Electronic supplementary information

Multifunctional mixed ligand metal organic frameworks: X-ray structure, adsorption, luminescence and electrical conductivity with theoretical correlation

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Tables related to X-ray structure:

Table S1 Selected bond Lengths (Å) and bond angles (°) for **1**.

Zn1 -O1	2.564(2)	Zn1-O1W	2.056(2)
Zn1 -O2	2.013(2)	Zn1-N1	2.202(2)
Zn1-O4^{a}	1.994(2)	Zn1-N4^{b}	2.215(2)
O1-Zn1-O1W	88.16(7)	O1-Zn1-O2	55.76(7)
O1-Zn1-N1	88.57(7)	O1-Zn1-N4^{b}	92.40(9)
O1-Zn1-O4^{a}	165.40(7)	O1W-Zn1-O2	143.67(8)
O1W-Zn1-N1	90.31(7)	O1W-Zn1-N4^{b}	87.91(7)
O1W-Zn1-O4^{a}	106.42(8)	O2-Zn1-N1	92.61(8)
O2-Zn1-N4^{b}	89.44(9)	O2-Zn1-O4^{a}	109.76(8)
N1-Zn1-N4^{b}	177.94(9)	O4^{a}-Zn1-N1	90.40(7)
O4^{a}-Zn1-N4^{b}	89.12(9)		

Symmetry code: *a* =1+x, y, z; *b* = x, y, -1+z.

Table S2 π-π interactions in **1**, **2** and C-H... π interaction in **1**.

	Ring(i) → Ring(j)	Distance of centroid(i) from ring(j),(Å)	Dihedral angle (i,j) (deg)	Distance between the (i,j) ring centroids,(Å)
1	R(1) → R(5)^{i}	3.889(3)	0.8(2)	3.542(2)
	R(2) → R(4)^{ii}	3.873(3)	2.2(2)	3.5408(19)
	R(3) → R(3)^{iii}	3.874(2)	0	3.5626(9)
	R(4) → R(2)^{ii}	3.873(3)	2.2(2)	3.5744(19)
	R(4) → R(4)^{iv}	3.639(3)	0	3.5238(19)
	R(5) → R(1)^{i}	3.889(3)	0.8(2)	3.5481(12)
2	R(1) → R(6)^{v}	3.8375(19)	14.14(16)	3.5213(14)
	R(6) → R(1)^{v}	3.8374(19)	14.14(16)	3.5408(11)

	C-H→ ring(j)	H...R distance (Å)	C-H...R angle (deg)	C...R distance (Å)
1	C(15) –H(15) → R(1)^{iii}	2.80	162	3.700(3)

Symmetry code: i = 1-x, -y, 2-z; ii = x, y, z; iii = -x, 1-y, 1-z; iv = -x, 1-y, 2-z; v = 1-x, 1-y, 1-z.

R(i)/R(j) denotes the ith/jth rings: R(1) = N(1)/C(1)/C(2)/C(3)/C(4)/C(5); R(2) = N(4)/C(6)/C(7)/C(8)/C(9)/C(10); R(3) = C(12)/C(13)/C(14)/C(15)/C(16)/C(18); R(4) = N(5)/C(19)/C(20)/C(21)/C(22)/C(23); R(5) = N(8)/C(24)/C(25)/C(26)/C(27)/C(28); R(6) = C(7)/C(8)/C(9)/C(10)/C(11)/C(13).

Table S3 Hydrogen bonding interactions (Å, °) of **1** and **2**.

	D-H···A	D-H	H···A	D···A	<D-H···A
1	O1W- H1WA···O1^{i}	0.8500	2.0100	2.769(3)	148.00
	O5- H5···N8^{ii}	0.8200	1.9300	2.732(5)	165.00
2	O5−H5A···O1W^{iii}	0.8200	1.9600	2.746(6)	162.00
	O1W−H2WB···O2	0.8500	1.9200	2.649(5)	144.00

Symmetry code: i = 1-x, -y, 1-z; ii = x, 1+y, -1+z; iii = 1-x, 2-y, 2-z.

Table S4 Selected Bond Lengths (Å) and Bond Angles (°) for **2**.

Zn1-O1	1.9460(18)	Zn1 -O1S	2.079(3)
Zn1-N1	2.035(2)	Zn1 -O4^{a}	1.9522(18)
Zn1-O4^{b}	2.5723(19)		
O1-Zn1-O1S	97.87(9)	O1-Zn1-N1	102.39(9)
O1-Zn1-O4^{a}	125.35(8)	O1-Zn1-O4^{b}	84.23(7)
O1S-Zn1-N1	92.54(10)	O1S-Zn1-O4^{a}	100.81(9)
O1S-Zn1-O4^{b}	176.64(8)	O4^{a}-Zn1-N1	127.27(9)
O4^{b}-Zn1-N1	84.44(9)	O4^{a}-Zn1-O4^{b}	79.96(7)

Symmetry Code: *a* = 1+x, 1+y, z; *b* = -x, 1-y, 1-z.

Figures related to single crystal X-ray structure and the characterization of 1 and 2:

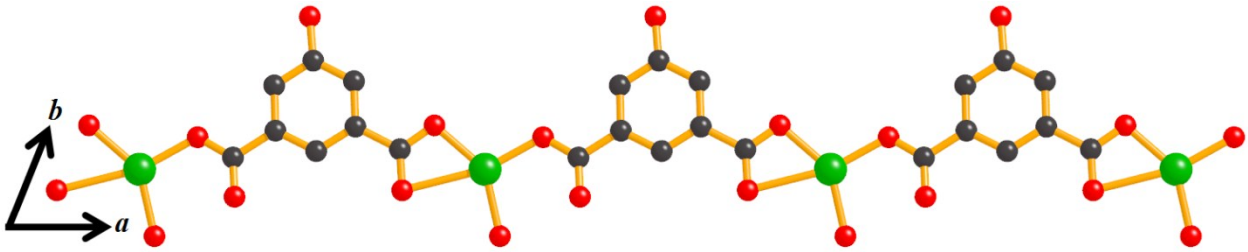


Fig. S1 View of $[Zn(HO\text{-}1,3\text{-}bdc)]_n$ one-dimensional (1D) chains in **1** (azbpy has been omitted for clarity).

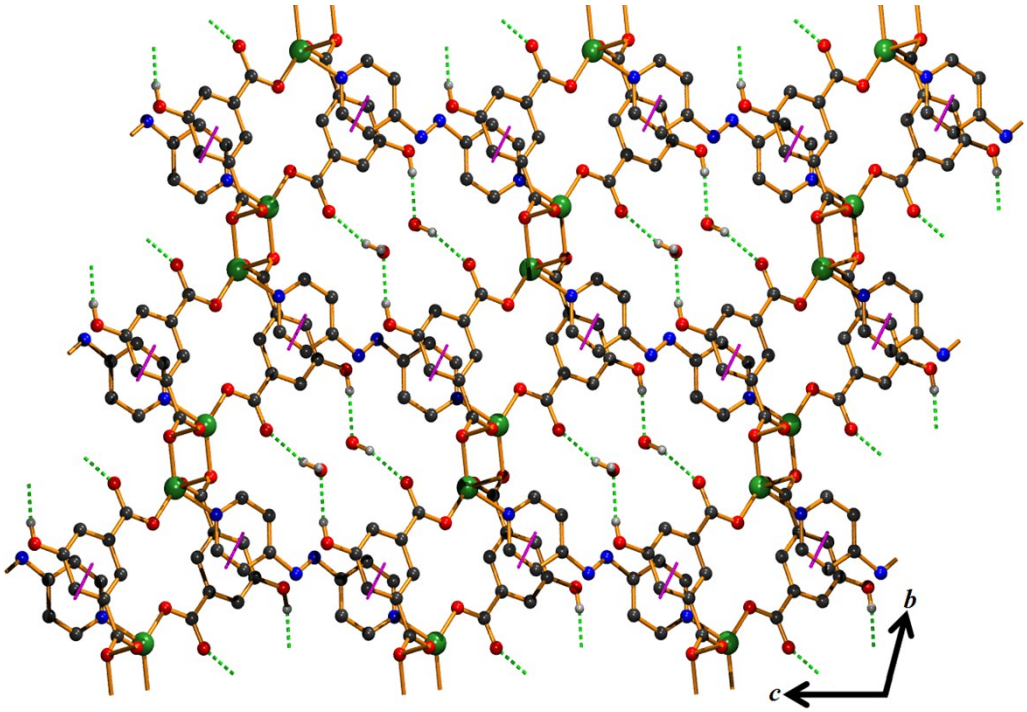


Fig. S2 Supramolecular 3D arrangement in **2** by locking the 2D sheets by H-bonding and π–π interaction (π–π interaction: pink dotted lines & H-bonding: green dotted lines).

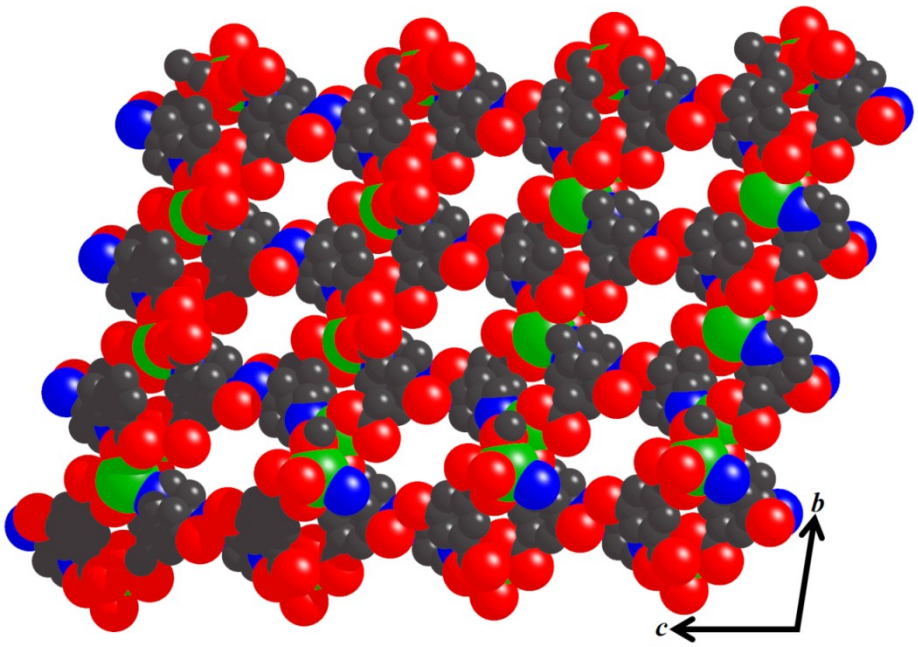


Fig. S3 Packing diagram of **2** in space fill model (view down *a* axis). Coordinated ethanol and guest water molecules have been removed for clarity.

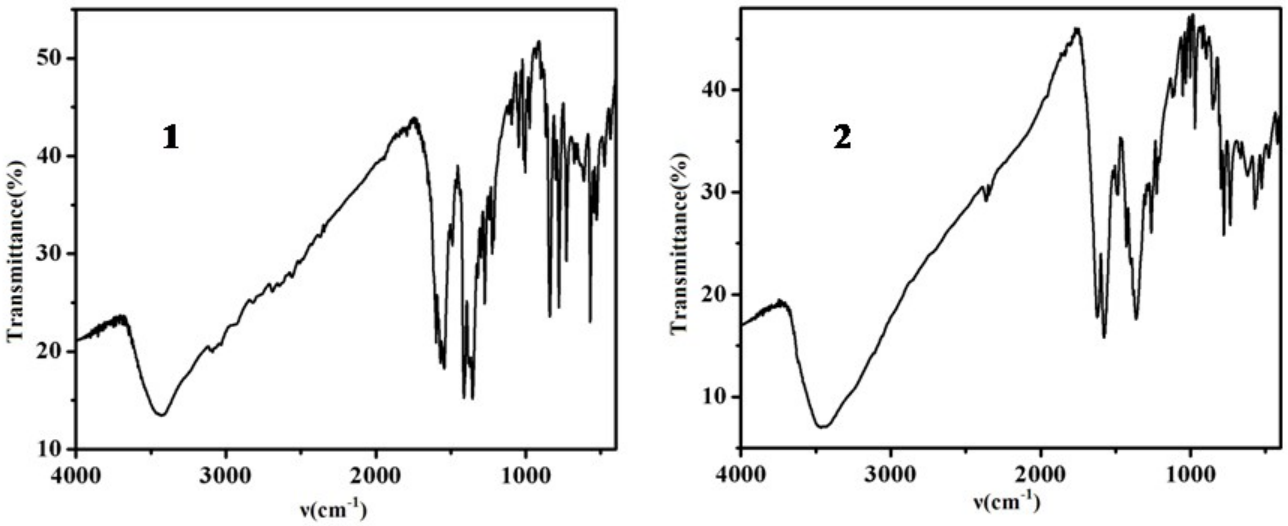


Fig. S4 FT-IR spectra of **1** and **2**.

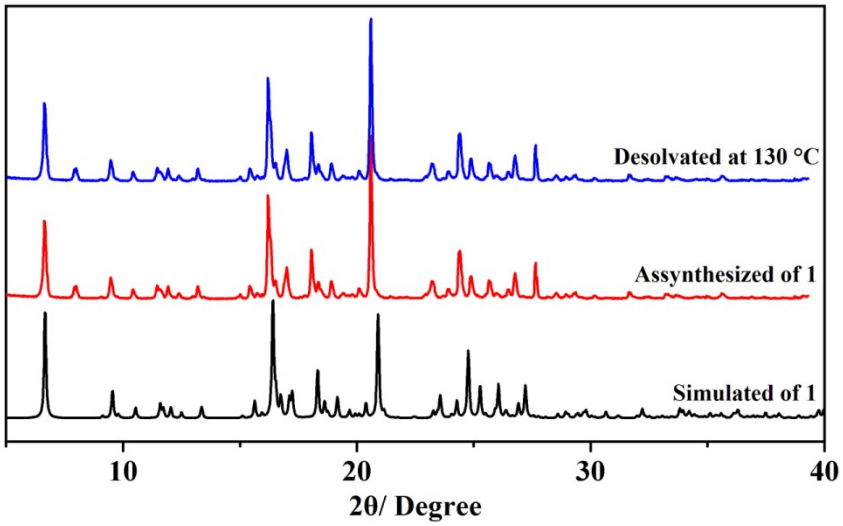


Fig. S5 Powder X-ray diffraction patterns of compound **1** in different state.

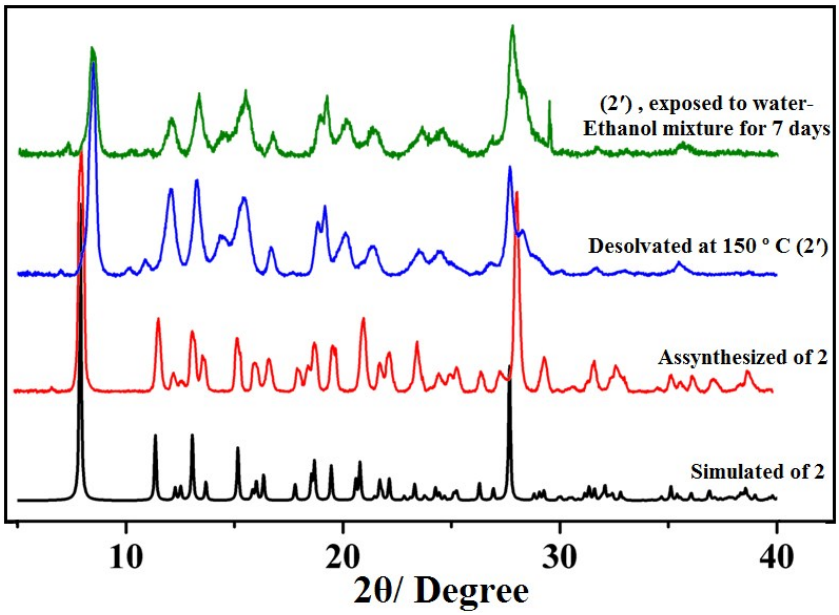


Fig. S6 Powder X-ray diffraction patterns of compound **2** in different state.

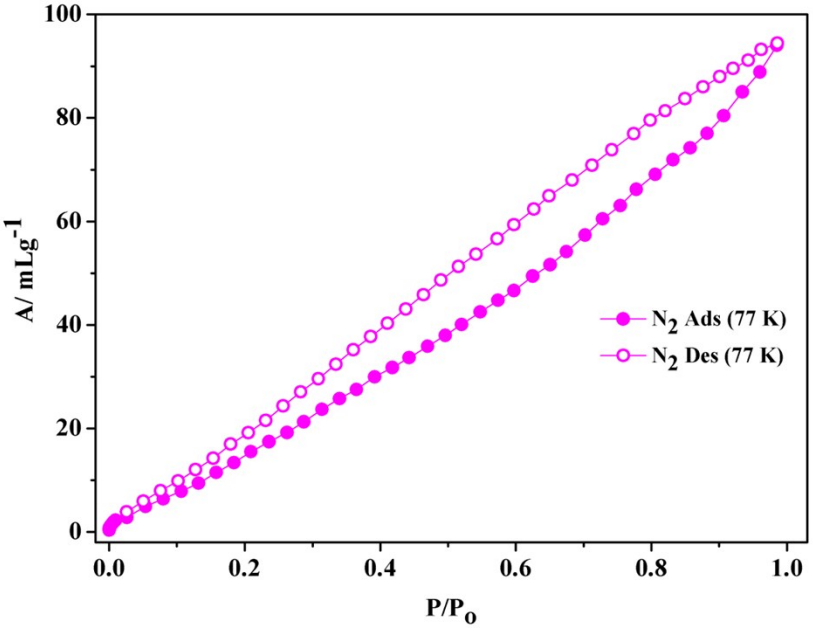


Fig. S7 N_2 adsorption isotherms of **2′** measured at 77 K. Filled and open circles represent adsorption and desorption respectively.

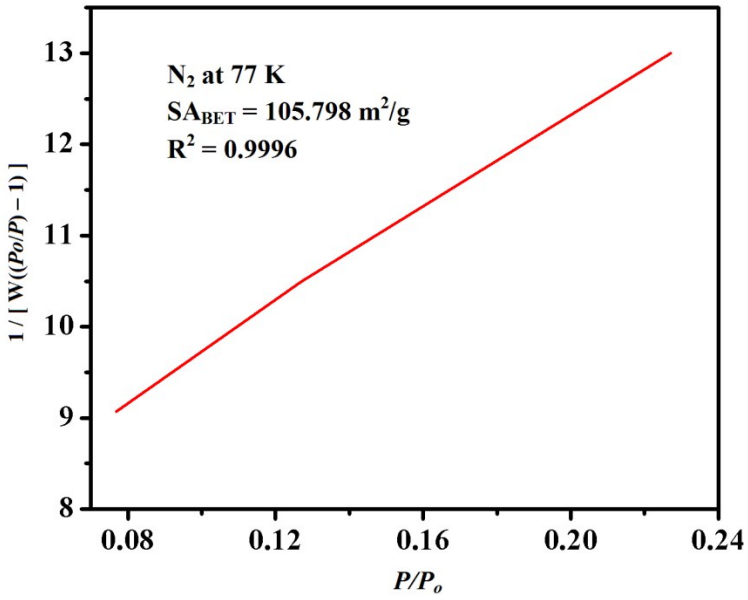


Fig. S8 BET plots for **2′** calculated from the N_2 adsorption isotherm at 77 K. The model was applied from *P/Po* = 0.08-0.24. The correlation factor is indicated. (W = Weight of gas absorbed at a relative pressure *P/Po*).

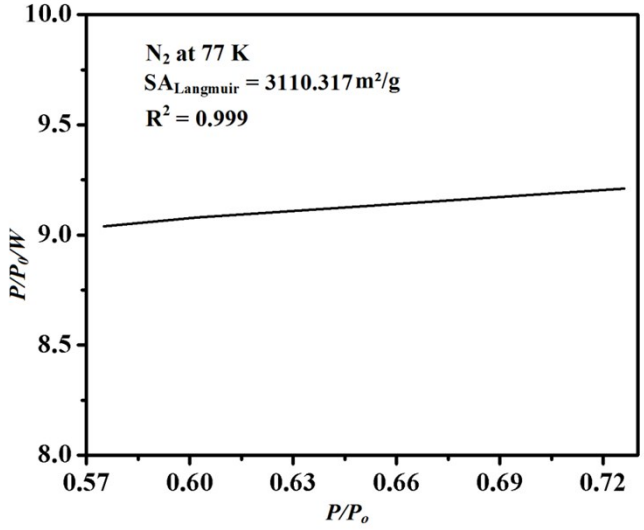


Fig. S9 Langmuir plots for **2′** calculated from the N_2 adsorption isotherm at 77 K. The model was applied from *P/Po* = 0.57-0.73. The correlation factor is indicated. (W = Weight of gas absorbed at a relative pressure *P/Po*).

UV-Vis spectral studies and band gap:

The optical band gap of **1** and **2** were calculated from UV-vis absorption spectrum using Tauc's equation:

$$\alpha = \frac{A\left(h\gamma - E_g\right)^{1/2}}{h\gamma}$$

Where 'α' is the absorption coefficient, 'E_g' is the band gap, and 'A' is a constant. The direct band gap of **1** and **2** were obtained as 2.89 eV and 2.92 eV respectively by extrapolating the linear region near the onset in a plot of $(\alpha h\gamma)^2$ versus hγ (Fig. S10(a) and S10(b)).

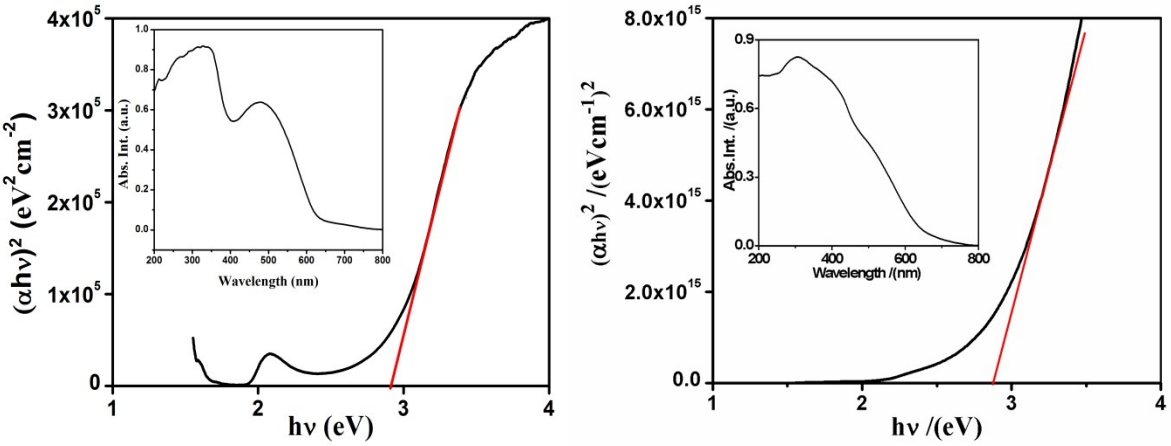
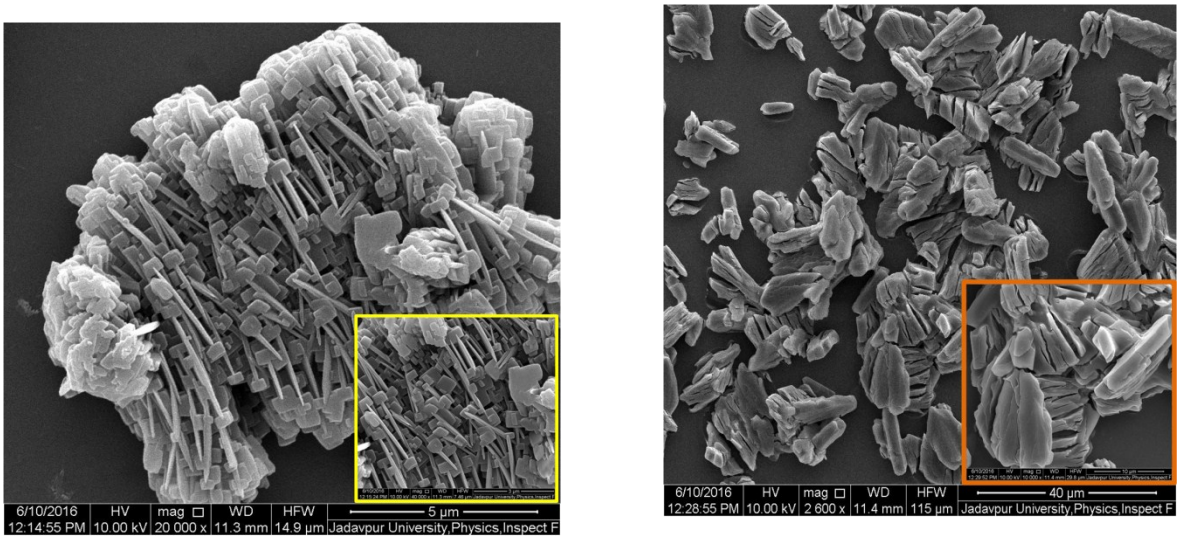


Fig. S10 (a) and (b) UV-vis absorption spectra and Tauc's plots of **1** and **2** respectively.



(a) **(b)**

Fig. S11 FESEM images along with their corresponding higher resolution images of compound (a) **1** and (b) **2** respectively.