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Supplementary Information

Band structure engineering of boron-oxygen based materials for efficient charge separation

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1 Experimental and computations details

1.1 LC-MS and FL characterization

The intermediate products during the chlorophenol degradation were qualitatively analyzed by a liquid chromatography- mass spectrometry (LC-MS, Agilent 1290) with a C18 column (4.6 mm ×250 mm). A mixture of methanol and water [80/20 (v/v)] was used as an effluent with the flow rate 1 mL/min, detector wavelength 282 nm. Fluorescence spectra were measured on a Hitachi fluorescence spectrophotometer F-7000.

1.2. Computational Details.

The exchange-correlation interaction was described by the generalized gradient approximation (GGA) and the Perdew-Burke-Ernzerhof (PBE) functional. A double-numerical basis set with polarization functions (DNP) was used, and spin unrestricted DFT calculations were performed. The convergence criteria included threshold values of 2 × 10-5 Ha, 0.004 Ha/Å, and 0.005 Å for energy, max force, and max displacement, respectively. Moreover, a self-consistent-field (SCF) density convergence threshold value of 1.0×10^{-5} Ha was used. A 15 Å vacuum was employed between the repeating slabs along the z-direction. A (3 × 3 × 1) k-point mesh was used to sample the surface Brillouin zone.

1.3 Photocatalytic degradation of CPs

During the experiment, 50 mg of a tested photocatalyst sample was dispersed in 100 mL solution of CPs (2,4-DCP, 2,6-DCP and 2,4,6-TCP) in a 200 mL glass beaker with a concentration 50 mg/L and stored for 30 min while being stirred in the dark to attain adsorption equilibrium. Then, the reactor was illuminated by a 500 W mercury light ($\lambda > 254$ nm). The intensity of light irradiated on the sample was measured to be 0.15-0.18 W/cm^2 with an optical densitometer. The same amount of solution was periodically extracted from the reactor. The percentage of residual CPs solution for the corresponding selected irradiation time is expressed as C/C_0, where C_0 is the concentration of the CP solution at the initial stage, and C is the concentration at selected irradiation times (0, 4, 8, 12, 16, and 20 min). For comparison, the blank experiments were also carried out under the same condition. Throughout the experiment, the concentration of chlorophenol was detected by HPLC.

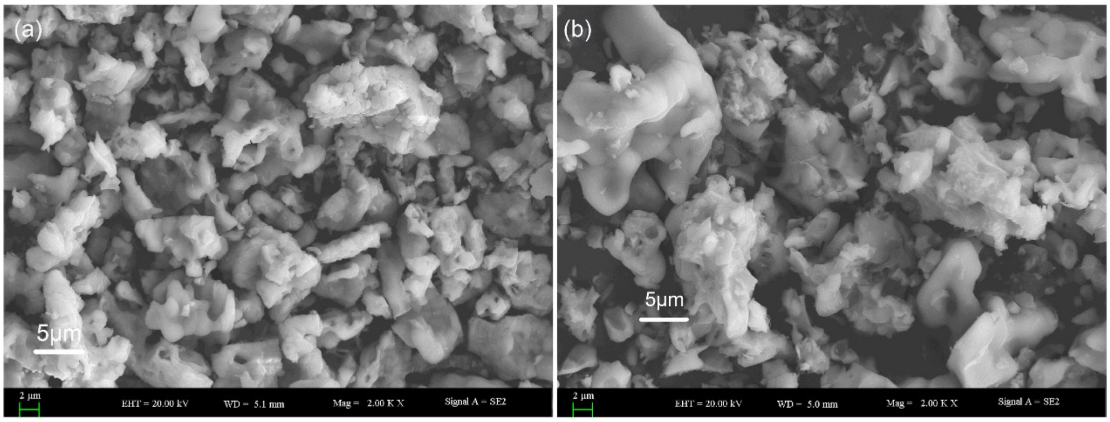

Figure S1. SEM images of (a) KBBO and (b)NBBO samples.

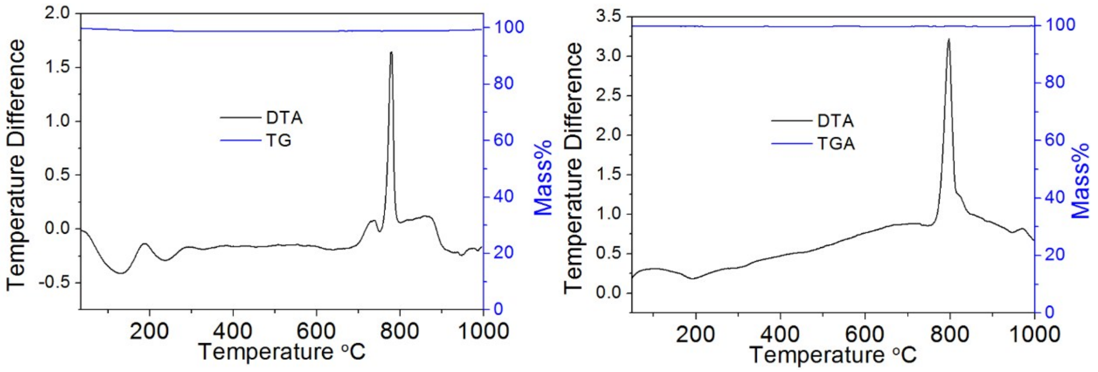

Figure S2. TGA/DTA curve of the KBBO(a) and NBBO(b) samples.

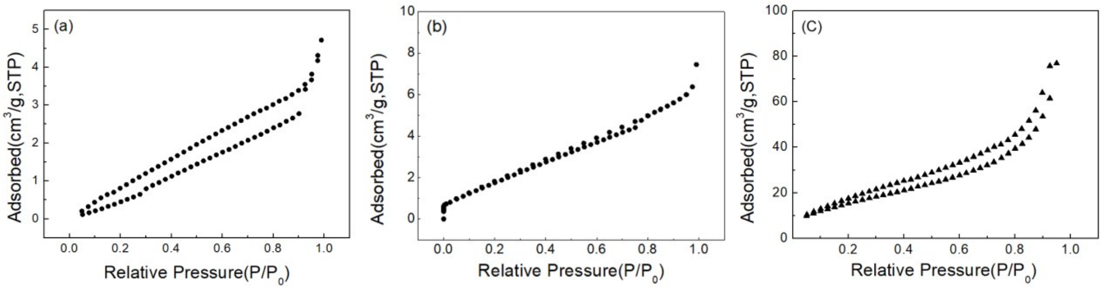

Figure S3. BET spectra of the KBBO(a), NBBO(b) and TiO_2 (c) samples

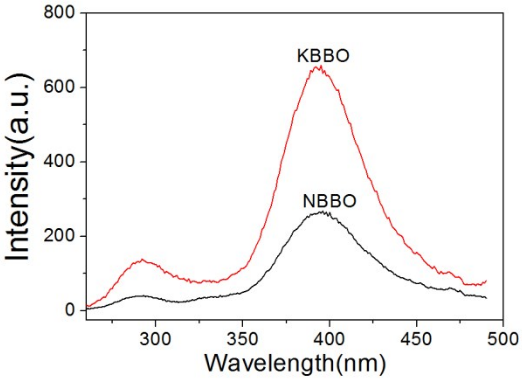

Figure S4. Photoluminescence spectra of KBBO and NBBO samples.

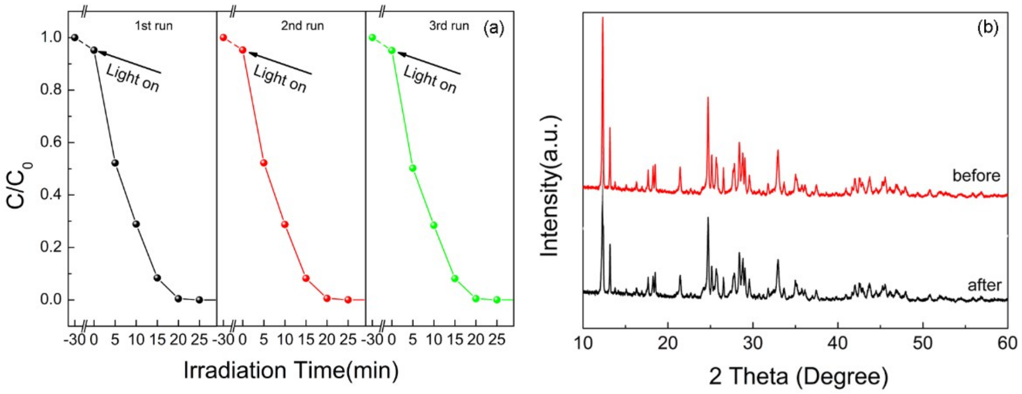

Figure S5. The stability test for three cycling 2,4-DCP degradation of KBBO under UV-visible light irradiation.

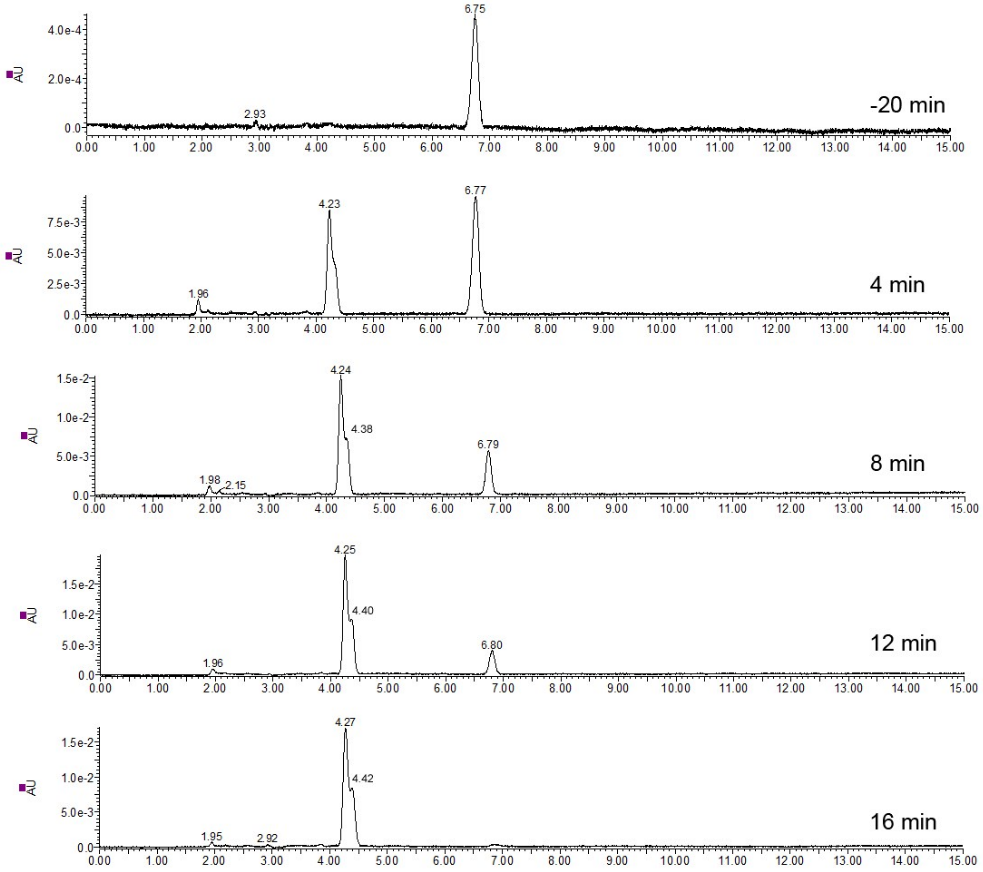

Figure S6. The LC of 2,4-DCP the photodechlorination in the presence of KBBO samples under UV-visible light.

Table S1. LC-MS data of photodegraded products of 2, 4-DCP.

Retention time (min)	Mw (m/z)	Assignment	CAS no.
6.77-6.8	162.19	2, 4-dichlorophenol	120-83-2
4.38-4.42	143.15	2-chlorohydroquinone	615-67-8
4.23-4.27	128.35	4-chlorophenol	106-48-9
2.15	108.19	1,4-benzoquinone	106-51-4
1.95-1.98	95.06	phenol	108-95-2