

Electric Supplemental Information for:

Self-assembly of polyoxometalate-based hybrid aggregates: from monomer to dimer by changing pH value of reaction systems

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Table S1. The BVS for the W and Cu atoms in compounds **1-3**.

Compounds	Atoms	BVS	Oxidation states
1	Cu1	1.89	II
	W1	5.76	VI
	W2	5.81	VI
	W3	5.92	VI
	W4	5.93	VI
	W5	5.87	VI
	W6	5.83	VI
	W7	5.77	VI
	W8	5.72	VI
	W9	5.79	VI
	W10	5.83	VI
	W11	5.86	VI
	W12	5.69	VI
	W13	5.71	VI
	W14	5.83	VI
	W15	5.77	VI
	W16	5.86	VI
	W17	5.78	VI
2	Cu1	1.74	II
	W1	5.86	VI
	W2	5.71	VI
	W3	5.82	VI
	W4	5.83	VI
	W5	5.77	VI
	W6	5.81	VI
	W7	5.83	VI
	W8	5.77	VI
	W9	5.72	VI
	W10	5.85	VI
	W11	5.76	VI
	W12	5.89	VI
	W13	5.81	VI
	W14	5.81	VI
	W15	5.87	VI
	W16	5.76	VI
	W17	5.89	VI
W18	5.87	VI	
3	Cu1	1.86	II
	W1	5.76	VI
	W2	5.82	VI

W3	5.86	VI
W4	5.73	VI
W5	5.87	VI
W6	5.71	VI
W7	5.73	VI
W8	5.69	VI
W9	5.77	VI
W10	5.87	VI
W11	5.77	VI
W12	5.79	VI
W13	5.71	VI
W14	5.83	VI
W15	5.77	VI
W16	5.79	VI
W17	5.83	VI
W18	5.81	VI

Table S2. The IR stretching frequencies of compounds 1–3.

Compounds	Stretching frequencies of POM (cm ⁻¹)	Stretching frequencies of bimb ligand (cm ⁻¹)
1	1045, 936, 871, 778	1638, 1534, 1275, 1198, 1151
2	1046, 937, 873, 780	1632, 1535, 1268, 1205, 1155
3	1047, 938, 875, 776	1629, 1531, 1271, 1211, 1157

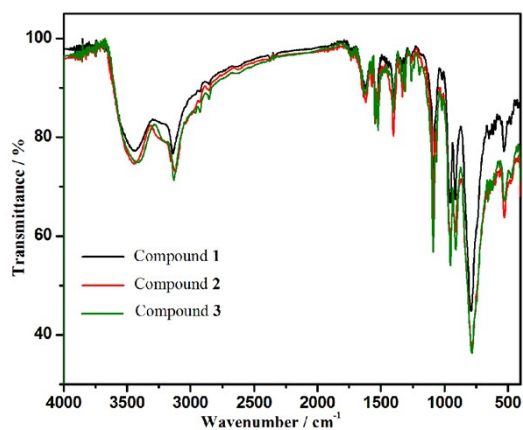


Fig. S1 The IR spectra of compounds 1-3.

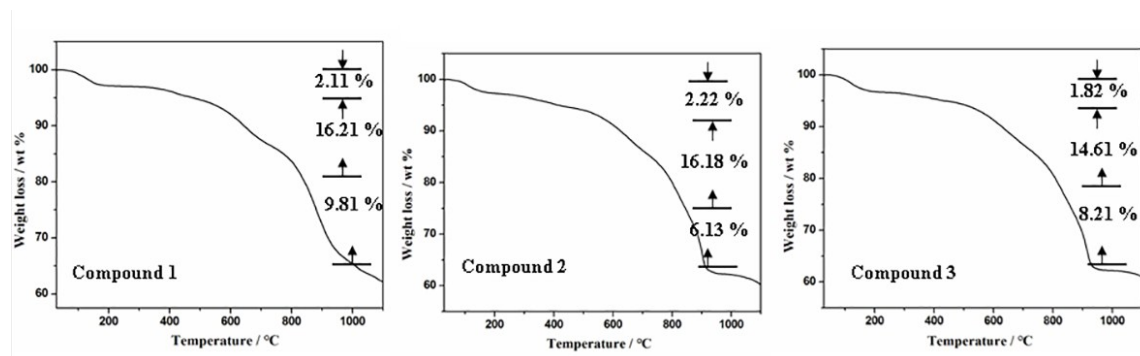


Fig. S2 The TG curves of compounds 1-3.

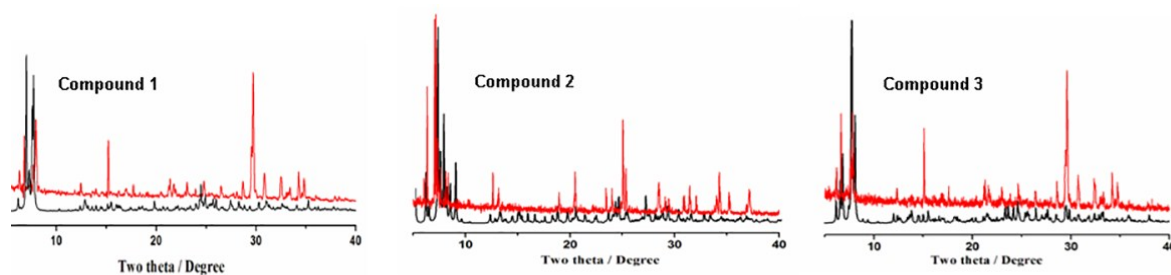


Fig. S3 The simulative (black) and experimental (red) powder X-ray diffraction patterns for compounds 1-3.

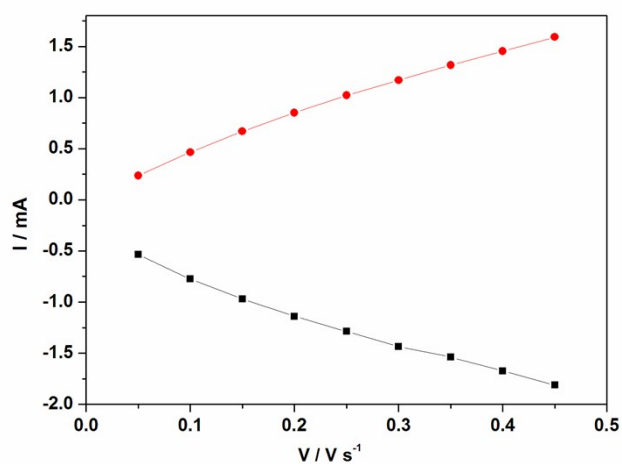


Fig. S4 The plots of the anodic and the cathodic peak currents for wave III of 1-CPE against scan rates.

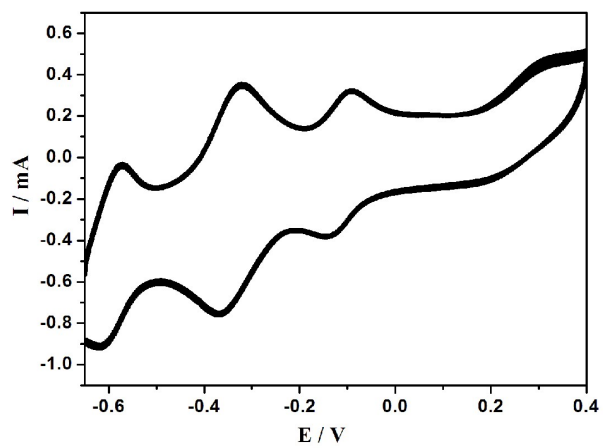


Fig. S5 The 100 consecutive CV cycles of the **1-CPE** at the scan rate of $0.1 \text{ V} \cdot \text{s}^{-1}$.