Supplementary Material (ESI) for Dalton Transactions

Two Copper(I) Cyanide Coordination Polymers Modified by Semi-rigid Bis(benzimidazole) Ligands: Syntheses, Crystal Structures, Electrochemical and Photocatalytic Properties

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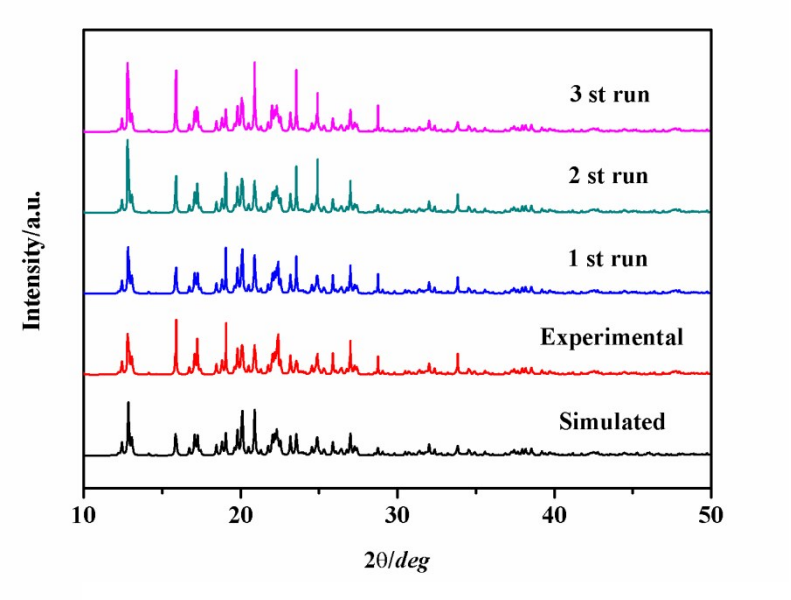
S1 Electrochemical experiment

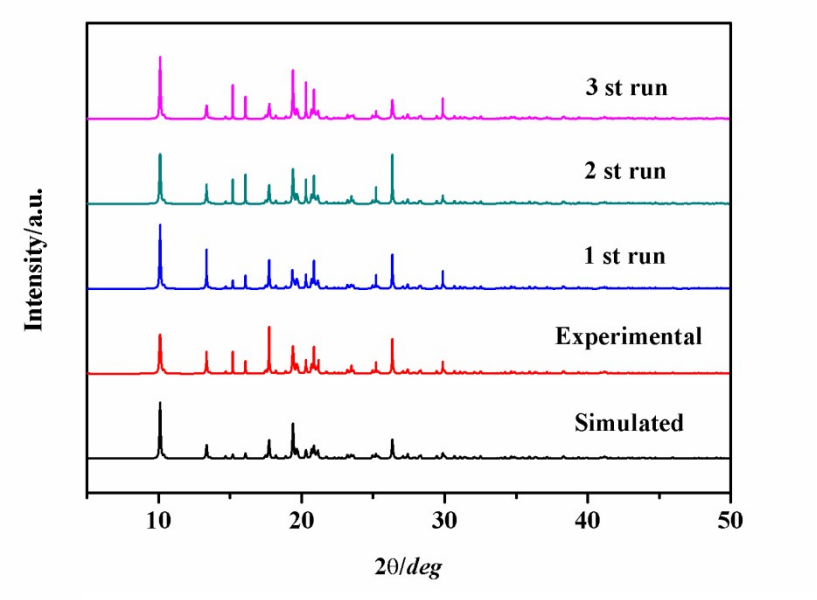
The electrochemical analysis was carried out using a CHI 660E electrochemical workstation (Chenhua Instrument, Shanghai, China). A conventional three-electrode system was used at room temperature. The CPs chemically bulk-modified carbon paste electrodes (**1**-CPE and **2**-CPE) were used as the working electrodes. A saturated calomel electrode and a platinum electrode were used as reference and auxiliary electrodes, respectively. The **1**-CPE or **2**-CPE was fabricated as follows: 0.5 g graphite powder and 0.04 g complex were mixed and ground together by agate mortar and pestle to achieve an even, dry mixture; and then 0.2 mL paraffin oil was added to the mixture and stirred with a glass rod. The homogenized mixture was used to pack a 3 mm inner diameter PTFE tube to a length of 1 cm, and the tube surface was wiped with weighing paper. Electrical contact was established with a copper rod through the back of the electrode. The same procedure was used for the preparation of the bare CPE.

S2 The photocatalytic experiment of CPs 1 and 2 for degrading Congo red

The photocatalytic experiment of CPs **1** and **2** for the degradation of Congo red through a typical process as follows: 50 mg crystal sample of each title coordination polymer was mixed with 100 mL of Congo red aqueous solution (10 $mg \cdot L^{-1}$). The mixture was magnetically stirred for half an hour in a dark environment to get a uniform working solution. Then, a 500 W high-pressure mercury lamp was used as the UV light source to irradiate the above solution, which was continuously stirred during the photodegradation. Aliquots (3.5 mL) of the suspension was taken at given time intervals, separated through centrifugation and then subsequently analyzed by using a UV-visible spectrometer at a special wavelength. Under the same conditions of photodegrading methylene blue, both of **1** and **2** also show promising photocatalytic activities (photocatalytic efficiency: 84.4% for **1** and 82.3% for **2**) for the degradation of Congo red (Figure S13-Figure S15).

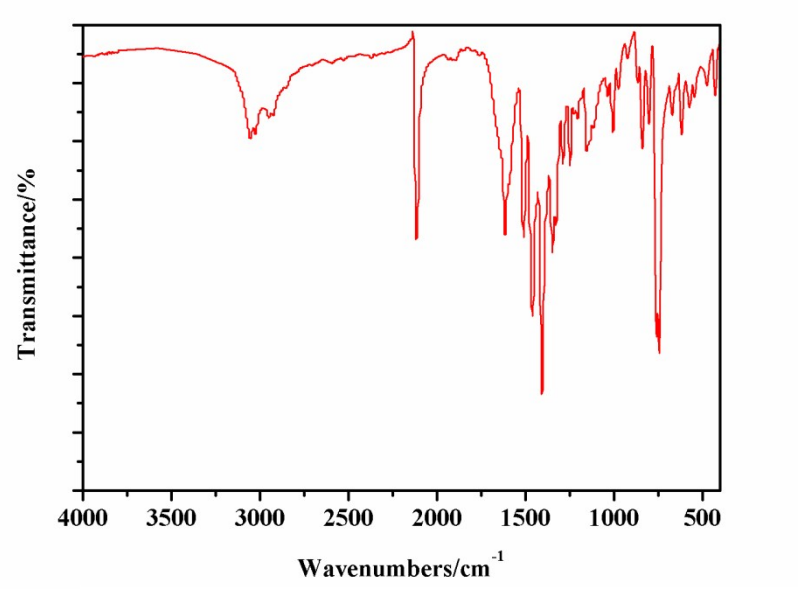


(a)

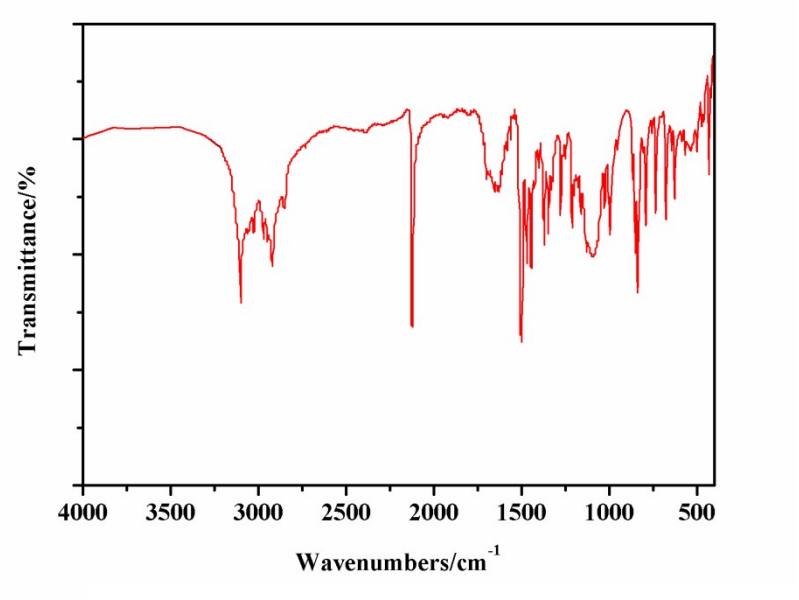


(b)

Fig. S1 PXRD patterns of CPs **1** and **2** simulated from single-crystal X-ray data, as-synthesized and after the photocatalytic reactions using the MB solution.



(a)



(b)

Fig. S2 IR spectra of CPs **1** and **2**.

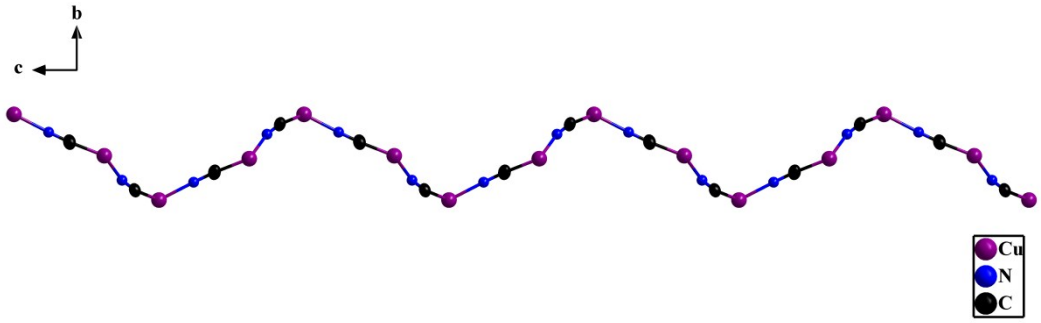
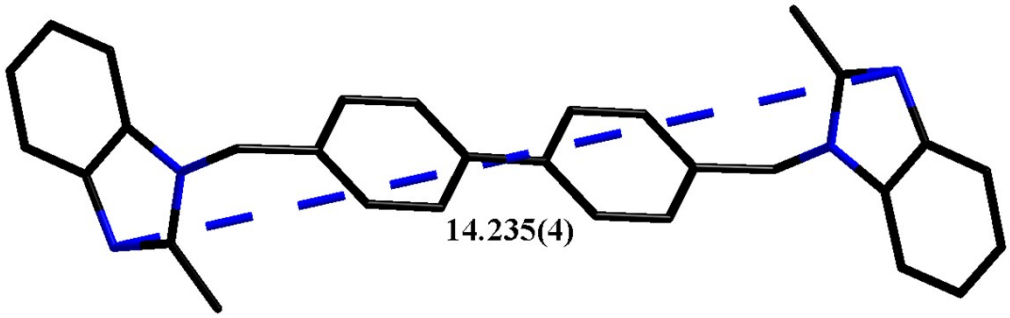
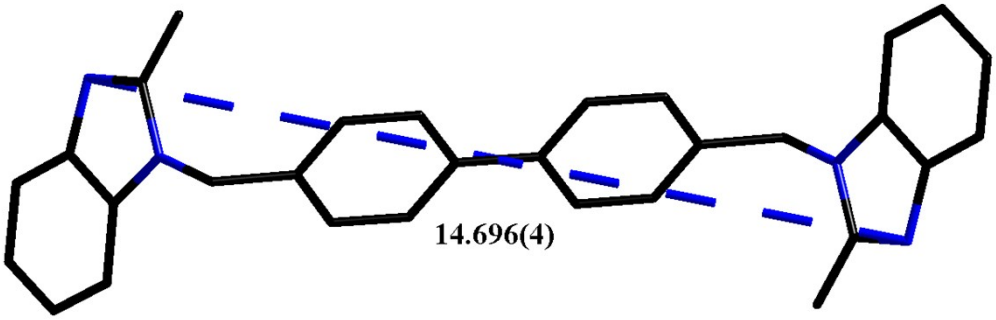


Fig. S3 Ball-and-stick representation of the 1D zigzag chain structure along the *a* axis in CP **1**.



(a)



(b)

Fig. S4 Coordination modes of the L1 ligand.

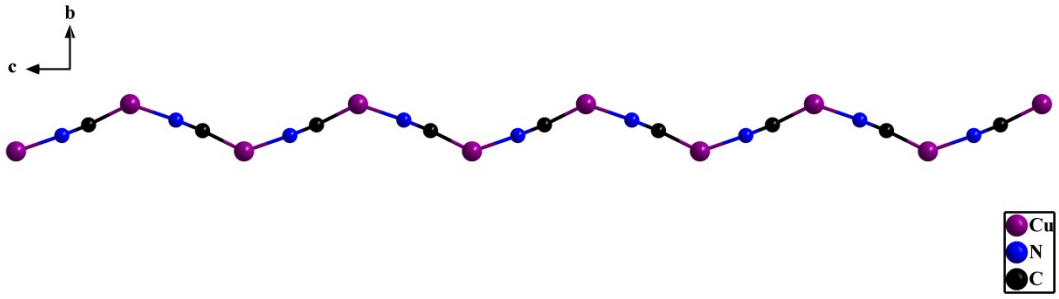


Fig. S5 Ball-and-stick representation of the 1D zigzag chain structure along the *a* axis in CP **2**.

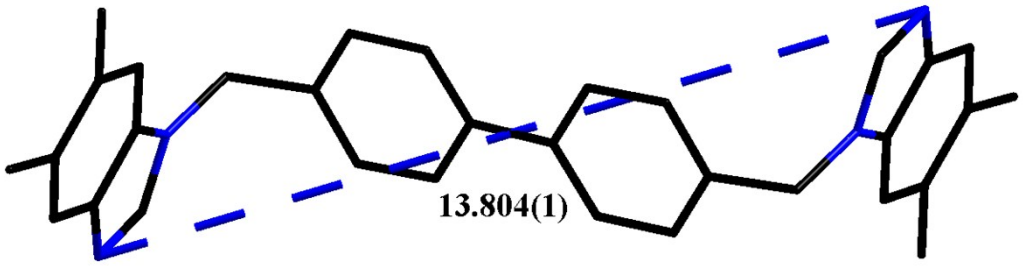
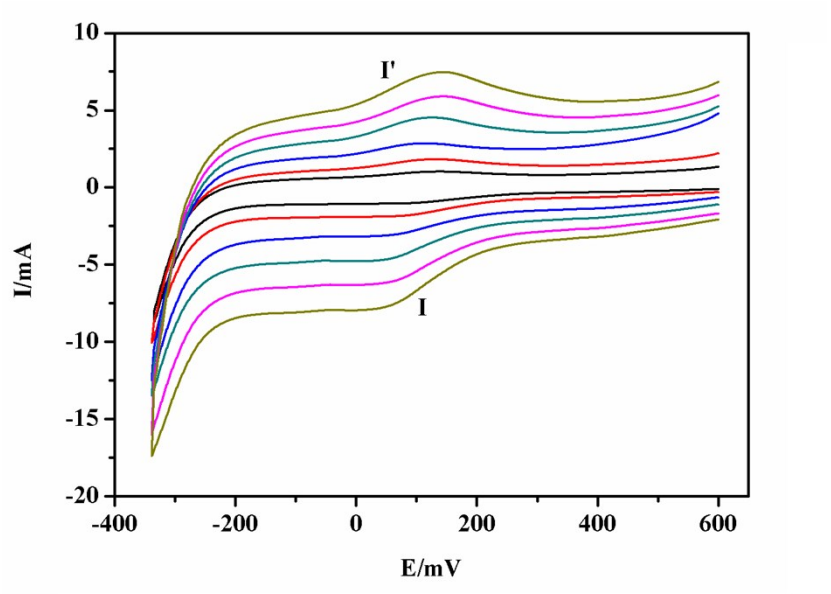
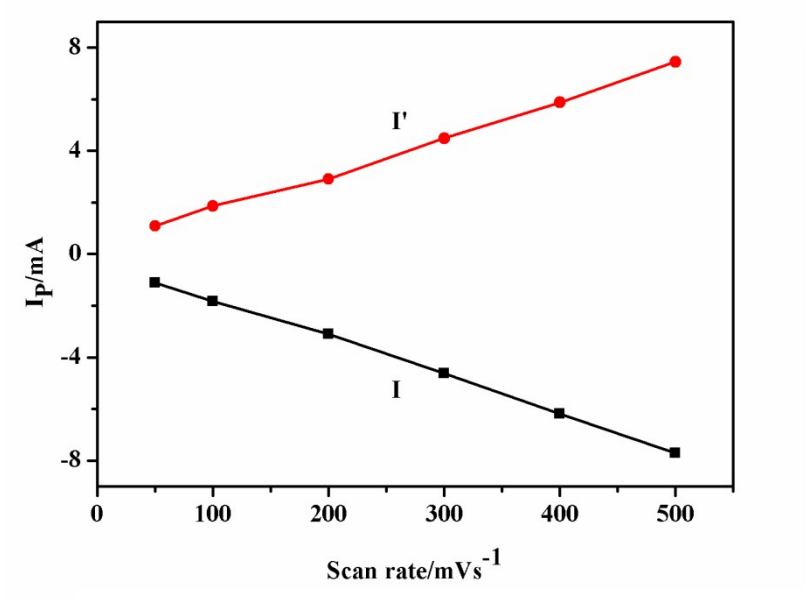


Fig. S6 Coordination mode of the L2 ligand.



(a)



(b)

Fig. S7 (a) Cyclic voltammograms of the CP **2** in 0.5 M Na_2SO_4 aqueous solution at different scan rates (from inner to outer: 50, 100, 200, 300, 400, 500 mV/s); (b) Dependence of cathodic peak and anodic peak currents of the CP **2** on the scan rates.

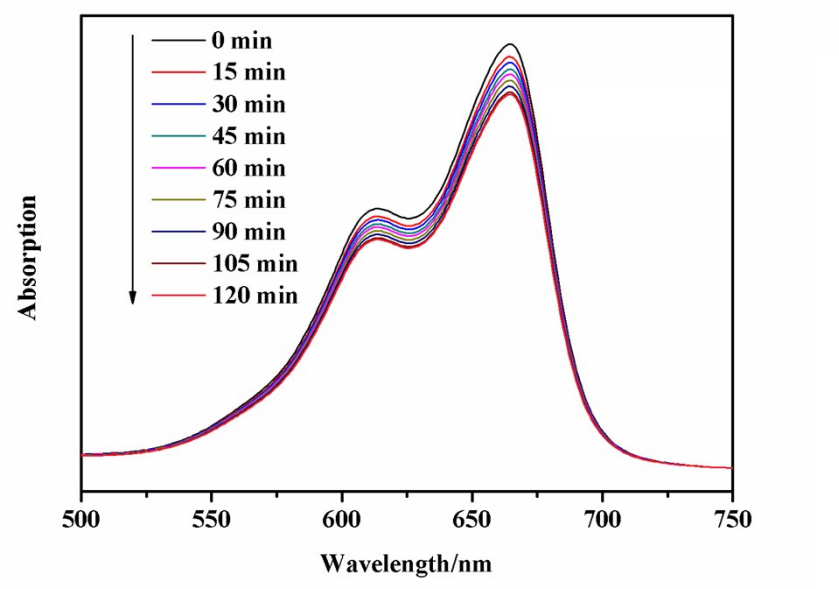


Fig. S8 Absorption spectra of the MB solution during the photodegradation reaction under UV irradiation without catalyst.

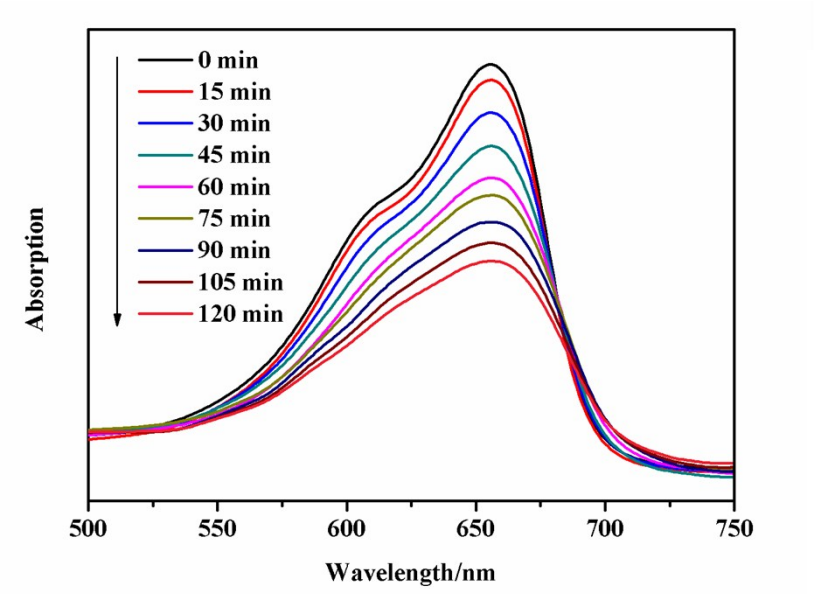


Fig. S9 Absorption spectra of the MB solution during the photodegradation reaction under UV irradiation in the presence of CP **1** and TBA.

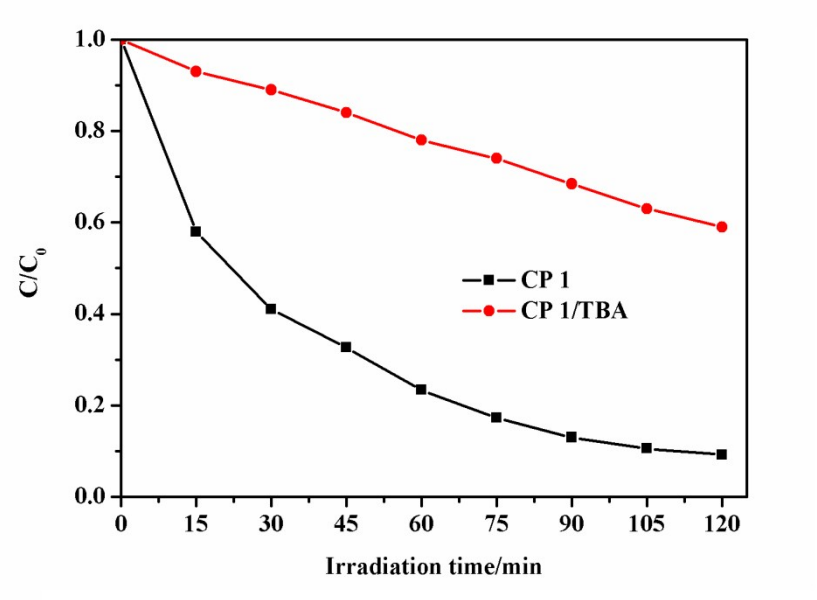


Fig. S10 Photocatalytic degradation of the MB solution under UV irradiation with the use of CP **1** and CP **1** in the presence of TBA.

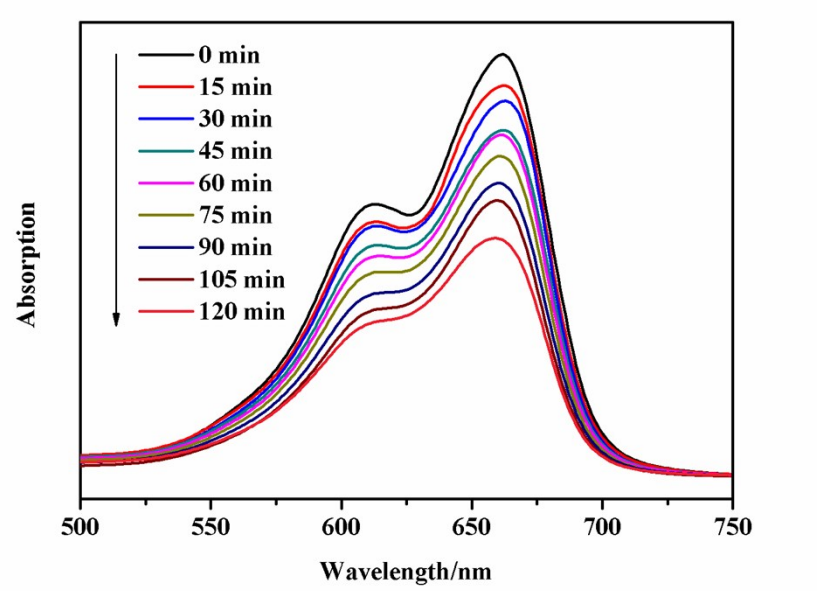


Fig. S11 Absorption spectra of the MB solution during the photodegradation reaction under UV irradiation in the presence of CP **2** and TBA.

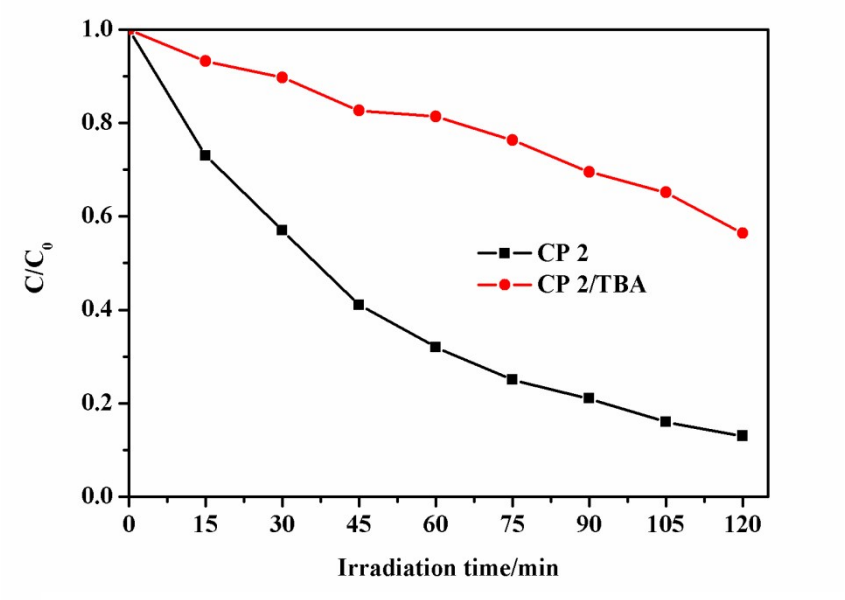


Fig. S12 Photocatalytic degradation of the MB solution under UV irradiation with the use of CP **2** and CP **2** in the presence of TBA.

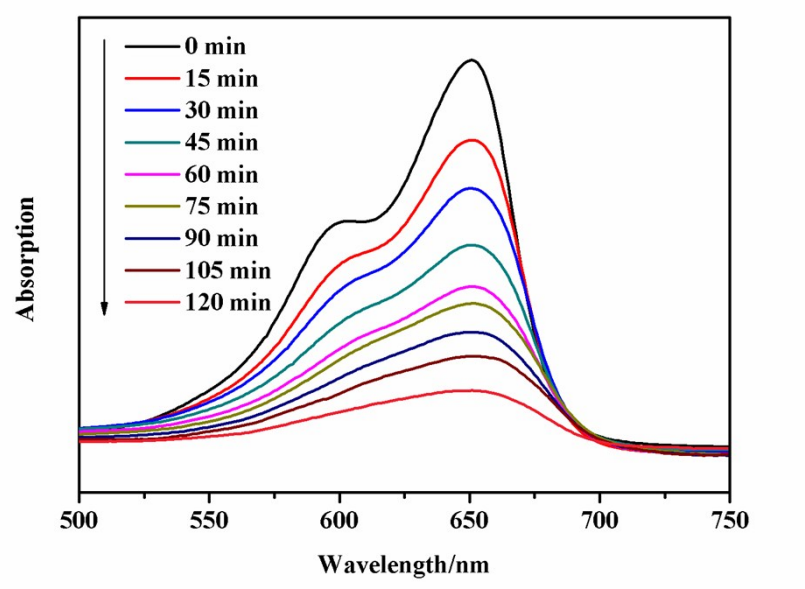


Fig. S13 Absorption spectra of the Congo red solution during the photodegradation reaction under UV irradiation in the presence of CP **1**.

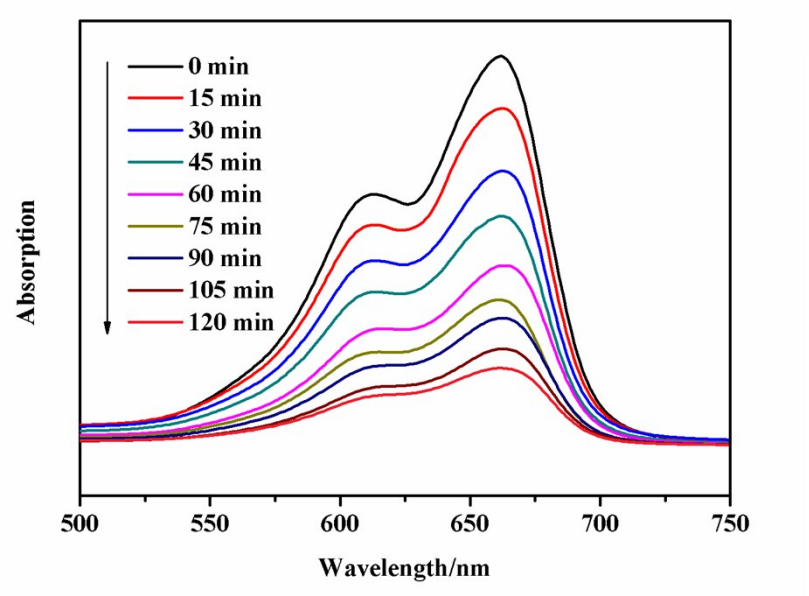


Fig. S14 Absorption spectra of the Congo red solution during the photodegradation reaction under UV irradiation in the presence of CP **2**.

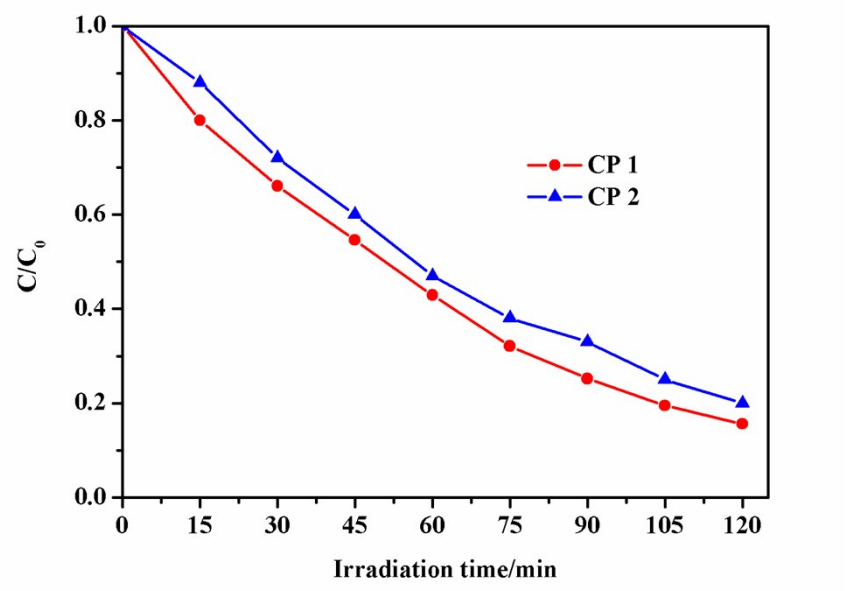


Fig. S15 Photocatalytic degradation of the Congo red solution under UV irradiation with the use of CP **1** and CP **2**.