Supplementary material

Copper phosphide-phosphorus (Cu_3P/P) hybrid nanomaterials: an in-situ dioxygen activator in ambident aqueous condition for advanced oxidation process

Jiaojiao Hu,[a] Guoxi Deng,[a] Jiayi Ru,[a] Xiaodan Chen*[a,b]

*Corresponding authors

[a]Guangdong Provincial Key Laboratory of Functional Supramolecular Coordination Materials and Applications, College of Chemistry and Materials Science, College of Chemistry and Materials Science, Jinan University, Guangzhou 510632, China

[b]International Innovation Center for Forest Chemicals and Materials, Nanjing Forestry University, Nanjing 210037, China

E-mail: chxdlzhsh@jnu.edu.cn

Chemicals and reagents:

Whahaha's bottled water was used as the ultrapure water (UPW) for all the reactions. SMX (purity > 99%), polyvinylpyrrolidone (PVP), p-benzoquinone (BQ) were provided by Macklin Reagent Co., Ltd (Shanghai, China). Copper(I) iodide (CuI), red phosphorus (P), sodium (Na), diethyl carbonate (DEC), sodium bicarbonate ($NaHCO_3$), sodium chloride (NaCl), sodium acetate (NaOAc) and catalase (Cat) were purchased from Aladdin Reagent Co., Ltd (Shanghai, China). Nitroblue tetrazolium (NBT) and N, N-diethyl-1, 4-phenylenediamine (DPD) were bought from TCI (Shanghai) Development Co. Ltd. Coumarin was purchased from Energy Chemical (Shanghai,China). 5,5-dimethyl-1-pyrroline N-oxide (DMPO) was bought from DOJINDO (Japan). Acetonitrile and methanol (HPLC grade) were supplied by Sigma Aldrich (St. Louis, MO, USA). All other reagents were of analytical grade, which were purchased from Tianjin Chemical Reagents Company (Tianjin, China). All the chemical reagents except sodium phosphathynolate (NaOCP) were used directly as we received. Sodium phosphathynolate (NaOCP) was prepared according to the procedure reported in the literatures.[1]

This supplementary information (SI) contains one table, four figures, and this cover page.

Table S1. Reaction of NaOCP with CuI as a copper source under different synthesis conditions

CuI:NaOCP Ratio	Solvent	stabilizer	Temperature	Reaction time	Results
1:1	UPW	CTAB	Room temperature	12 h	×
1:3	UPW	CTAB	Room temperature	12 h	×
1:6	UPW	CTAB	Room temperature	12 h	×
1:3	Oleylamine	CTAB	Room temperature	12 h	×
1:3	Oleylamine	CTAB	60 ℃	12 h	×
1:3	Oleylamine	CTAB	100 ℃	12 h	×
1:3	THF	CTAB	Room temperature	12 h	×
1:3	THF	CTAB	60 ℃	12 h	×
1:3	THF	CTAB	100 ℃	12 h	×
1:3	UPW	PEG	Room temperature	12 h	×
1:3	UPW	PEG	60 ℃	12 h	×
1:3	UPW	PEG	100 ℃	12 h	×
1:3	UPW	PVP	Room temperature	12 h	×
1:3	UPW	PVP	60 ℃	12 h	×
1:3	UPW	PVP	100 ℃	12 h	√
1:3	UPW	PVP	100 ℃	8 h	√

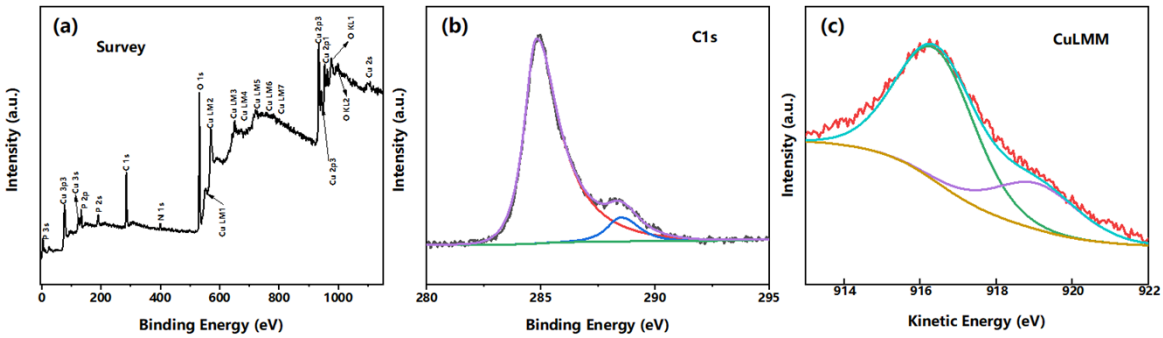

Fig. S1. The XPS spectrum of Cu_3P/P : **(a)** survey spectra **(b)** C1s peaks **(c)** Auger spectrum of Cu.

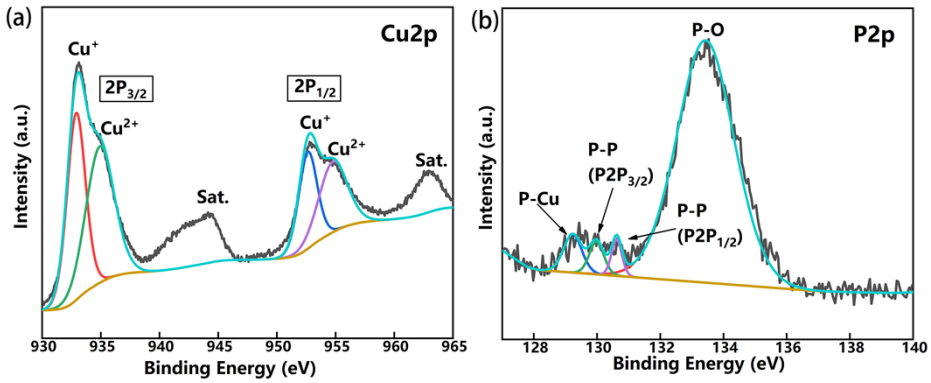

Fig. S2. XPS spectra of Cu_3P/P after the degradation in pH3 conditions corresponding to Cu 2p (a) and P2p (b). Reaction conditions: [SMX] = 18 mg/L [Cu_3P/P] = 120 mg/L.

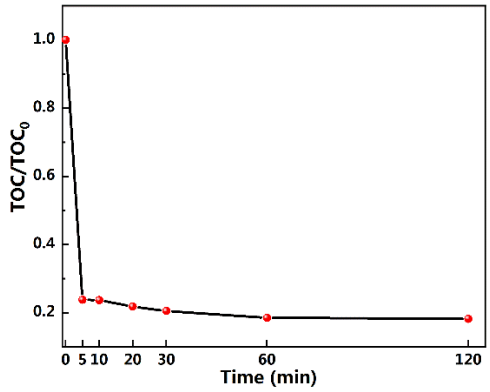

Fig. S3. Mineralization degree of SMX in Cu_3P/P UPW suspension. Experimental condition: [Cu_3P/P] = 60 mg/L, [SMX] = 18 mg/L, $[TOC]_0$ = 10 mg/L.

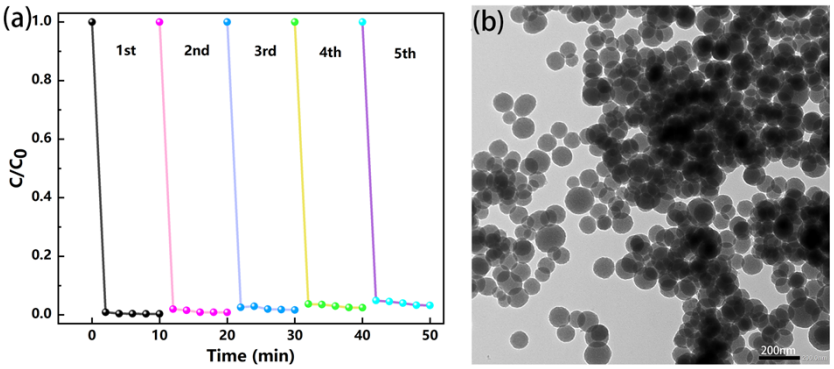

Fig. S4. (a) Degradation of SMX during five different batch runs using Cu_3P/P, (b) TEM images of Cu_3P/P nanoparticle after five degradation cycles. Reaction conditions: [SMX] = 18 mg/L [Cu_3P/P] = 120 mg/L.

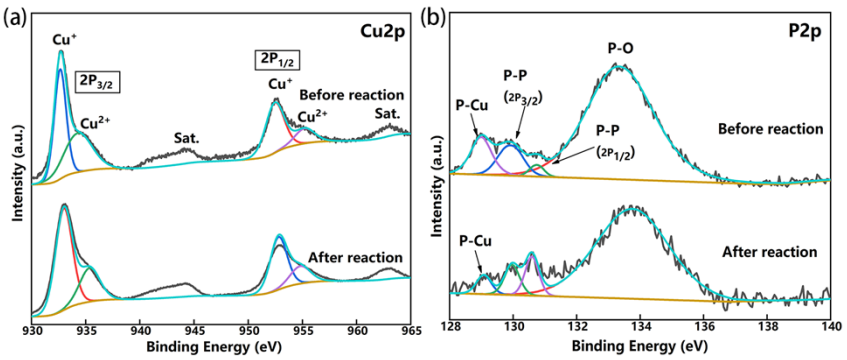

Fig. S5. XPS spectra of Cu_3P/P before and after five degradation cycles corresponding to Cu 2p (a) and P2p (b). Reaction conditions: [SMX] = 18 mg/L [Cu_3P/P] = 120 mg/L.

1 F. F. Puschmann, D. Stein, D. Heift, C. Hendriksen, Z. A. Gal, H.-F. Grützmacher and H. Grützmacher, *Angew. Chem. Int. Ed.*, 2011, **50**, 8420–8423.