Electronic Supplementary Information

Semiconducting properties of pyridyl appended linear dicarboxylate based coordination polymers: theoretical prediction via DFT study

Faruk Ahmed,[a,b] Joaquín Ortega-Castro,[c] Antonio Frontera*[c] and Mohammad Hedayetullah Mir*[a].

a. Department of Chemistry, Aliah University, New Town, Kolkata 700 156, India.

Email: chmmir@gmail.com

b. Department of Chemistry, Saheed Nurul Islam Mahavidyalaya, Tentulia, West Bengal 743 286, India.

c. Departament de Química, Universitat de les Illes Balears, Crta. de Valldemossa km 7.5, 07122 Palma de Mallorca, Baleares, Spain. E-mail: toni.frontera@uib.es

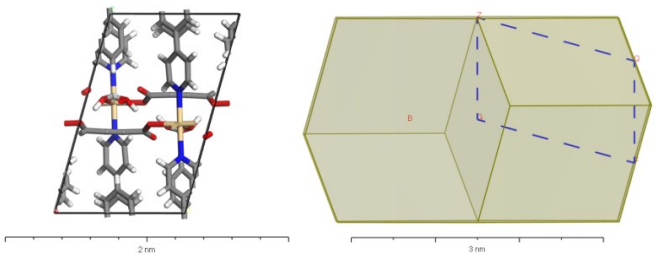
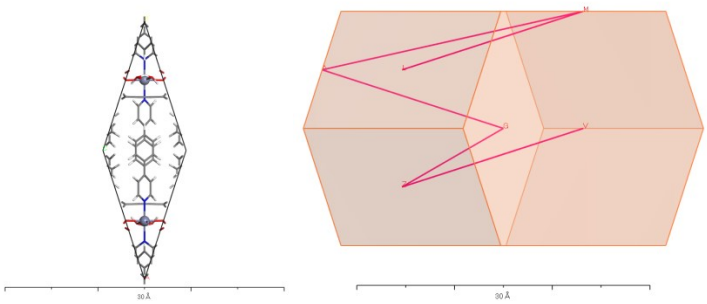
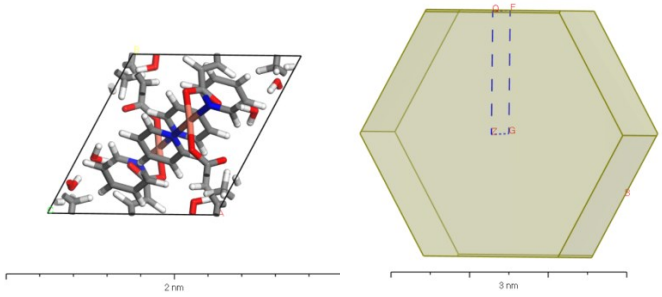
Compound **1**	
Compound **2**	
Compound **3**	

Fig. S1 Unit Cells of the polymers studied theoretically in this work. On the right, the used brillouin zones are shown, as well as the special k-points represented in the band diagram.

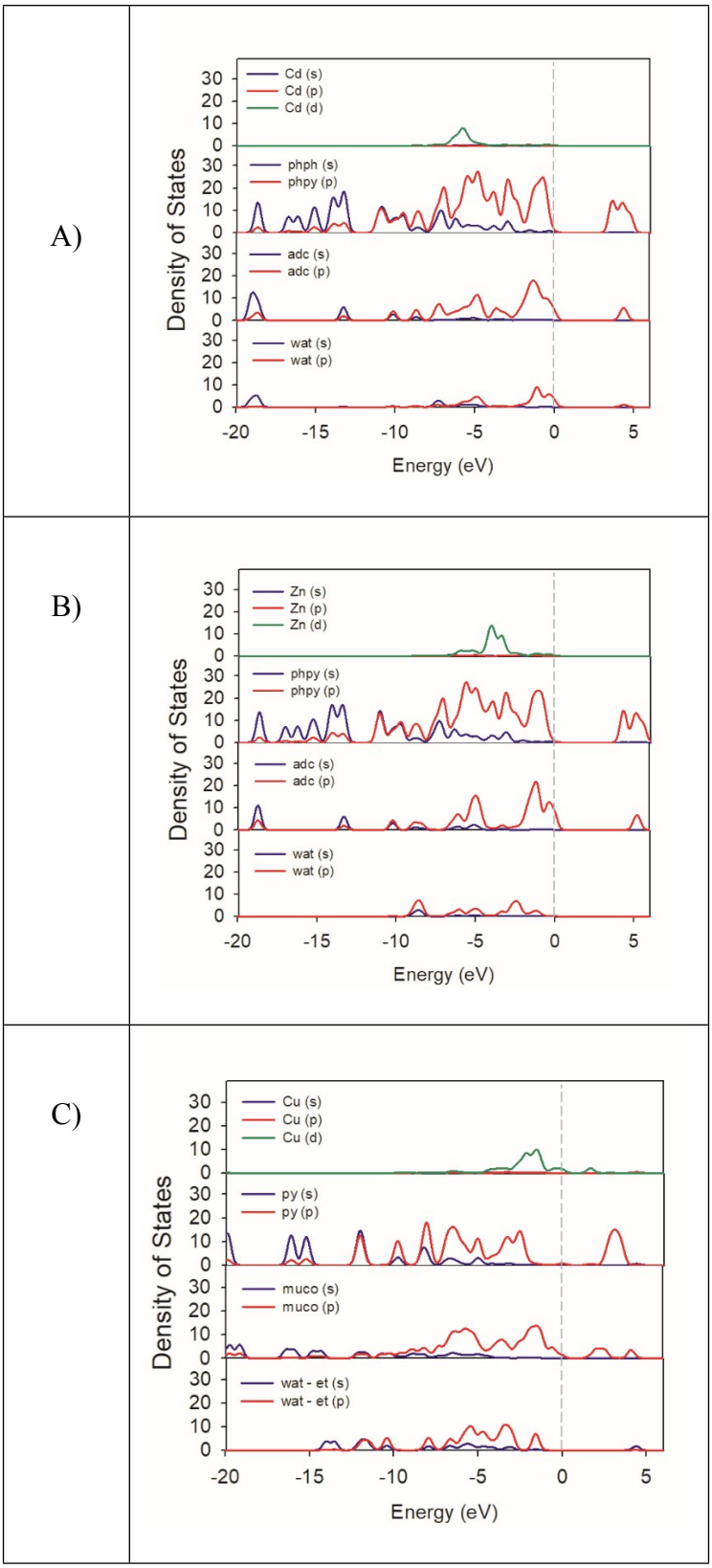
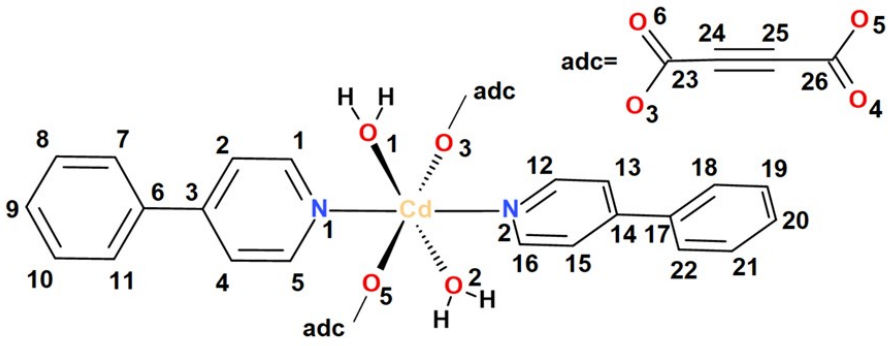


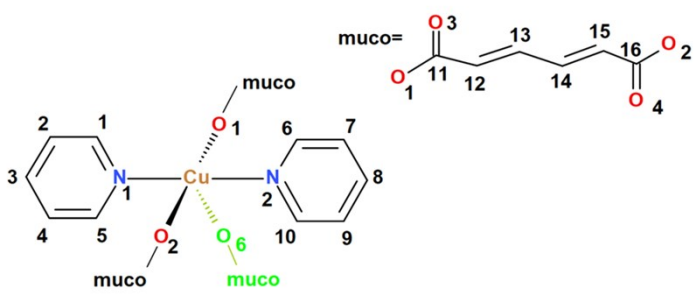
Fig. S2 Completed PDOS of the CPs calculated in this work; A) compound **1**, B) compound **2**, C) compound **3**.

Table S1. Geometric measurements (bond length (Å), bond angles (°) and dihedral angles (°)) of the ground state, 1st and 2nd excited states of compound **1**.



4-Phpy	GS	1st	2nd	Adc	GS	1st	2nd
Cd-N1	2.34	2.34	2.34	O3-C23	1.29	1.28	1.28
Cd-N2	2.33	2.33	2.37	O6-C23	1.26	1.25	1.25
Cd-O1	2.35	2.36	2.35	C23-C24	1.45	1.46	1.46
Cd-O2	2.36	2.35	2.35	C24-C25	1.22	1.21	1.21
Cd-O3	2.33	2.33	2.33	C25-C26	1.45	1.46	1.46
Cd-O5	2.32	2.32	2.32	O4-C26	1.26	1.25	1.25
N1-C1	1.35	1.36	1.36	O5-C26	1.29	1.28	1.28
C1-C2	1.39	1.39	1.39				
C2-C3	1.41	1.41	1.41	O1-Cd-O3	89.9	85.9	86.0
C3-C4	1.40	1.41	1.41	O3-Cd-O2	90.9	91.6	91.5
C4-C5	1.38	1.39	1.39	O2-Cd-O5	92.5	96.2	86.7
C5-N1	1.35	1.36	1.36	O5-Cd-O1	87.7	86.9	96.5
C3-C6	1.47	1.48	1.48	N1-Cd-O3	97.0	97.5	97.8
C6-C7	1.41	1.41	1.41	N2-Cd-O3	80.0	81.7	98.9
C7-C8	1.39	1.40	1.40	C2-C3-C6-C7	16.6	19.5	19.5
C8-C9	1.40	1.40	1.40	C13-C14-C17-C18	18.8	10.0	9.2
C9-C10	1.39	1.40	1.40				
C10-C11	1.39	1.40	1.40				
C11-C6	1.41	1.41	1.41				
N2-C12	1.35	1.36	1.36				
C12-C13	1.39	1.36	1.38				
C13-C14	1.40	1.38	1.43				
C14-C15	1.40	1.43	1.43				
C15-C16	1.38	1.43	1.38				
C16-N2	1.35	1.38	1.36				
C14-C17	1.47	1.44	1.44				
C17-C18	1.40	1.43	1.44				
C18-C19	1.39	1.38	1.38				
C19-C20	1.40	1.41	1.41				
C20-C21	1.40	1.41	1.41				
C21-C22	1.39	1.38	1.38				
C22-C17	1.40	1.43	1.44				

Table S2. Geometric measurements (bond length (Å) and bond angles (°)) of the ground state, 1st and 2nd excited states of compound **3**.



Py	GS	1st	2nd	Muco	GS	1st	2nd
Cu-N1	2.07	2.12	2.11	O1-C11	1.29	1.28	1.30
Cu-N2	2.06	2.12	2.11	O3-C11	1.26	1.27	1.26
Cu-O1	1.99	2.06	2.04	C11-C12	1.47	1.47	1.47
Cu-O2	2.01	2.06	2.08	C12-C13	1.35	1.35	1.35
Cu-O6		2.22	2.23	C13-C14	1.43	1.43	1.43
N1-C1	1.35	1.35	1.35	C14-C15	1.35	1.35	1.35
C1-C2	1.39	1.39	1.39	C15-C16	1.47	1.47	1.47
C2-C3	1.39	1.40	1.40	O2-C16	1.29	1.28	1.30
C3-C4	1.40	1.40	1.40	O4-C16	1.26	1.27	1.26
C4-C5	1.39	1.39	1.39				
C5-N1	1.35	1.35	1.35	N1-Cu-O1	89.8	90.0	89.4
N2-C6	1.35	1.35	1.35	N1-Cu-O2	90.7	91.6	91.7
C6-C7	1.39	1.39	1.39	N2-Cu-O2	88.1	87.6	87.3
C7-C8	1.40	1.40	1.39	N2-Cu-O2	91.7	91.8	92.4
C8-C9	1.40	1.40	1.40				
C9-C10	1.39	1.39	1.39				
C10-N2	1.35	1.35	1.35				

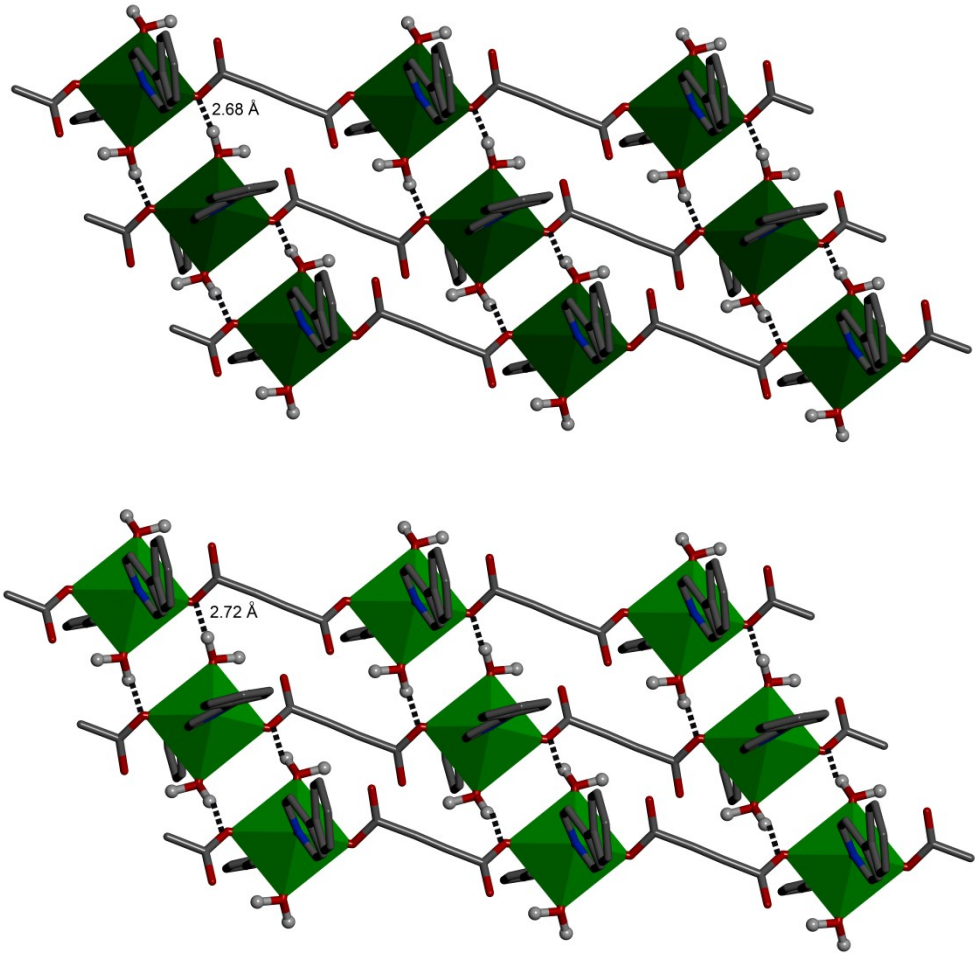


Fig. S3 View of hydrogen bonding interactions in **1** (top) and **2** (bottom) forming 2D networks.