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Keggin-based 3D Frameworks Tuned by Silver Polymeric Motifs: Effect of Substituent Group of Bi(triazole) on the Architectures

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Table S1. Selected bond lengths (Å) and bond angles (°) for compounds **1**, **2** and **3**.

Compound **1**

Ag(1)-N(1)	2.236(9)	Ag(1)-N(2)	2.251(11)
Ag(1)-O(18)#2	2.418(10)	Ag(1)-O(20)	2.527(9)
Ag(2)-N(3)#3	2.194(10)	Ag(2)-N(4)#4	2.200(10)
Ag(2)-O(12)	2.696(9)	Ag(2)-O(23)#1	2.583(10)
Ag(2)-O(21)	2.506(9)		
O(18) #2-Ag(1)-O(20)	139.3(4)	N(1)-Ag(1)-N(2)	152.8(4)
N(1)-Ag(1)-O(18)#2	102.7(4)	N(2)-Ag(1)-O(18)#2	94.6(4)
N(1)-Ag(1)-O(20)	89.6(3)	N(2)-Ag(1)-O(20)	90.9(3)
N(3)#3 -Ag(2)-O(21)	93.9(4)	N(3)#3-Ag(2)-N(4)#4	166.9(4)
O(21)-Ag(2)-O(23)#1	93.2(3)	N(4)#4-Ag(2)-O(21)	90.3(4)
N(3)#3-Ag(2)-O(23)#1	104.7(3)	N(4)#4-Ag(2)-O(23)#1	87.5(3)

Symmetry codes for **1**: #1 *–x, y* + 1/2, *z;* #2 *–x* + 1, *y* + 1/2, *z;* #3 *x*, *–y* + 3/2, *–z;* #4 *x* – 1, *y, z ;* #5 *x, y, –z* + 1/2.

Compound **2**

Ag(1)-N(1)	2.20(2)	Ag(1)-N(6)	2.25(2)
Ag(1)-O(15)	2.515(19)	Ag(1)-O(24)#1	2.44(2)
Ag(2)-N(4)	2.19(2)	Ag(2)-N(5)#2	2.18(2)
Ag(2)-O(2)	2.667(2)	Ag(2)-O(14)	2.732(18)

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Ag(2)-O(19)#3	2.58 (2)	N(1)-Ag(1)-O(15)	93.7(8)
N(1)-Ag(1)-O(24)#1	103.0(10)	N(1)-Ag(1)-N(6)	153.6(10)
O(24) -Ag(1)-O(15)	133.8(9)	N(6)-Ag(1)-O(24)#1	89.7(10)
N(6)-Ag(1)-O(15)	93.7(9)	N(5)#7-Ag(2)-O(19)#3	96.7(7)
N(5)#2-Ag(2)-N(4)	169.7(8)	N(4)-Ag(2)-O(19)#3	87.3(8)

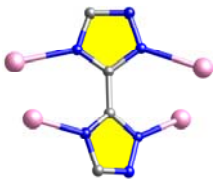
Symmetry codes for **2**:#1 *–x, y* + 1/2, *–z* + 1/2; #2 *x* + 1, *–y* – 1/2, *–z*; #3 *x* + 1, *y, z*.

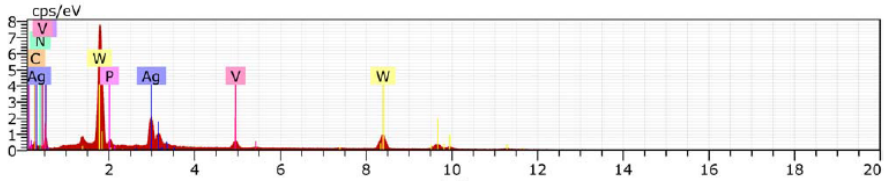
Compound **3**

Ag(1)-N(5)	2.143(18)	Ag(1)-O(2W)	2.28(3)
Ag(1)-N(14)	2.515(19)	Ag(1)-O(13)	2.670(7)
Ag(1)-O(9)	2.614(15)	Ag(2)-N(1)#2	2.131(18)
Ag(2)-N(2)	2.199(16)	Ag(2)-O(10)#3	2.54(4)
Ag(3)-N(7)#4	2.301(19)	Ag(3)-N(9)#4	2.478(17)
Ag(3)-O(12)#3	2.471(14)	Ag(3)-O(20)	2.488(16)
Ag(3)-O(1W)	2.58(7)	Ag(4)-N(11)#5	2.16(2)
Ag(4)-N(12)	2.64(2)	Ag(4)-O(1)#1	2.400(13)
Ag(4)-O(18)	2.437(14)	N(5)-Ag(1)-O(2W)	101.6(9)
N(5)-Ag(1)-N(14)	121.1(6)	O(2W)-Ag(1)-N(14)	120.8(9)
N(1)#2-Ag(2)-N(2)	169.6(7)	N(1)#2-Ag(2)-O(10)#3	89.9(13)
N(7)#4-Ag(3)-O(12)#3	119.1(6)	N(7)#4-Ag(3)-N(9)#4	98.0(6)
O(12)#3-Ag(3)-N(9)#4	88.6(5)	N(7)#4-Ag(3)-O(20)	85.1(6)
O(12)#3-Ag(3)-O(20)	82.8(5)	N(9)#4-Ag(3)-O(20)	171.3(5)
N(11)#5-Ag(4)-O(1)#1	137.4(6)	N(11)#5-Ag(4)-O(18)	99.8(6)
O(1)#1-Ag(4)-O(18)	114.3(5)		

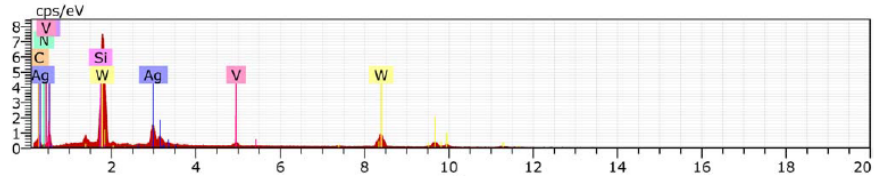
Symmetry codes for **3**: #1 *–x* + 2, *–y* + 1, *–z* + 1*;* #2 *–x* + 2, *y* – 1/2, *–z* + 3/2*;* #3 *x* + *1*, *–y* + 1/2, *z* + 1/2*;* #4 *x*, *–y* + 1/2, *z* – 1/2*;* #5 *–x* + 2, *y* + 1/2, *–z* + 3/2.

Table S2. The conformations of ligands and the dihedral angles between the triazoles

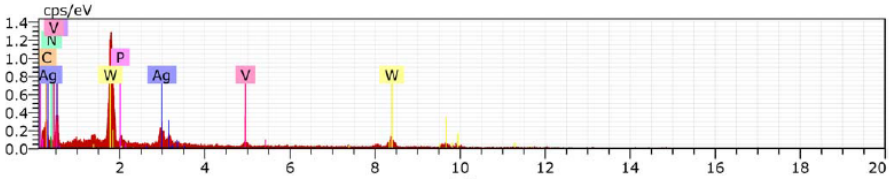
Configuration				
Ligands	a- **L**[1]	b- **L**[1]	a- **L**[2]	b- **L**[2]
Dihedral angle (°)	20.72	40.37	10.56	40.07



(a)



(b)



(c)

Fig. S1. The EDS spectra of compounds **1** (a), **2** (b) and **3** (c).

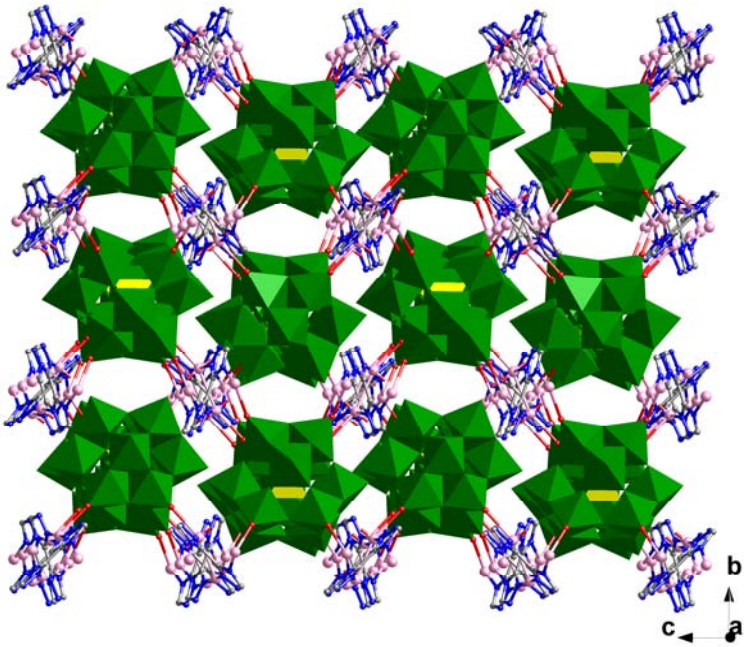


Fig. S2. Polyhedral and ball/stick view of the 3D framework of compound **1**.

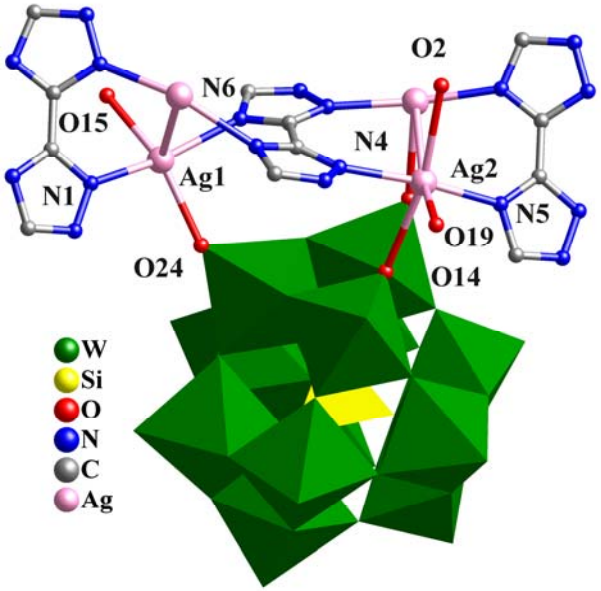


Fig. S3. Ball/stick and polyhedral view of the asymmetric unit of compound **2**.
Compared with compound **1**, Ag1 ion in compound **2** is five-coordinated and there is no coordiantion water molecule.

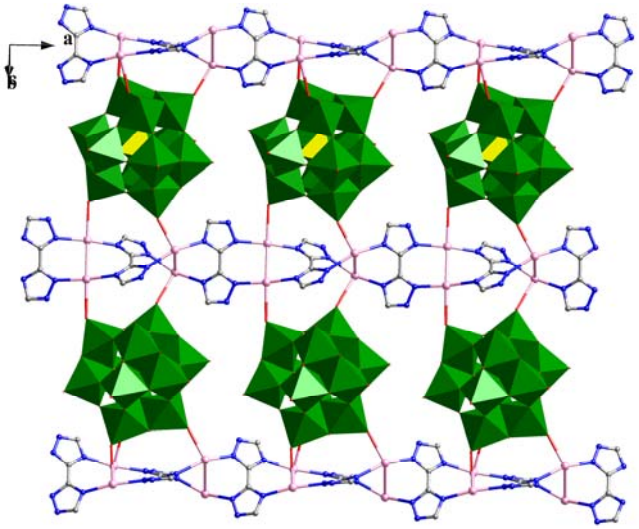


Fig. S4. Polyhedral and ball/stick view of the 2D network of compound **2**.

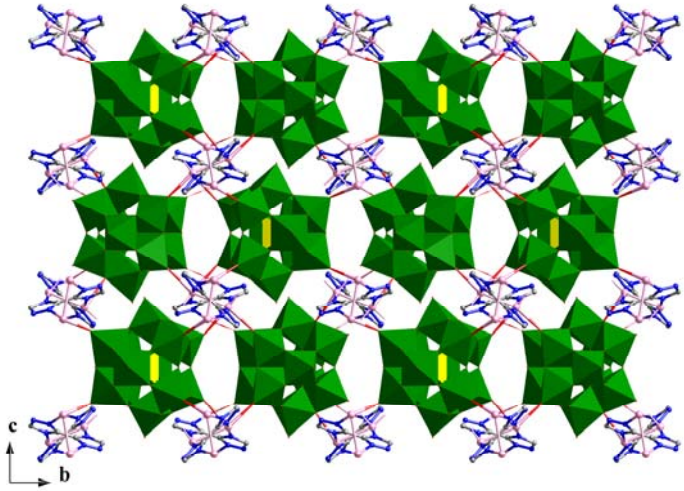


Fig. S5. Polyhedral and ball/stick view of the 3D framework of compound **2**.

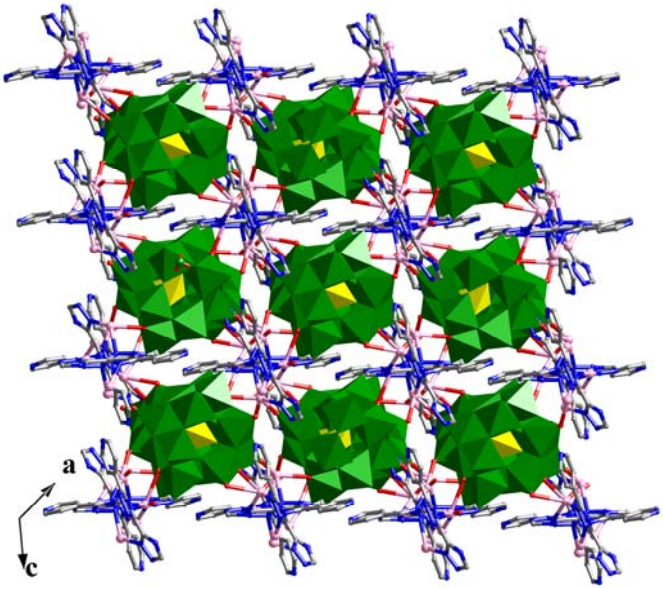
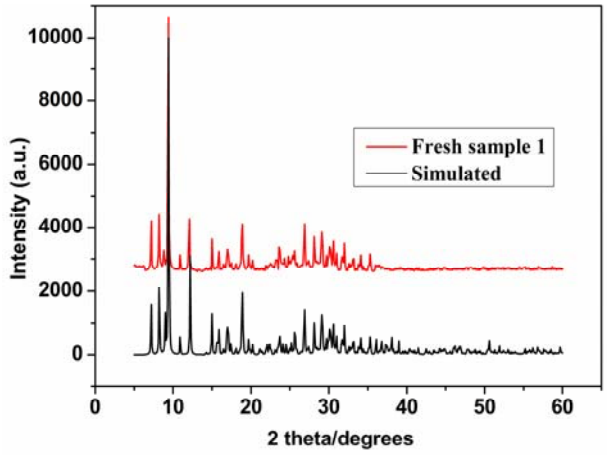
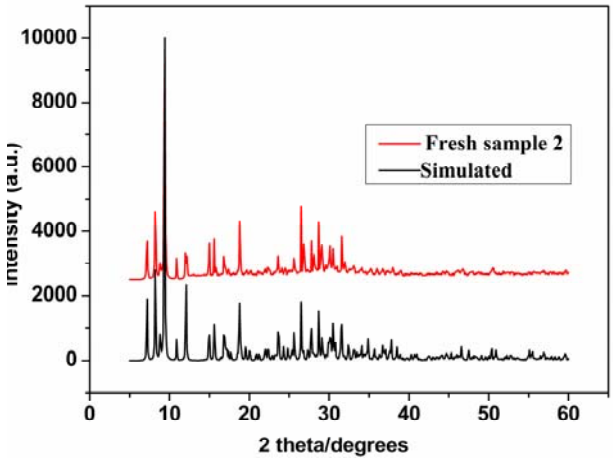


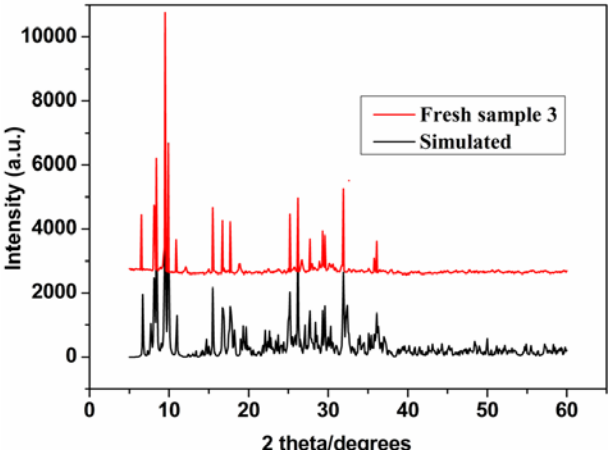
Fig. S6. Polyhedral and ball/stick view of the 3D framework of compound **3**.



(a)

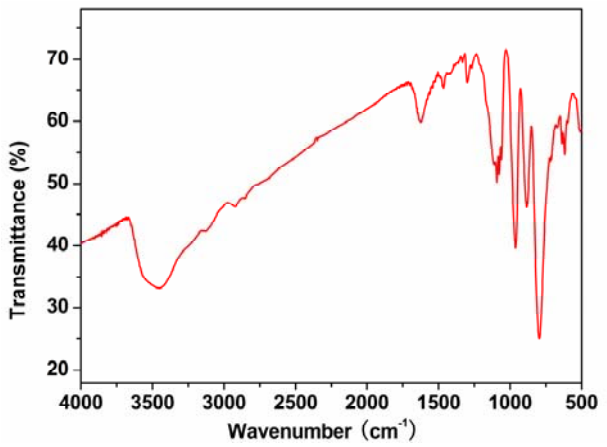


(b)

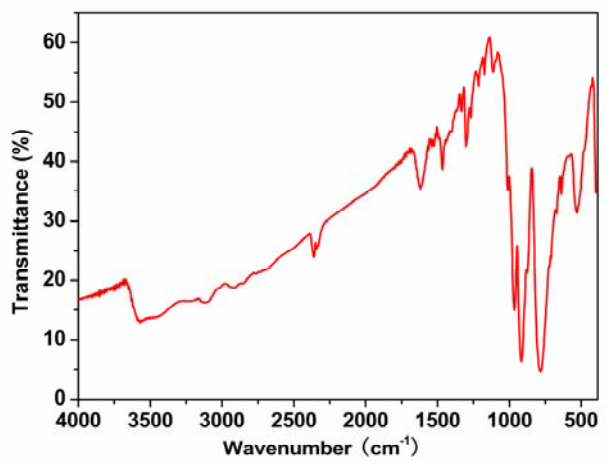


(c)

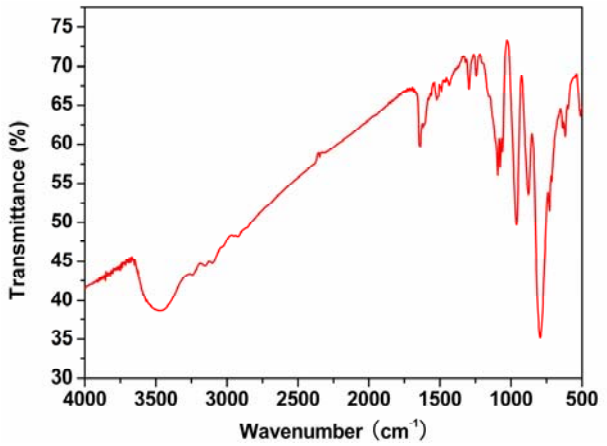
Fig. S7. The PXRD patterns of compounds **1** (a), **2** (b) and **3** (c).



(a)



(b)



(c)

Fig. S8. The IR spectra of compounds **1** (a), **2** (b) and **3** (c).

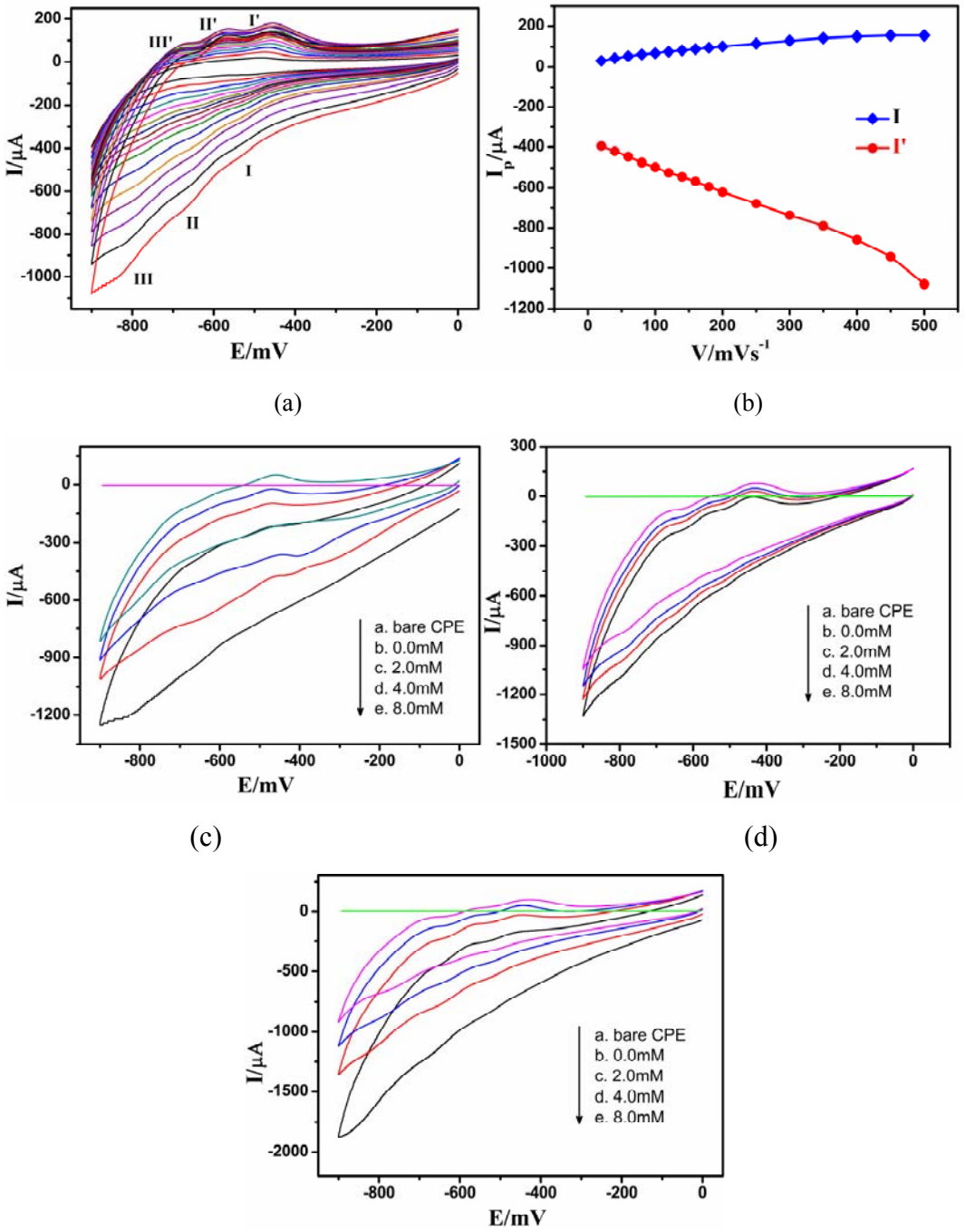
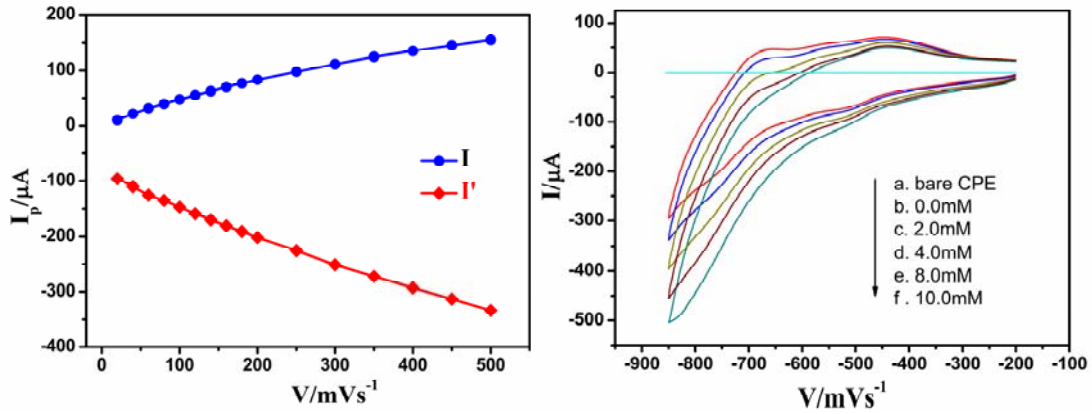


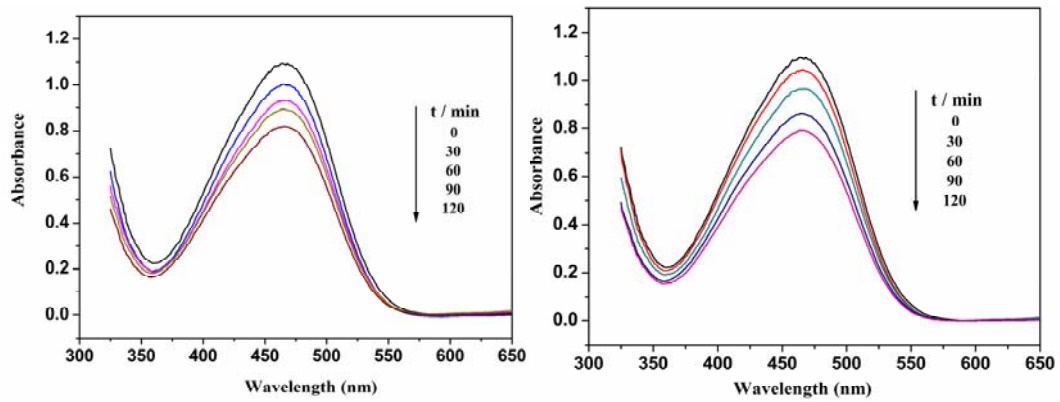
Fig. S9. (a) Cyclic voltammograms of **2**-CPE in a 0.1 M H_2SO_4 + 0.5 M Na_2SO_4 aqueous solution at different scan rates (from inner to outer: 20, 40, 60, 80, 100, 120, 140, 160, 180, 200, 250, 300, 350, 400, 450 and 500 mV/s). (b) The plots of the anodic and cathodic peak currents against scan rates of **2**-CPE. (c) Cyclic voltammograms of **2**-CPE in a 0.1 M H_2SO_4 + 0.5 M Na_2SO_4 aqueous solution containing 0.0−8.0 mM KNO_2 and a bare CPE in a 0.1 M H_2SO_4 + 0.5

M Na_2SO_4 mixed solution. Scan rate: 200 mV/s. (d) Cyclic voltammograms of **2**-CPE in a 0.1 M H_2SO_4 + 0.5 M Na_2SO_4 aqueous solution containing 0.0−10.0 mM H_2O_2 and a bare CPE in a 0.1 M H_2SO_4 + 0.5 M Na_2SO_4 mixed solution. Scan rate: 200 mV/s. (e) Cyclic voltammograms of **2**-CPE in a 0.1 M H_2SO_4 + 0.5 M Na_2SO_4 aqueous solution containing 0.0−8.0 mM $KBrO_3$ and a bare CPE in a 0.1 M H_2SO_4 + 0.5 M Na_2SO_4 mixed solution. Scan rate: 200 mV/s.



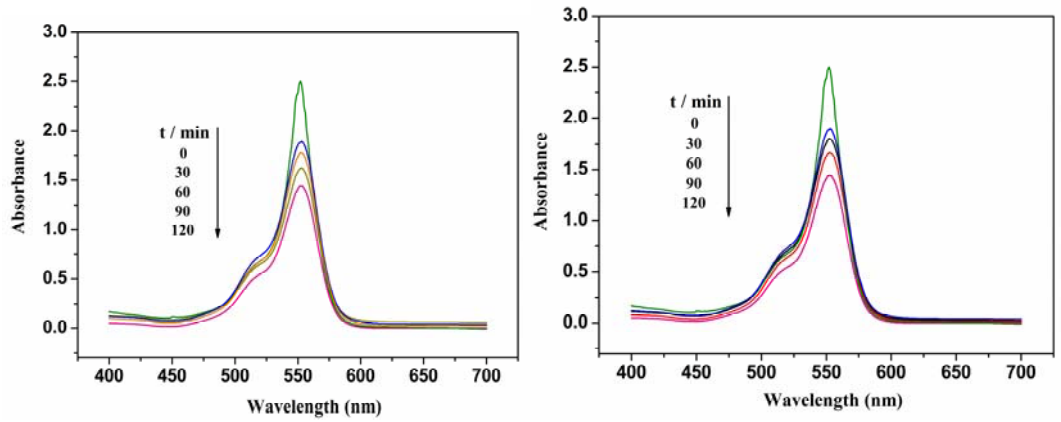
(a) (b)

Fig. S10. (a) The plots of the anodic and cathodic peak currents against scan rates of **3**-CPE. (b) Cyclic voltammograms of **3**-CPE in a 0.1 M H_2SO_4 + 0.5 M Na_2SO_4 aqueous solution containing 0.0−8.0 mM KNO_2 and a bare CPE in a 0.1 M H_2SO_4 + 0.5 M Na_2SO_4 mixed solution. Scan rate: 200 mV/s.



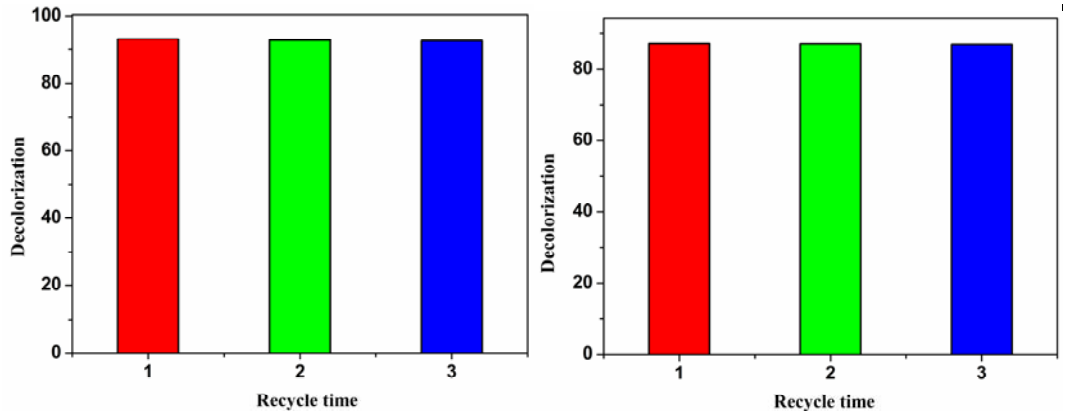
(a) (b)

Fig. S11. Absorption spectra of the MO solution during the decomposition reaction with the use of compounds **2**(a) and **3**(b).



(a) (b)

Fig. S12. Absorption spectra of the RhB solution during the decomposition reaction with the use of compounds **2** (a) and **3** (b).



(a) (b)

Fig. S13. Cycling runs of **2**(a) and **3**(b) in the degradation of MB solution.