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Five POM-based compounds modified by mono- and bis-triazole derivatives: photocatalytic, electrochemical and supercapacitor properties

Xi Xu, Yanping Zhang, Jun Ying*, Liang Jin, Aixiang Tian, Xiuli Wang*

Table S1. Selected bond lengths (Å) and angles (°) of compounds **1–5.**

Compound **1**

Ni(1) – O(1)	2.0215(16)	Ni(1) – N(1)	2.0454(19)
Ni(1) – O(7)^{2}	2.0732(16)	Ni(1) – N(2)	1.388(3)
O(1) – Ni(1) –O3W	88.76(7)	N(1) – Ni(1) – O(7)^{2}	90.49(7)
O1W – Ni(1) – O(7)^{2}	87.59(7)	O(1) – Ni(1) – O(7)^{2}	92.93(7)
O(1) – Ni(1) – O2W	174.58(7)	O(1) – Ni(1) – N(1)	93.17(8)

Symmetry codes: #1 1-X, -Y,1-Z #2 1-X, 1-Y, 1-Z

Compound **2**

Zn(1) – O3W	2.1862(17)	Zn(1) – O(12)	2.0815(17)
Zn(1) – N(1)	2.087(2)	Zn(1) – O(5)^{2}	2.1390(16)
O(12) – Zn(1) – O3W	87.67(7)	O(12) – Zn(1) – O(5)^{2}	94.10(7)
O2W – Zn(1) – N(1)	175.18(8)	O(12) – Zn(1) – N(1)	93.13(8)
N(1) – Zn(1) – O3W	85.30(8)	N(15) – Zn(1) – O(5)^{2}	89.92(7)

Symmetry codes: #1 1-X, 2-Y,1-Z #2 1-X, 1-Y, 1-Z

Compound **3**

Co(1) – O(12)	2.089(3)	Co(1) – O1W^{2}	2.070(3)
Co(1) – N(1)	2.095(3)	Co(1) – N(1)^{2}	2.095(3)
O1W – Co(1) – O1W^{2}	180.00	O(12)^{2} – Co(1) – N(1)	80.10(12)
O(12) – Co(1) – N(1)	99.90(12)	O1W^{2} – Co(1) – O(12)	90.85(11)
O1W – Co(1) – N(1)	89.06(13)	O1W^{2} – Co(1) – N(1)	90.94(13)

Symmetry codes: #1 -X, 1-Y,1-Z #2 -X, 1-Y, -Z

Compound **4**

Cu(1) – O(9)^{1}	2.099(3)	Cu(1) – O(5)	2.063(3)
Cu(1) – N(1)	1.975(5)	Cu(1) – N(2)^{2}	2.003(5)

Mo(3) – O(9) – Cu(1)[1]	138.05(19)	Mo(1) – O(5) – Cu(1)	134.3(2)
N(2) – N(1) – Cu(1)	118.8(4)	C(1) – N(1) – Cu(1)	132.6(4)
N(1) – N(2) – Cu(1)[2]	119.5(3)	C(2) – N(2) – Cu(1)[2]	133.6(4)

Symmetry codes: #1 -X, 1-Y,2-Z #2 1-X, 1-Y, 1-Z

Compound **5**

Cu(1) – O(47)	2.280(13)	Cu(1) – N(1)	2.014(15)
Cu(2) – O2W	2.059(14)	Cu(2) – N(14)	1.981(16)
Cu(3) – O1W	1.949(14)	Cu(3) – N(7)	2.001(15)
N(1) – Cu(1) – O(47)	88.3(5)	N(10) – Cu(1) – O(8)	77.5(7)
N(8) – Cu(2) – N(14)	175.0(7)	N(14) – Cu(2) – O(47)	90.0(6)
N(7) – Cu(3) – N(2)	148.9(7)	O(47) – Cu(3) – N(7)	89.5(5)

Symmetry codes: #1 1-X, 1-Y,2-Z #2 1-X, 1-Y, 2-Z #3 +X, 1+Y, +Z #4 -X, 2-Y, 1-Z

Table S2. Comparison of the properties of the POM-based compounds with several published supercapacitors.

Electrode	Cs(F g^{-1})	Current density (A g^{-1})	Current collector	Ref.
2–GCE	412.77	1	glassy carbon	This work
3–GCE	580	1	glassy carbon	This work
4–GCE	823.09	1	glassy carbon	This work
$[Cu^{II}_2(C_{12}H_{12}N_6)_4(PMo^{VI}_9Mo^{V}_3O_{39})]$	154.5	3	glassy carbon	1
$[Cu^{I}H_2(C_{12}H_{12}N_6)(PMo_{12}O_{40})]\cdot[(C_6H_{15}N)(H_2O)_2]$	249.0	3	glassy carbon	1
$H_3[Cu_2(4\text{-dpye})_2(PMo_{12}O_{40})]$	260.0	0.5	carbon cloth	2
$H[Cu_2(4\text{-Hdpye})_2(PMo_{12}O_{40})(H_2O)_4]\cdot 2H_2O$	196.6	0.5	carbon cloth	2
$[PMo^{VI}_9Mo^{V}_3O_{40}]Cu^{I}_5[4\text{-atrz}]_6\cdot H_2O$	237.1	1	glassy carbon	3
$[HPW^{VI}_9W^{V}_3O_{40}]Cu^{I}_5[4\text{-atrz}]_6$	147.5	1	glassy carbon	3
$[H_2SiMo^{VI}_9MoV_3O_{40}]Cu^{I}_5[4\text{-atrz}]_6\cdot H_2O$	232.5	1	glassy carbon	3
$(H_2bipy)_{1.5}[Cu^{I}(bipy)(C_6H_5PO_3)_2Mo_5O_{15}]\cdot H_2O$	70.3	2	glassy carbon	4
$[Cu^{II}_2(bipy)(H_2O)_4(C_6H_5PO_3)_2Mo_5O_{15}]$	160.9	2	glassy carbon	4
$[H(C_{10}H_{10}N_2)Cu_2][PMo_{12}O_{40}]$	287	1	glassy carbon	5
$(C_{10}H_{10}N_2)Cu_2][PW_{12}O_{40}]$	153.43	1	glassy carbon	5

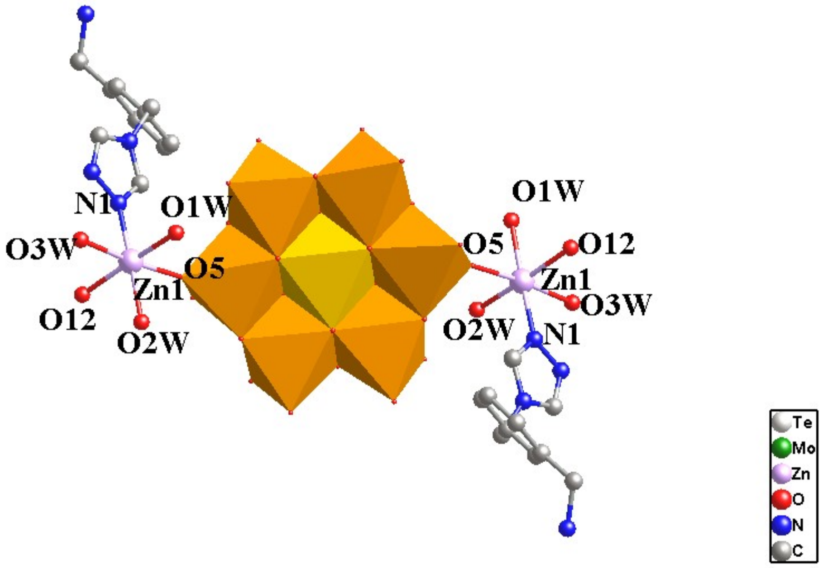

Fig. S1. Polyhedral/ball/stick view of the unit of compound **2**. The hydrogen atoms are omitted for clarity.

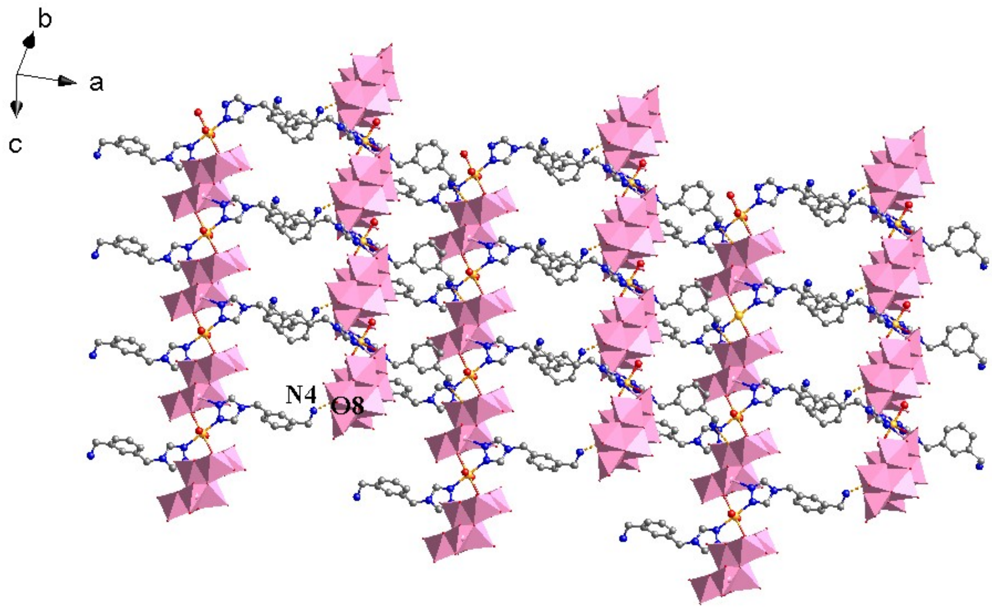

Fig. S2. The supramolecular 2D layer of **3** through the hydrogen bonding interactions of N4···O8 (2.863 Å).

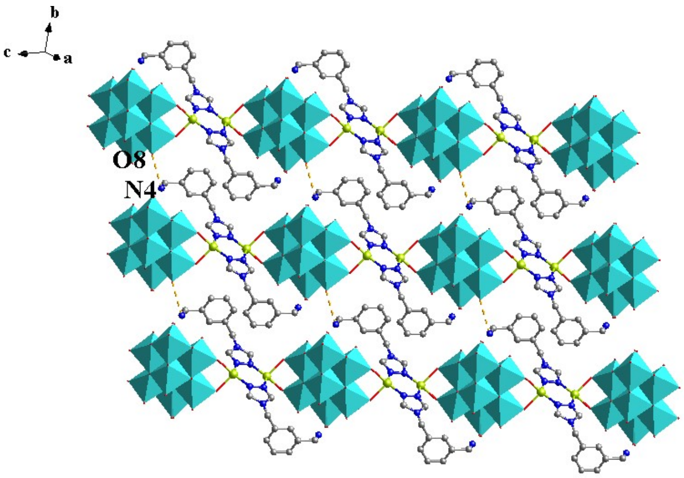

Fig. S3. The supramolecular 2D layer of **4** through the hydrogen bonding interactions.

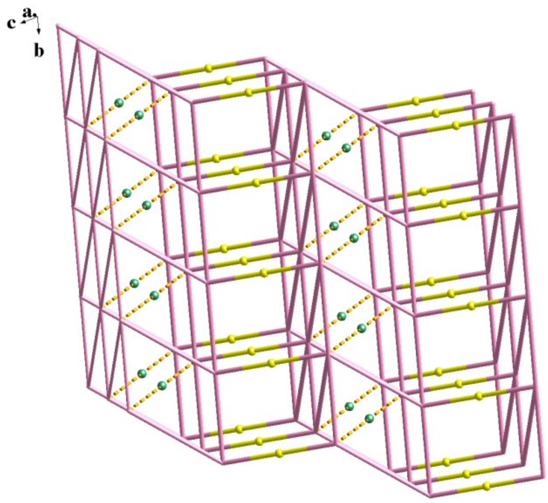

Fig. S4. The supramolecular 2D layer of **5** with dissociative PW_{12} anions dispersing between adjacent layers.

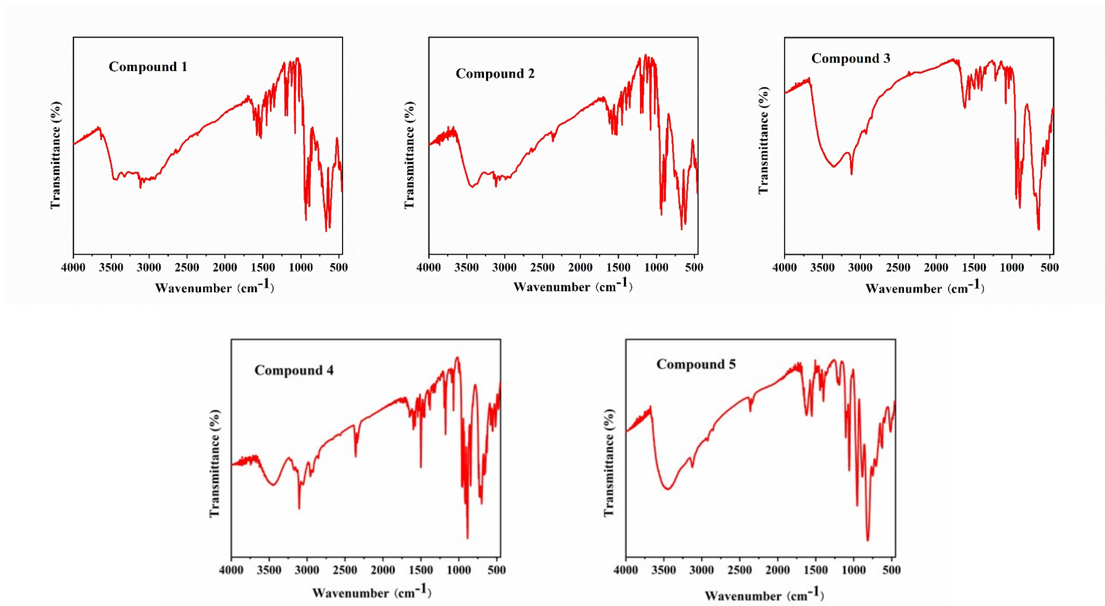

Fig. S5. The IR spectra of compounds **1–5**.

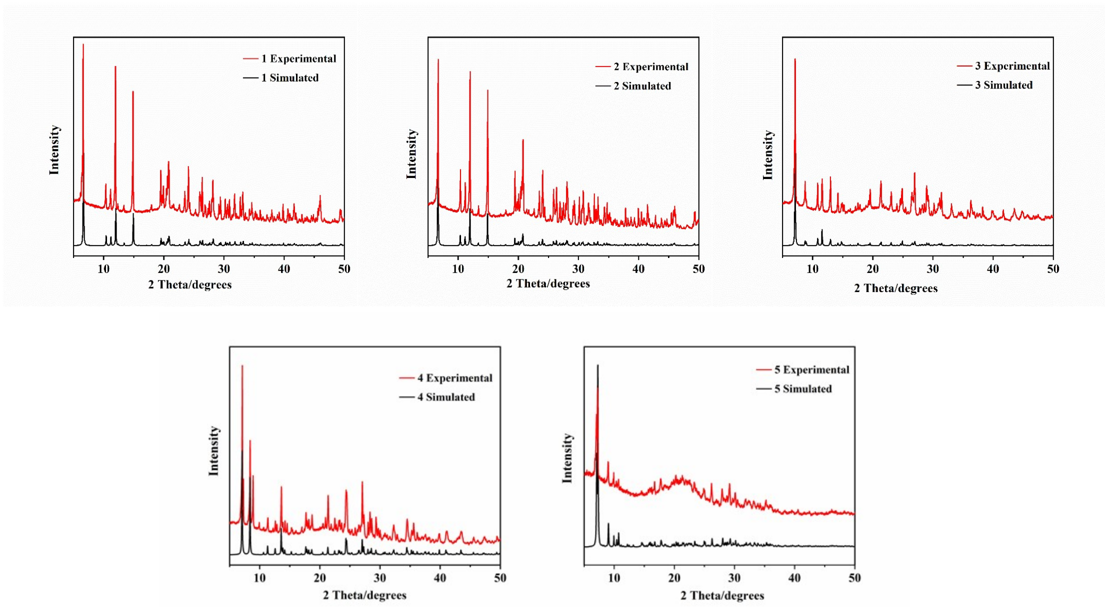

Fig. S6. The PXRD patterns of compounds **1–5**.

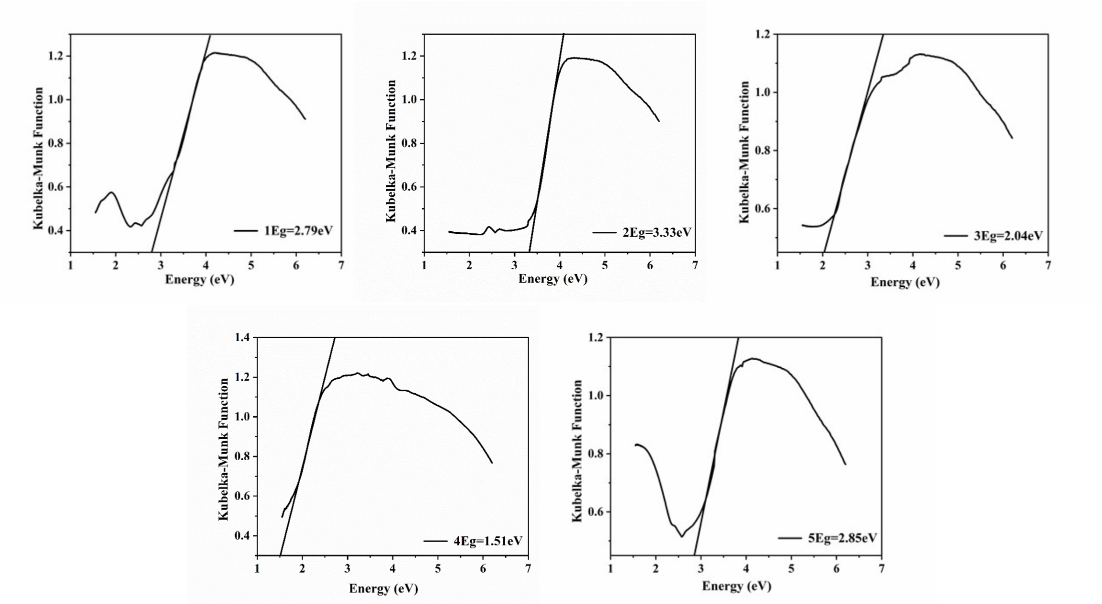

Fig. S7. The solid-state optical diffuse-reflectance spectra of compounds **1–5**.

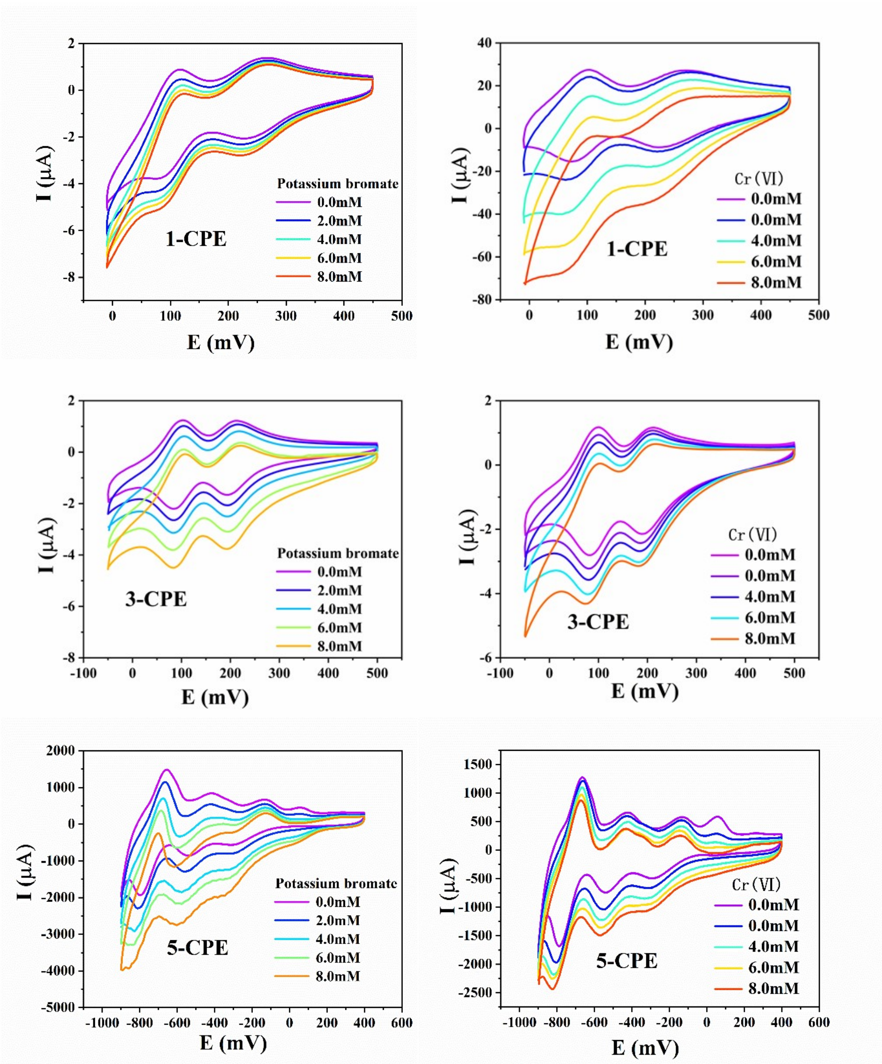

Fig. S8. Cyclic voltammograms of **1–**, **3–** and **5–**CPEs in 0.1 M H_2SO_4 + 0.5M

Na_2SO_4 aqueous solution containing 0–8 mM $KBrO_3$/Cr(VI). Scan rate: 200 mV s^{-1}.

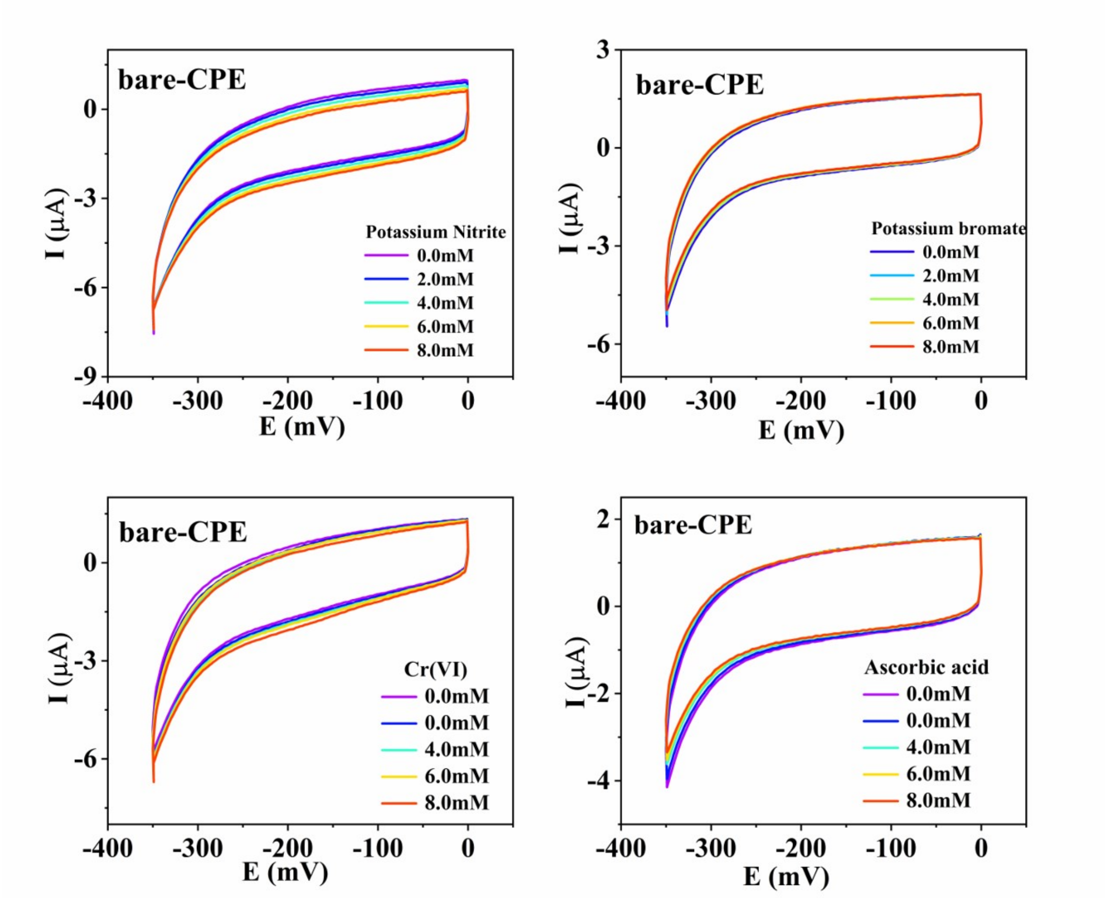

Fig. S9. Cyclic voltammograms of bare–CPE in 0.1 M H_2SO_4 + 0.5M Na_2SO_4 aqueous solution containing 0–8 mM KNO_2/$KBrO_3$/Cr(VI)/AA. Scan rate: 200 mV s^{-1}.

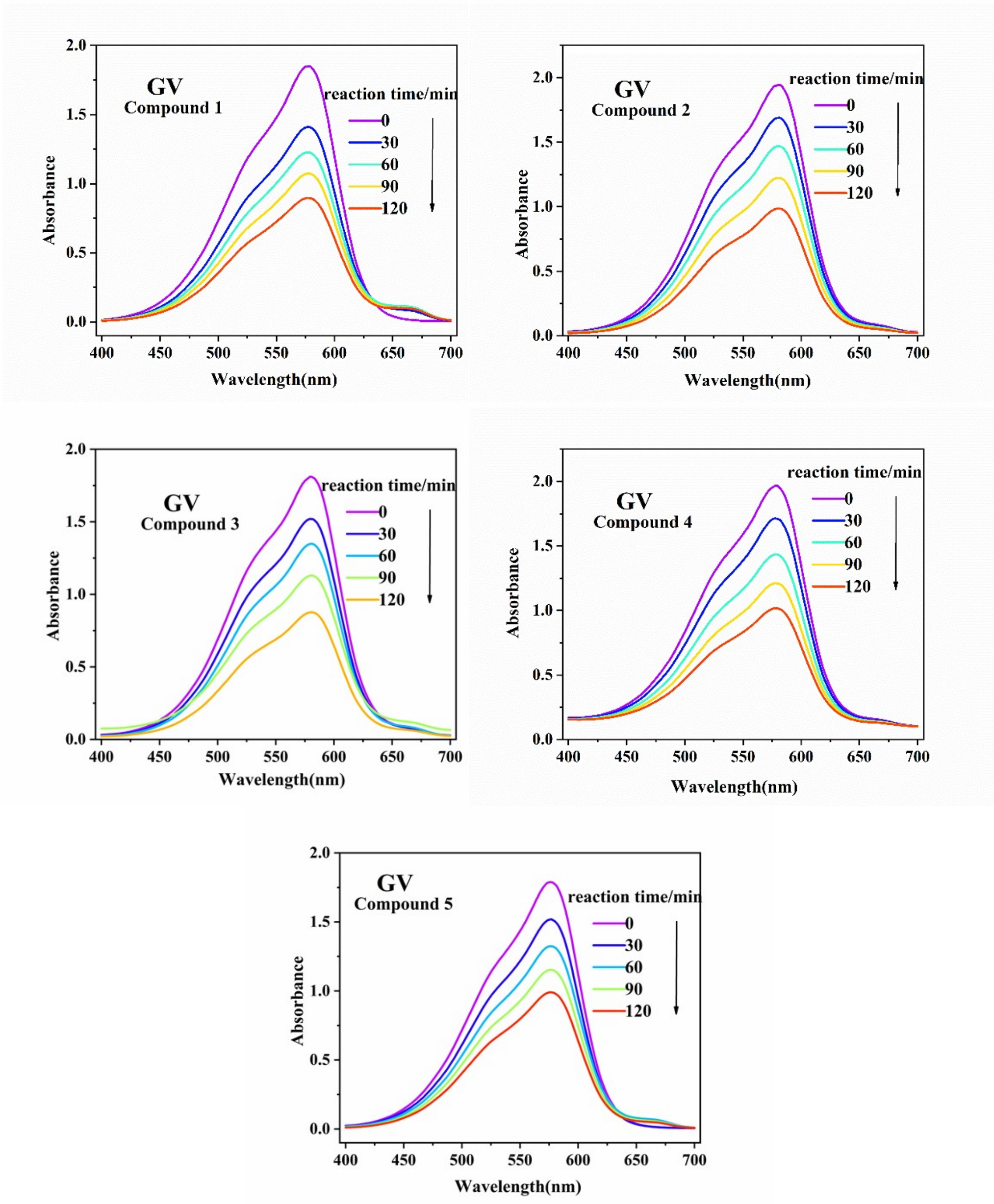

Fig. S10. The absorption spectra of GV solution during the decomposition reaction under UV irradiation with compounds **1–5** as catalysts.

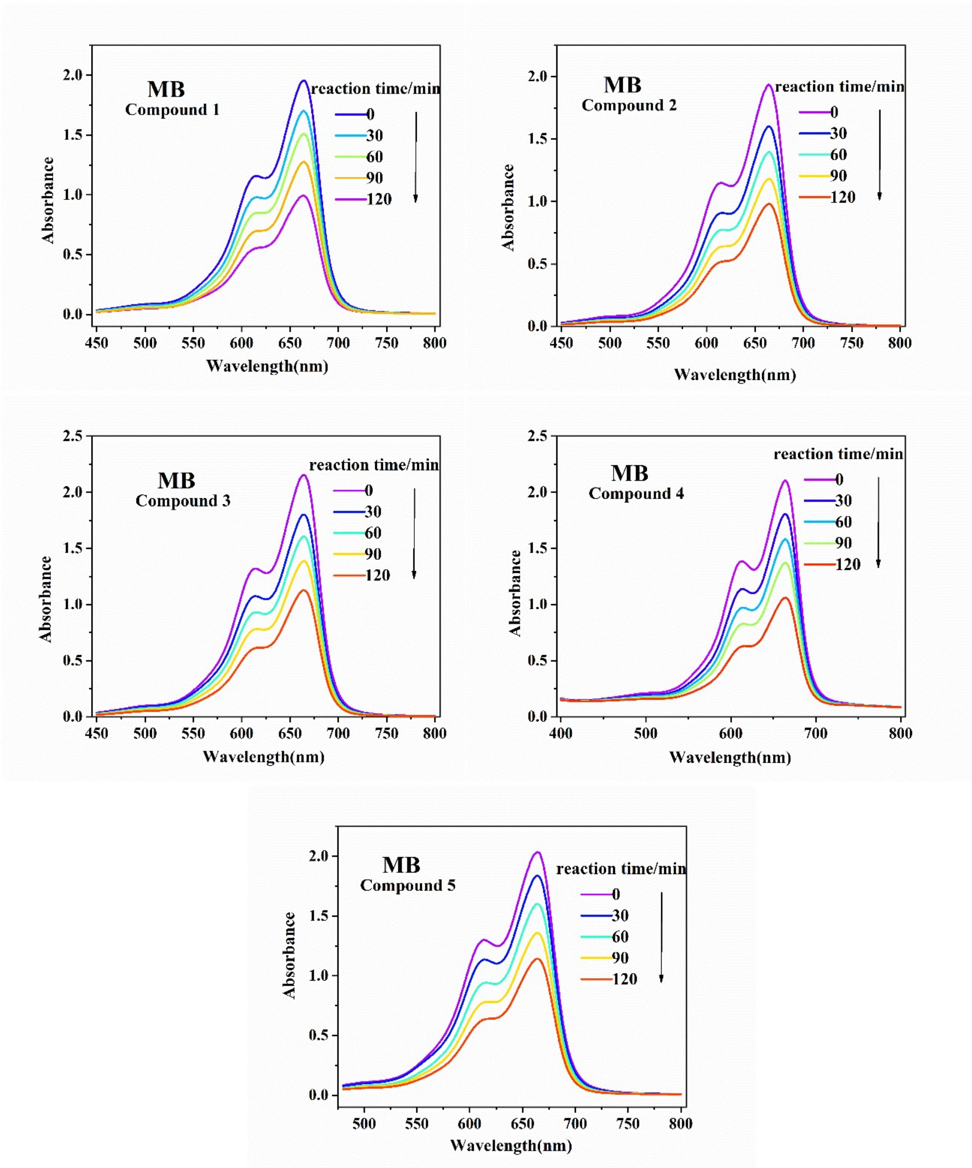

Fig. S11. The absorption spectra of MB solution during the decomposition reaction under UV irradiation with compounds **1–5** as catalysts.

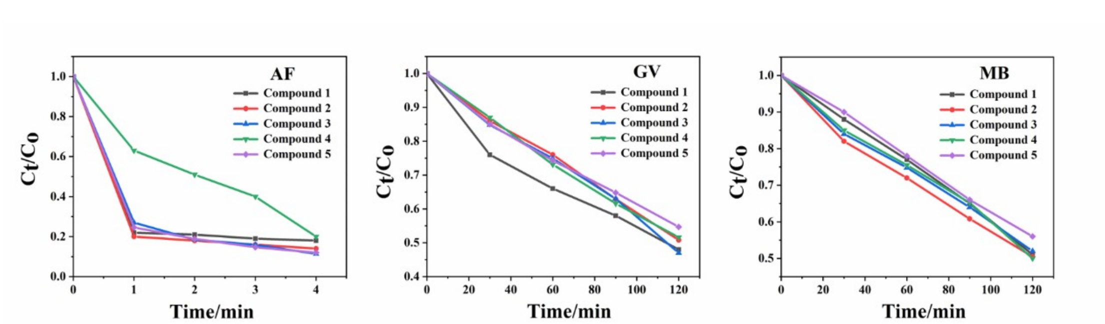

Fig. S12. The catalytic conversion curves of compounds **1–5**.

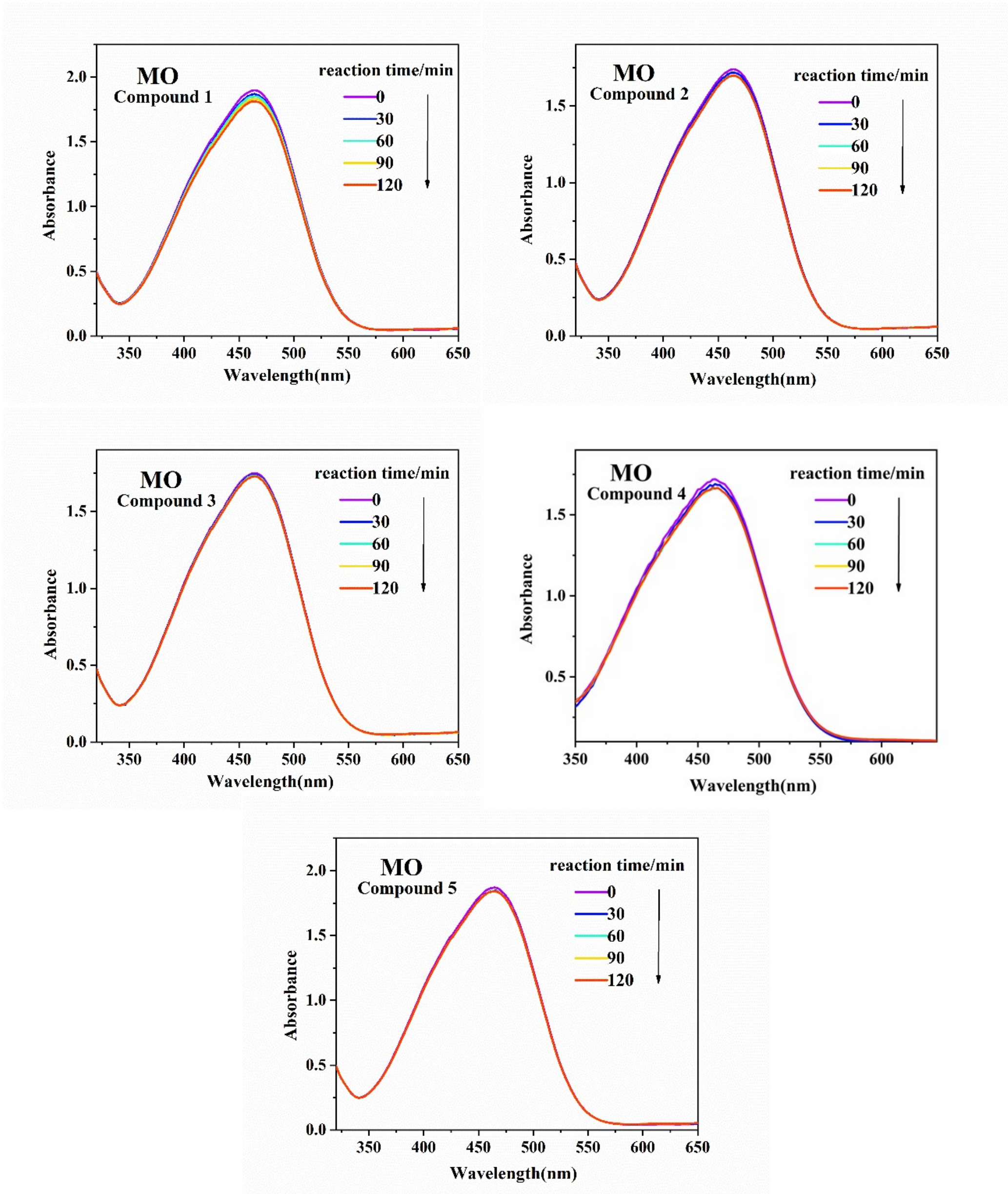

Fig. S13. The absorption spectra of MO solution during the decomposition reaction under UV irradiation with compounds **1–5** as catalysts.

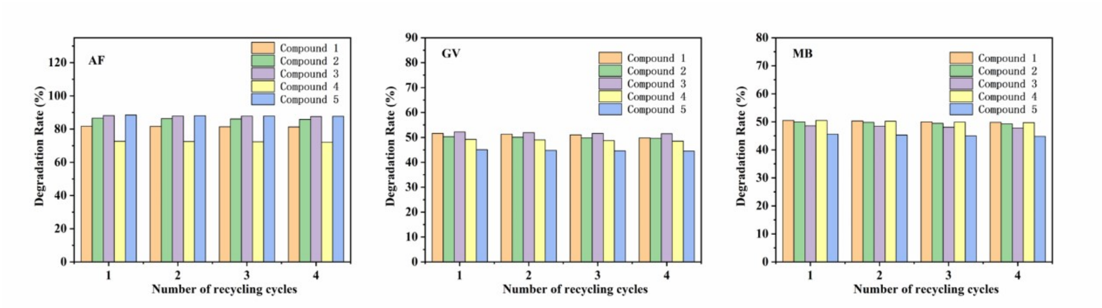

Fig. S14. Four cycles of photocatalytic degradation of compounds **1–5**.

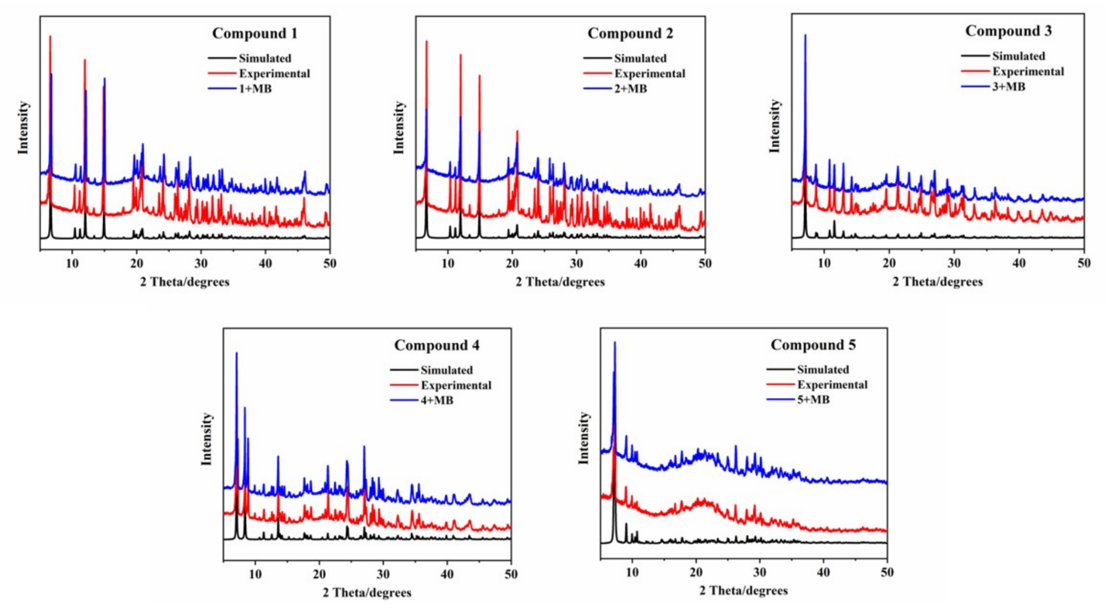

Fig. S15. The PXRD spectra of compounds **1–5**.

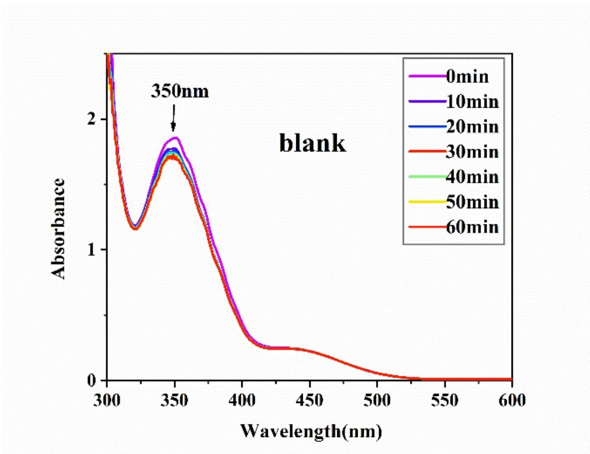

Fig. S16. The UV spectra of the Cr(VI) solution without compounds as the photoreduction catalysts.

Notes and references

1 D. F. Chai, J. J. Xin, B. Li, H. J. Pang, H. Y. Ma, K. Q. Li, B. X. Xiao, X. M. Wang and L. C. Tan, *Dalton Trans.,* 2019, **48**, 13026.

2 Q. Q. Liu, X. L. Wang, H. Y. Lin, Z. H. Chang, Y. C. Zhang, Y. Tian, J. J. Lu and L. Yu, *Dalton Trans.*, 2021, **50**, 9450

3 M. L. Yang, S. Rong, X. M. Wang, H. Y. Ma, H. J. Pang, L. C. Tan, Y. X. Jiang and K. Q. Gao, *ChemNanoMat*, 2021, **7**, 299

4 B. R. Lu, S. B. Li, J. Pan, L. Zhang, J. J. Xin, Y. Chen and X. G. Tan, *Inorg. Chem.*, 2020, **59**, 1702

5 S. Roy, V. Vemuri, S. Maiti, K. S. Manoj, U. Subbarao and S. C. Peter, *Inorg. Chem.*, 2018, **57**, 12078