

Morphology

Morphology of the film is given in Fig S1. From the image it is clear that the major portion of the film surface is smooth and continuous and good coverage is seen. However, there were some places with agglomeration and cracks which can degrade the device performance to some extent.

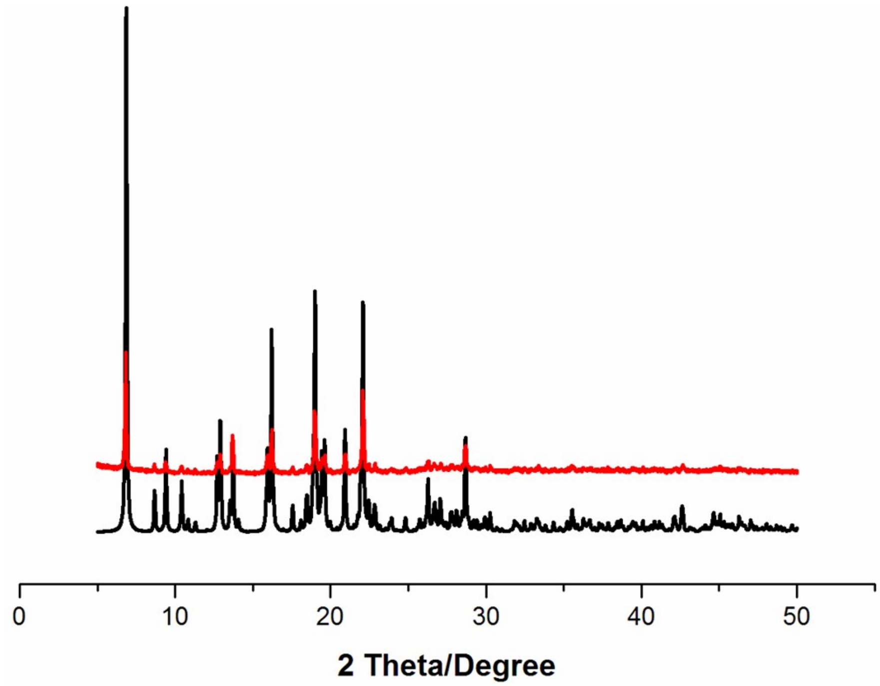


Fig. S2 Powder X-ray diffraction patterns of simulated **1** (Black) and as-synthesized **1** (Red).

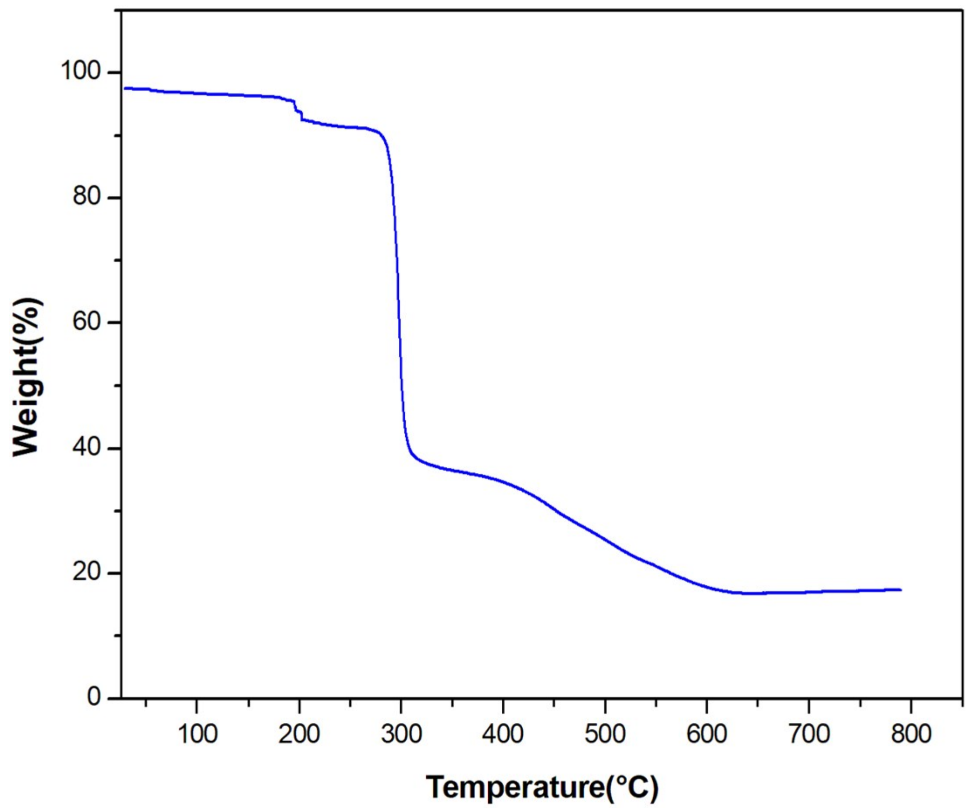


Fig. S3 TGA plot of compound **1** measured under N_2 atmosphere.

Device fabrication:

At first an indium tin oxide (ITO) coated glass substrate was properly cleaned with acetone, ethanol and distilled water sequentially using an ultrasonicator. Then the substrate was dried in N_2 atmosphere. To get a well dispersed homogeneous medium of the synthesized material, it was poured into dimethyl sulfoxide (DMSO) solvent, followed by ultrasonication. Later to prepare the film of synthesized material, the dispersion was spin-coated on pre-cleaned ITO coated glass substrate and followed by a dry in a vacuum chamber. The thickness of film (d) was measured ~1µm with a surface profiler. Finally vacuum coating unit 12A4D (HINDHIVAC) was used to deposit aluminum metal onto the film at a base pressure of 10^{-6} Torr. With the help of a shadow mask the effective diode area (A) was maintained as 7.065×10^{-6} m^2.

Electrical Characterization:

According to thermionic emission theory, J can be expressed as[1]

$$J = J_0\,[exp\left(\frac{qV}{nkT}\right) - 1] \tag{1}$$

where J_0 is the saturation current density, q is the electronic charge, V is the voltage across the diode, n is the ideality factor, k is the Boltzmann constant and T is the absolute temperature. The saturation current density J_0 can be expressed as:[1]

$$J_0 = AA^{*}T^2 exp\left(\frac{-q\varnothing_b}{kT}\right) \tag{2}$$

where A is the effective diode area, A* is the effective Richardson constant and $\varnothing_b$ is the barrier height. Here, the effective diode area was taken as 7.065 $\times 10^{-6}$ m^2. The effective Richardson constant was considered as 1.201 $\times 10^6$ $AK^{-2}m^{-2}$.

At low bias voltage, linear nature of current was observed. The ideality factor (n), barrier height and series resistance (R_s) for Schottky device were derived from the linear region using Cheung's equation. When a resistance is connected serially across a diode, then the voltage of the diode is substituted by the voltage drop across the series combination of diode and resistor. So, equation (1) can be written as[2],

$$J = J_0 exp[\frac{q(V - IR_s)}{nkT}] \tag{3}$$

where IR_s is the voltage drop across the series resistance of the device.

From equation (2) and equation (3), we get

$$V = R_sAJ + n\varnothing_b + \left(\frac{nkT}{q}\right)ln\left(\frac{J}{A^{*}T^2}\right) \tag{4}$$

Differentiating equation (4) with respect to lnJ, we get[2]

$$\frac{dV}{dln(J)} = \frac{nkT}{q} + JAR_s$$

Dielectric Constant measurement:

The relative dielectric constants for compound derived from capacitance versus logarithm of frequency graph at a constant bias voltage (Fig. S4). To determine the value of relative dielectric constants of synthesized material films the saturated capacitance value was put into the following equation[3]

$$\varepsilon_r = \frac{1}{\varepsilon_0} . \frac{C.d}{A} \quad (5)$$

Where C is the capacitance at saturation, d is the thickness of the film, ε_0 is the free space permittivity and A is the effective area.

From the above formula the relative dielectric constant of the compound was obtained 0.5.

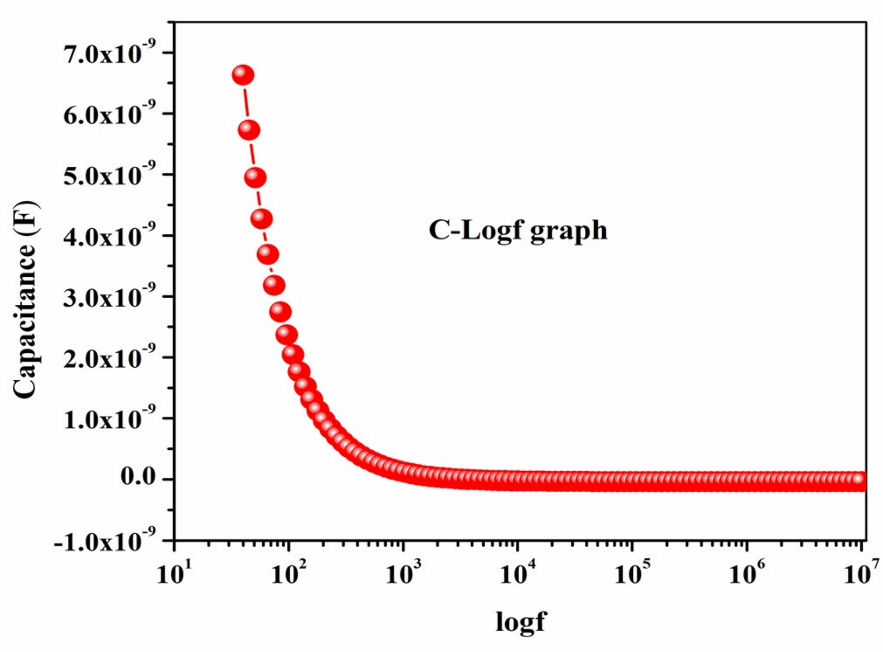


Fig. S4 Capacitance versus logarithm of frequency graph.

References:

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2. J. Datta, M. Das, S. Sil, S. Kumar, A. Dey, R. Jana, S. Bandyopadhyay and P. P. Ray, *Mater. Sci. Semicond. Process.*, 2019, **91**, 133-145.
3. J. Datta, A. Dey, S. K. Neogi, M. Das, S. Middya, R. Jana and P. P. Ray, *IEEE Trans. Electron Devices* 2017, **64**, 4724−4730.