

# Syntheses, structures, photoluminescence and photocatalysis of chiral 3D Cd(II) frameworks from achiral mixed flexible ligands by spontaneous resolution

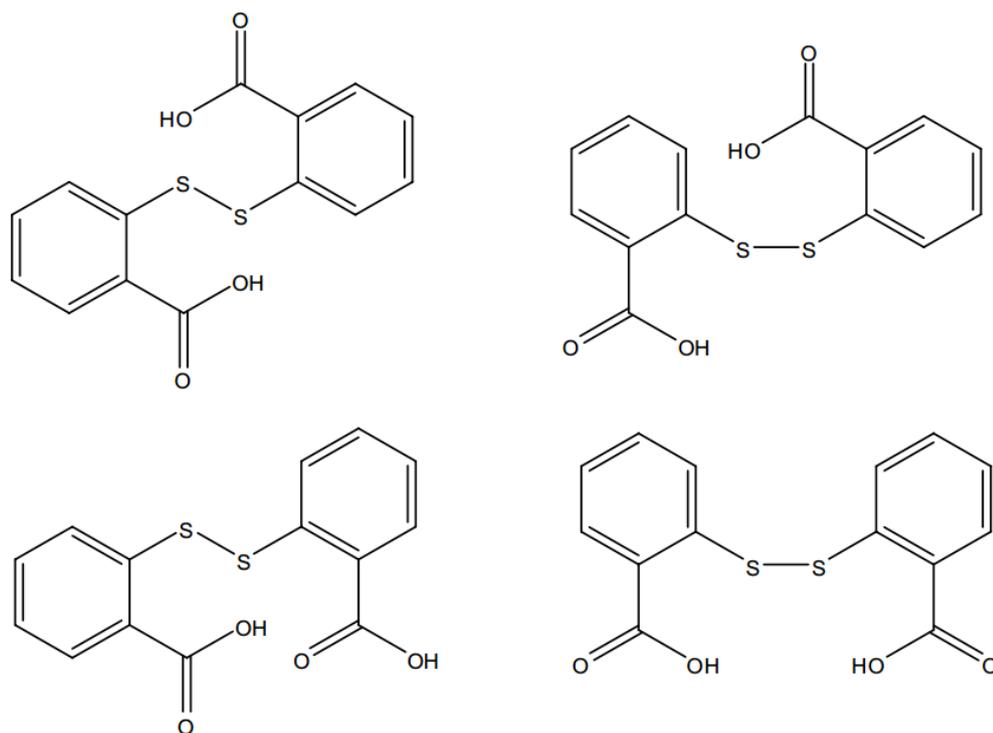
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**Fig.S1** The conformational isomers of H<sub>2</sub>dtba ligand.

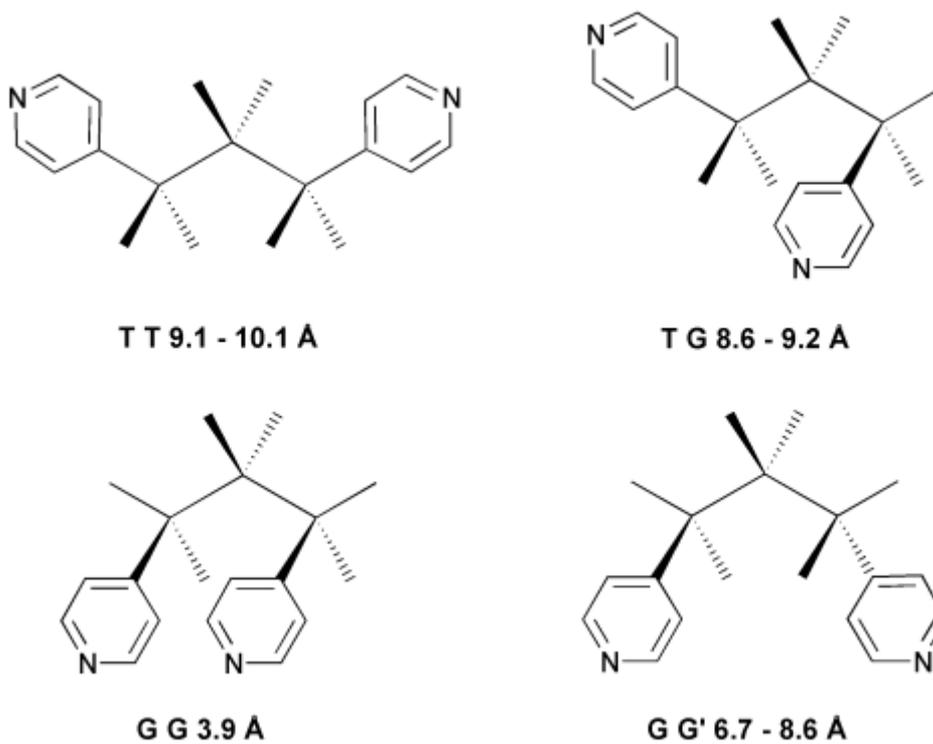


Fig.S2 The configurations of bpp ligands and the distance of -N-N-.

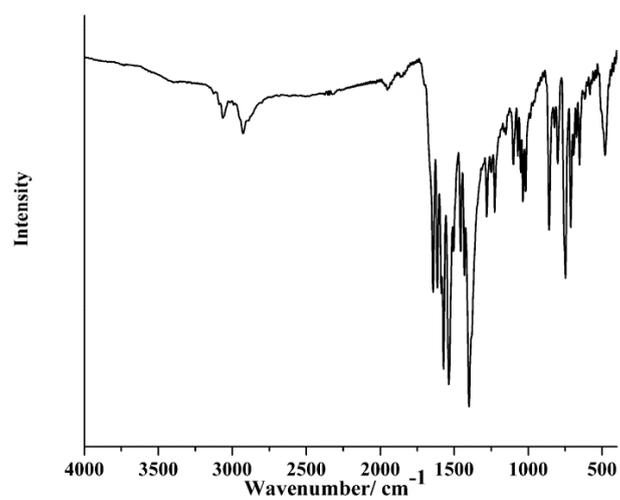
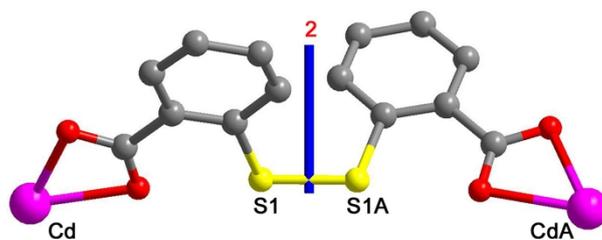
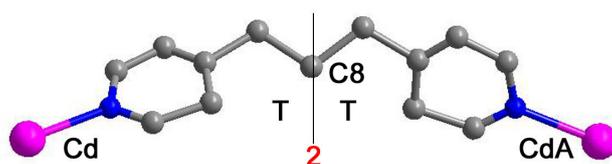


Fig.S3 The IR spectrum of compound 1.



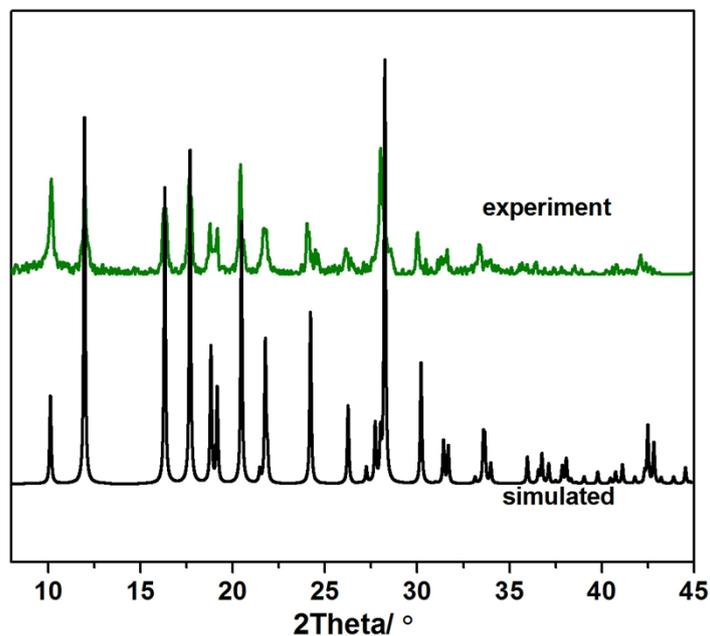
**Fig.S4** The coordination mode of dtba<sup>2-</sup> ligand of compound **1**.

The dtba<sup>2-</sup> ligand, with a two-fold axis passing through the middle of S-S bond, adopts a twist conformation with a C-S-S-C torsion angle of ca. 86°, which can show the axial chirality with the M- and P-forms of the enantiomers to construct interesting coordination frameworks. All the carboxylate groups of dtba<sup>2-</sup> ligand adopt chelating modes to connect two Cd(II) atoms.



**Fig.S5** The coordination mode of bpp ligand of compound **1**.

The bpp molecule, with a two-fold axis passing through C8 atom, has TT configuration and bridges two Cd(II) centers.



**Fig.S6** The good accordance of the experimental XRD patterns with the simulated patterns indicates phase purity of **1**.

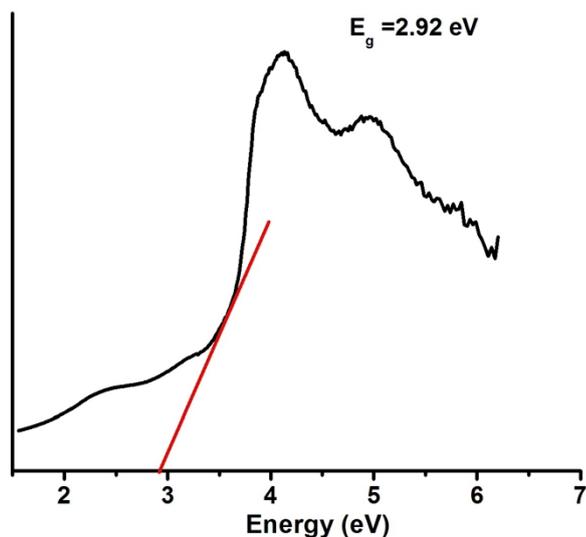


Fig.S7 The Solid UV spectrum for 1.

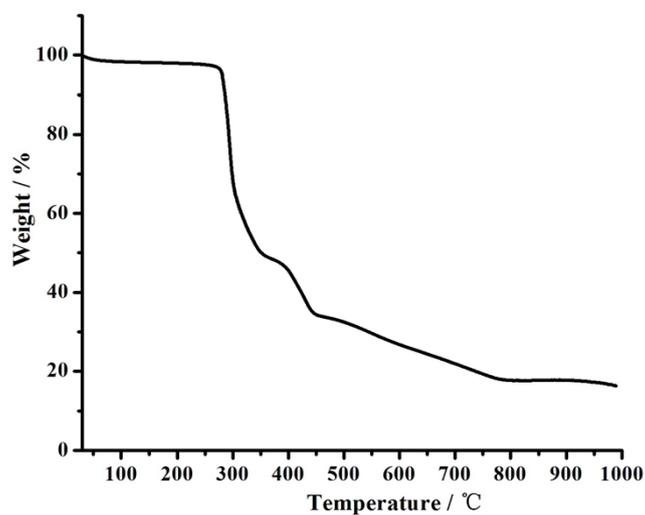


Fig.S8 The TGA curve of compound 1.

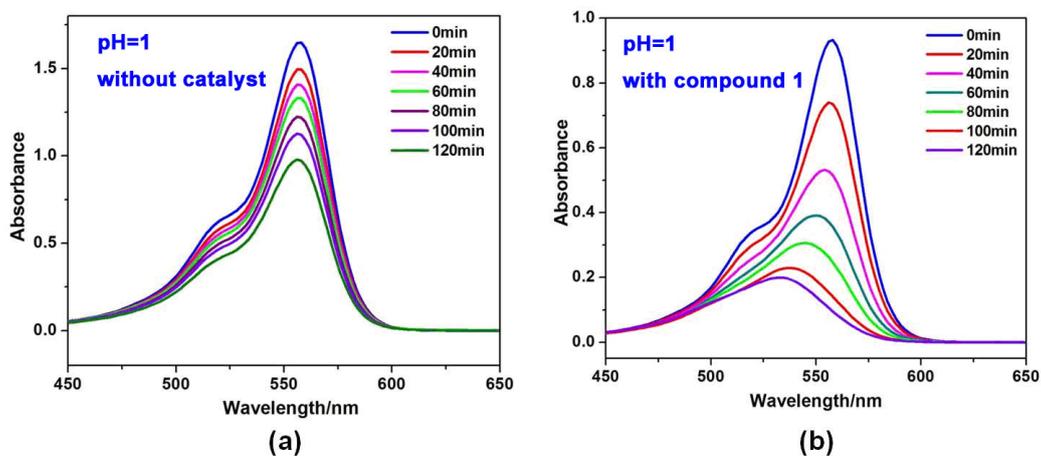
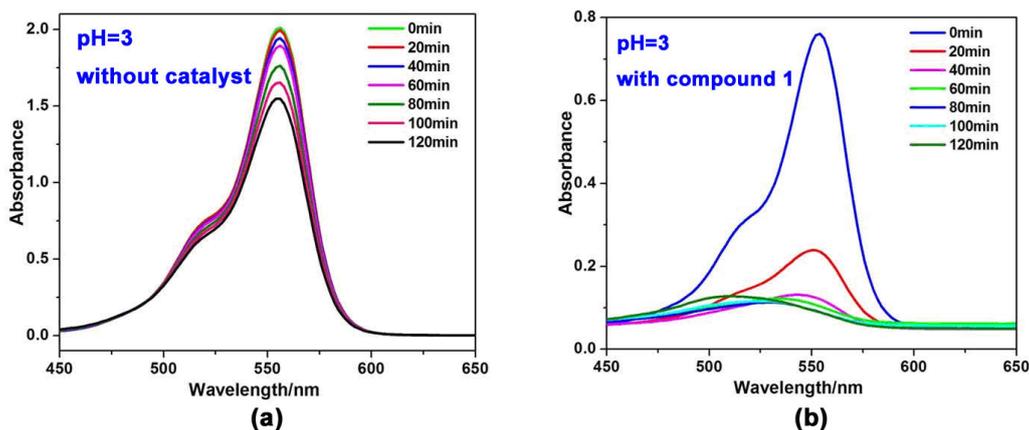
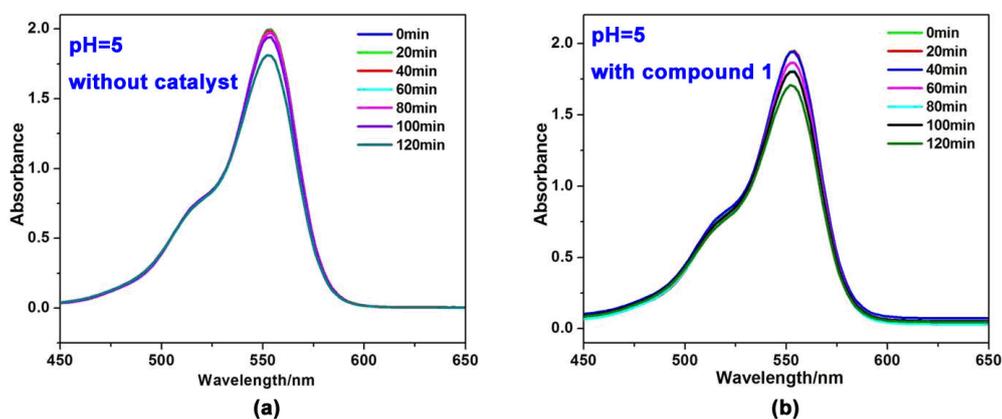


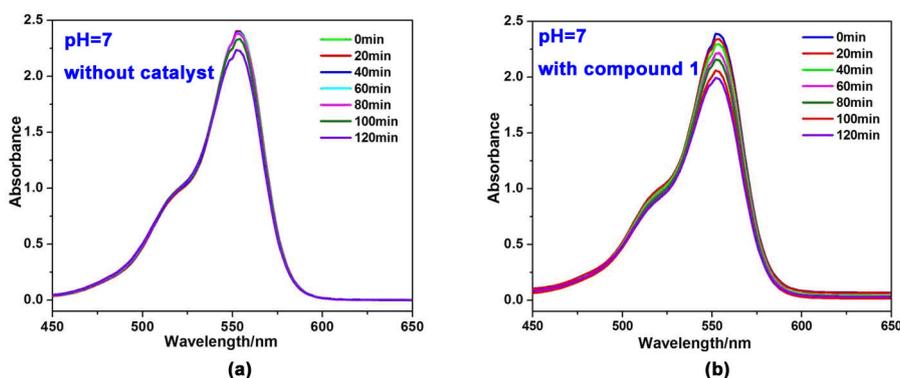
Fig.S9 Absorption spectra of the RhB aqueous solution with  $\text{pH} = 1$  during the photodegradation under 300 W high pressure Xe lamp irradiation without catalyst (a) and with compound 1 (b).



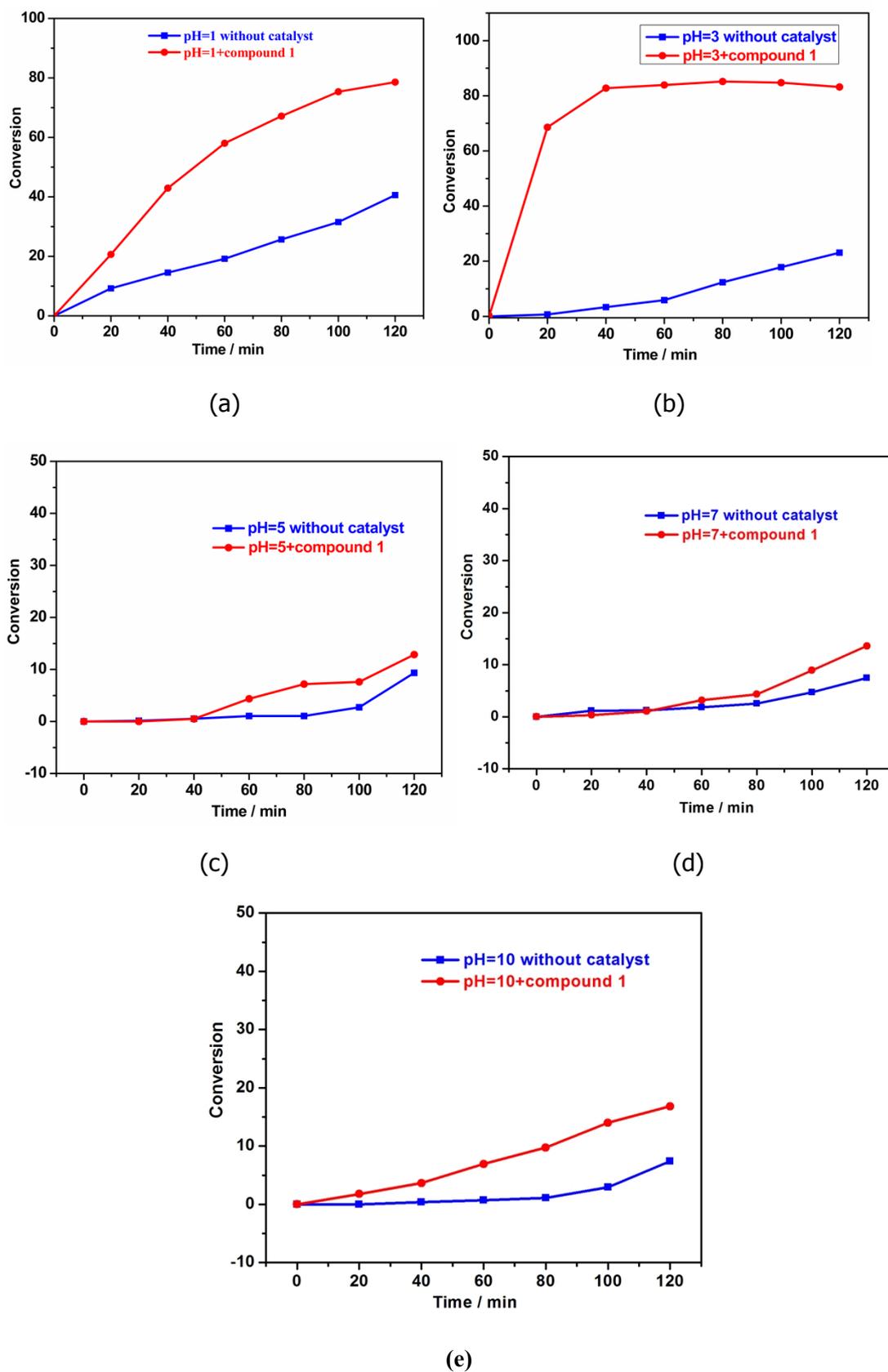
**Fig.S10** Absorption spectra of the RhB aqueous solution with pH = 3 during the photodegradation under 300 W high pressure Xe lamp irradiation without catalyst (a) and with compound 1 (b).



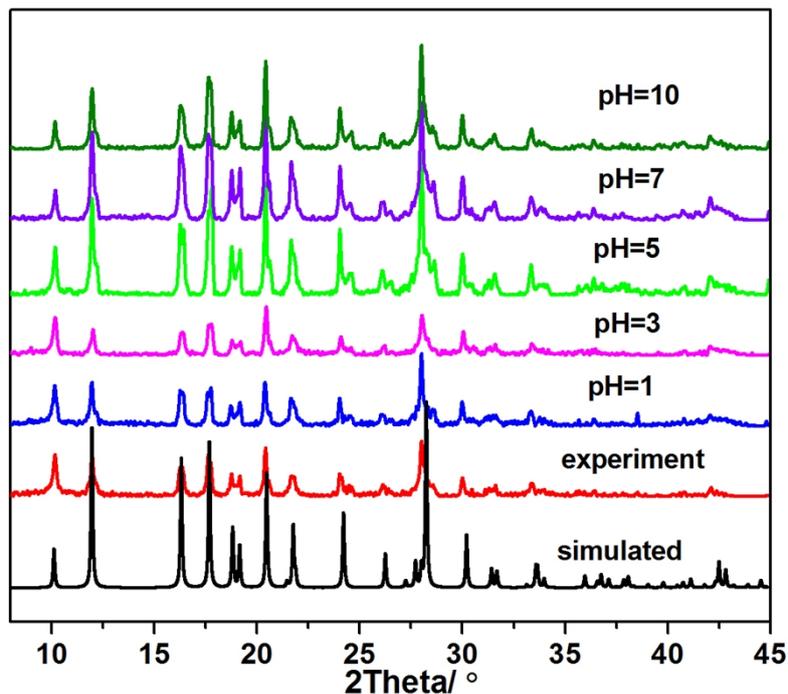
**Fig.S11** Absorption spectra of the RhB aqueous solution with pH = 5 during the photodegradation under 300 W high pressure Xe lamp irradiation without catalyst (a) and with compound 1 (b).



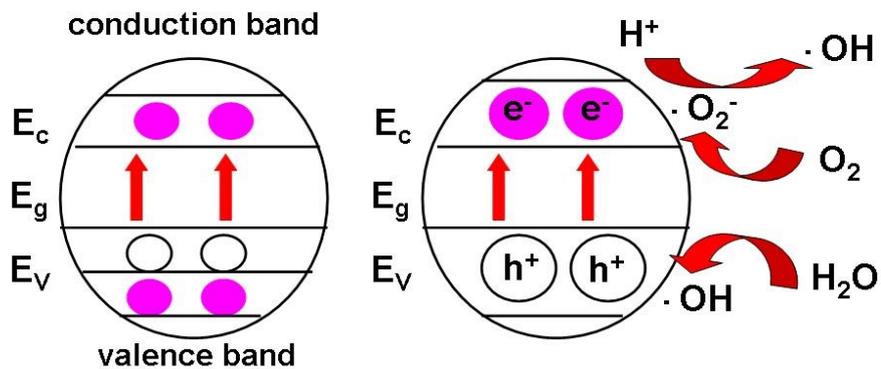
**Fig.S12** Absorption spectra of the RhB aqueous solution with pH = 7 during the photodegradation under 300 W high pressure Xe lamp irradiation without catalyst (a) and with compound 1 (b).



**Fig.S13** Conversion rate of RhB (K) with the reaction time (t) in different pH value solution (a) pH = 1; (b) pH = 3; (c) pH = 5; (d) pH = 7; (e) pH = 10 without catalyst and with compound 1.



**Fig.S14** PXRD patterns **1** (black, simulated; red, experimental; blue, activated in pH =1; purple, activated in pH =3; green, activated in pH =5; purple blue, activated in pH =7; dark green, activated in pH =10).



**Scheme S1** Schematic diagram of the photocatalytic mechanism of **1**.