Photo(electro)catalytic activity enhancement of PhC_2Cu by Fe doping induced energy band modulation and luminescence chromism switching

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Theoretical calculations

The theoretical calculations were carried out using the plane wave pseudopotential DFT[1] method using the projector augmented wave (PAW) pseudopotentials[2,3] implemented using the Vienna abinitio simulation program (VASP).[3] The GGA scheme was employed. The valence configurations including valence and semicore electrons are $2s^22p^2$ for carbon, $3d^{10}4p^1$ for copper and $3d^74s^1$ for iron according to the PAW scheme.[1] The cutoff energy is 450 eV and the Monkhorst–Pack[4] k-point mesh for the 56-atom-supercell was 2×5×3, 112-atom-supercell 2×3×3 and 168-atom-supercell 2×2×3, respectively. We performed structural relaxations of the crystal until the total energy was converged to 10^{-5} eV and the residual forces on atoms were below 0.02 eV $Å^{-1}$.

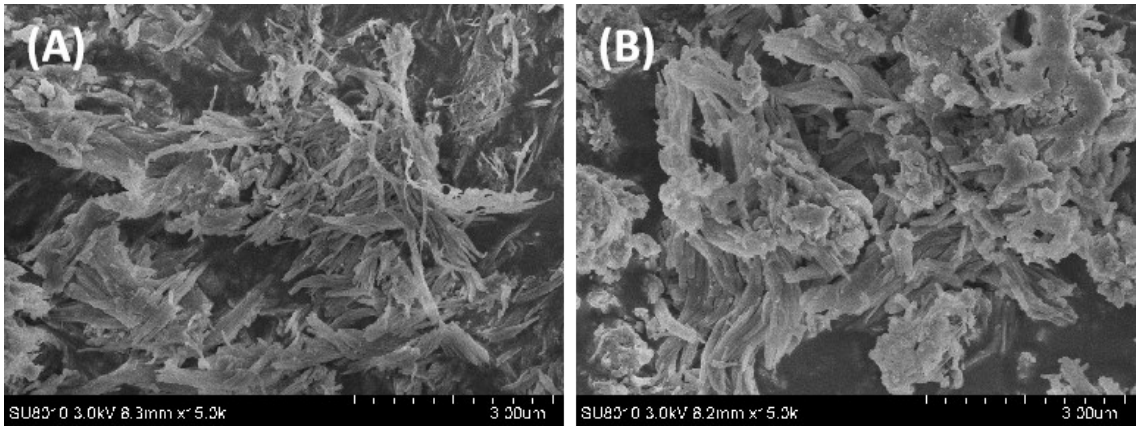

Figure S1 (A) SEM image of PhC_2Cu; (B) SEM image of 2% Fe/PhC_2Cu.

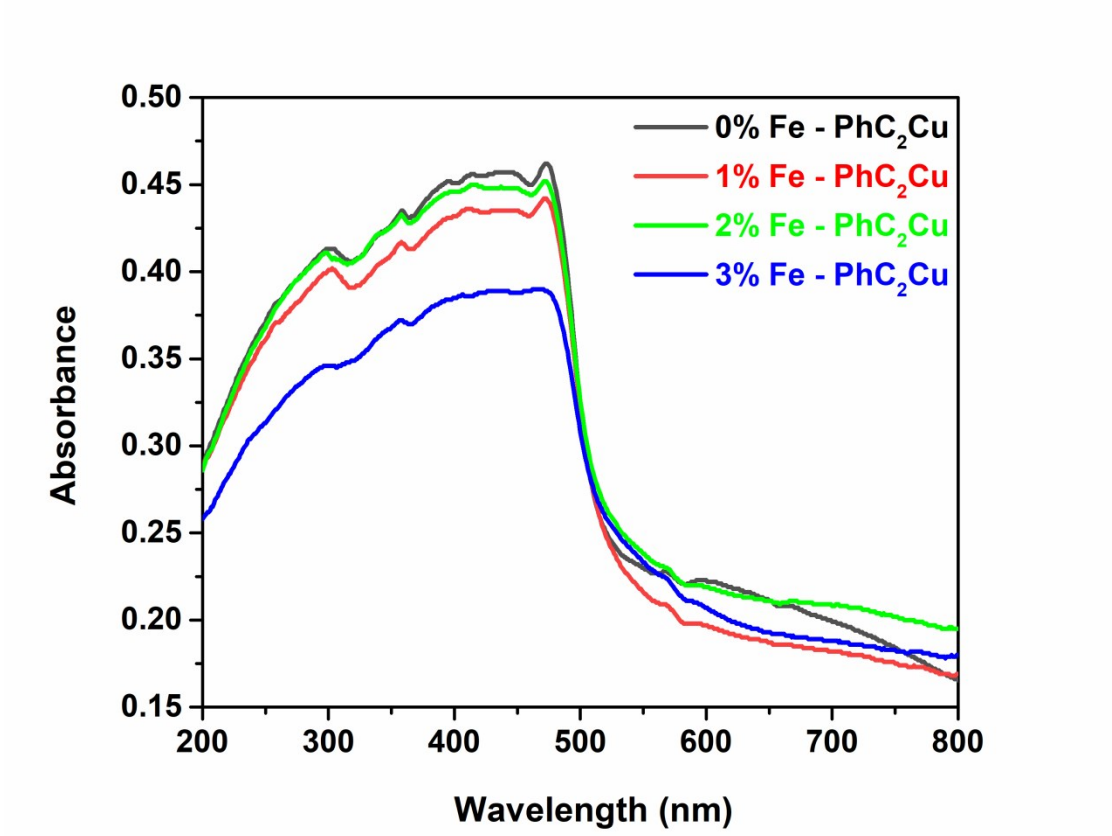

Figure S2 UV-vis DRS spectra of the as-prepared Fe-PhC_2Cu samples.

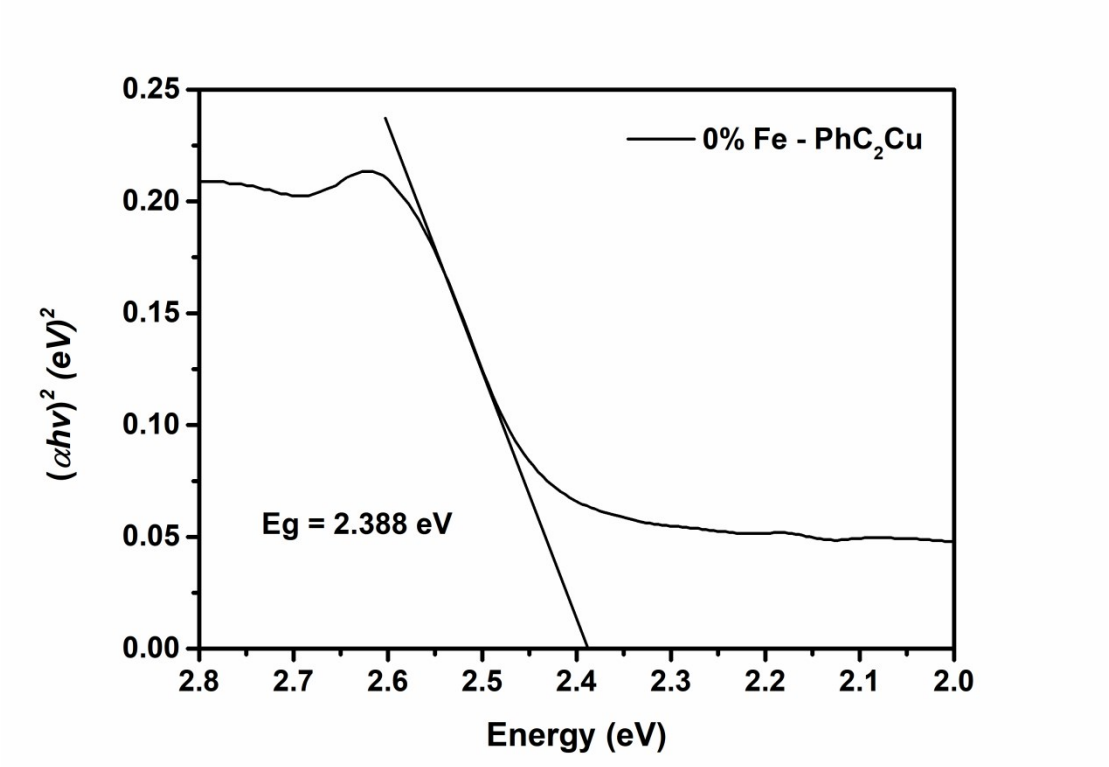

Figure S3 Tauc plot curve of 0% Fe-PhC_2Cu.

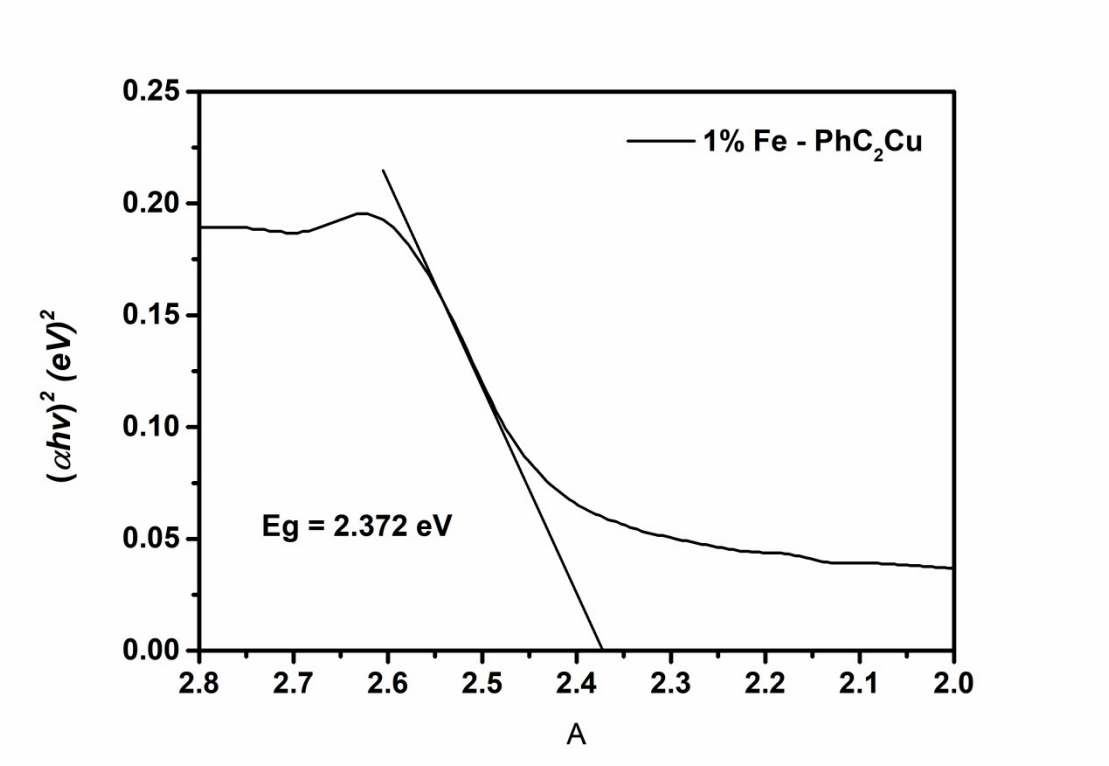

Figure S4 Tauc plot curve of 1% Fe-PhC_2Cu.

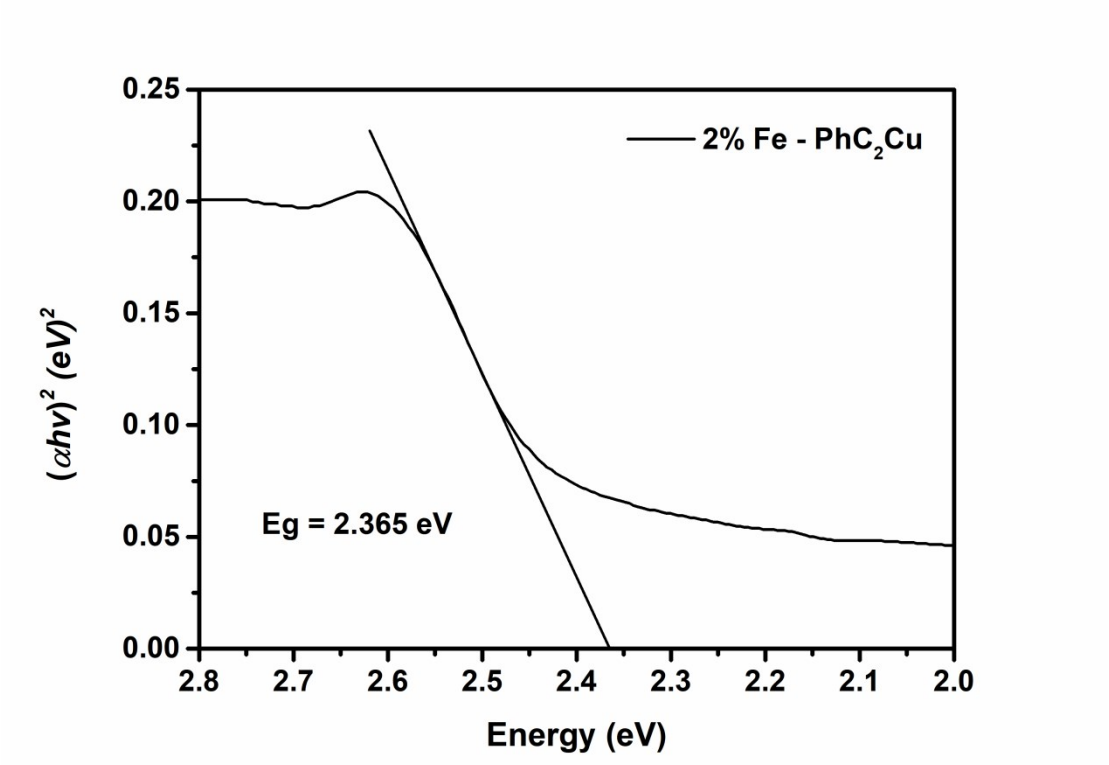

Figure S5 Tauc plot curve of 2% Fe-PhC_2Cu.

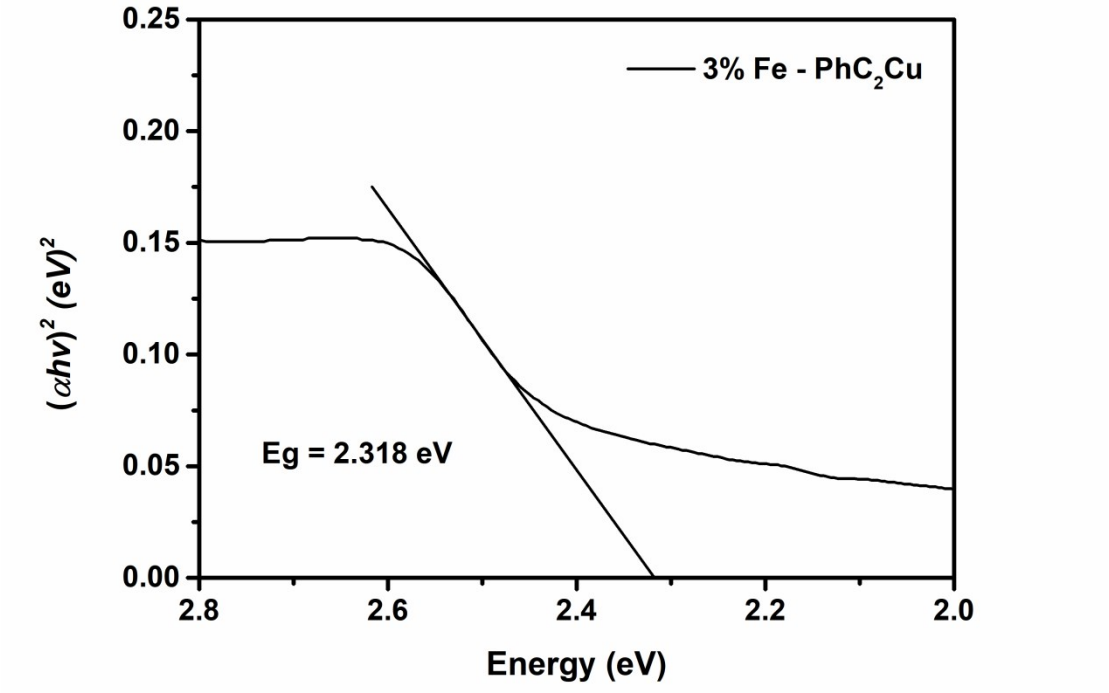

Figure S6 Tauc plot curve of 3% Fe-PhC_2Cu.

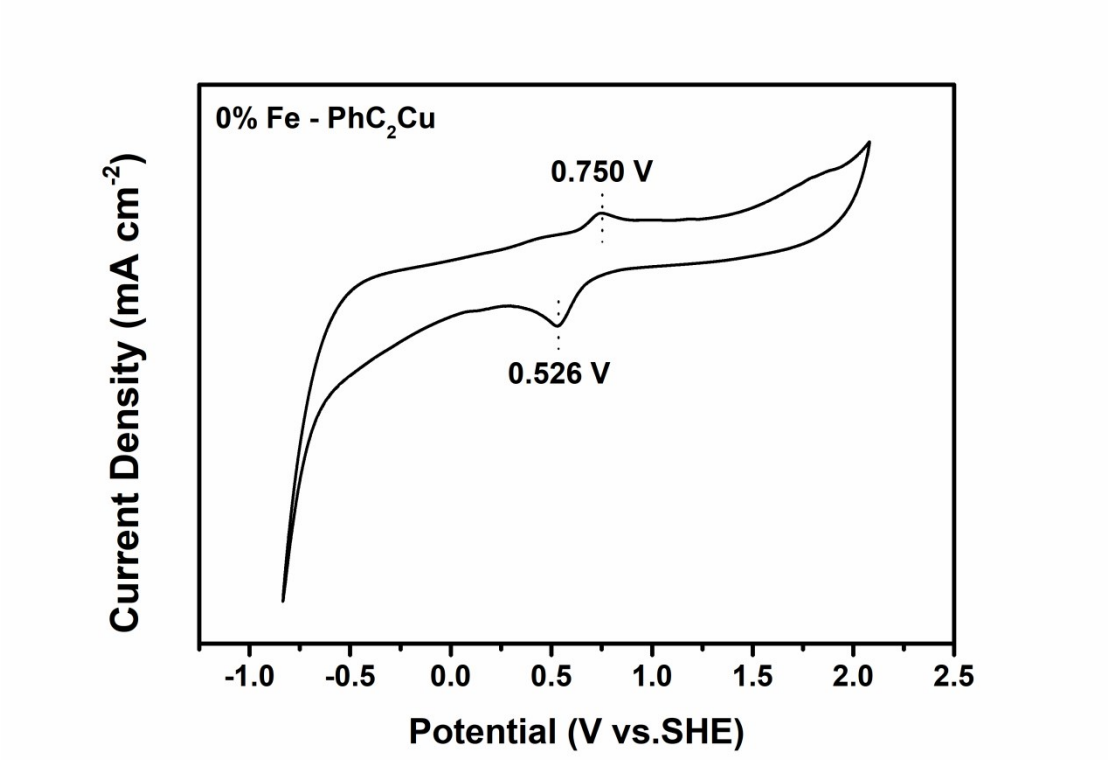

Figure S7 Cyclic voltammetry curve of 0% Fe-PhC_2Cu.

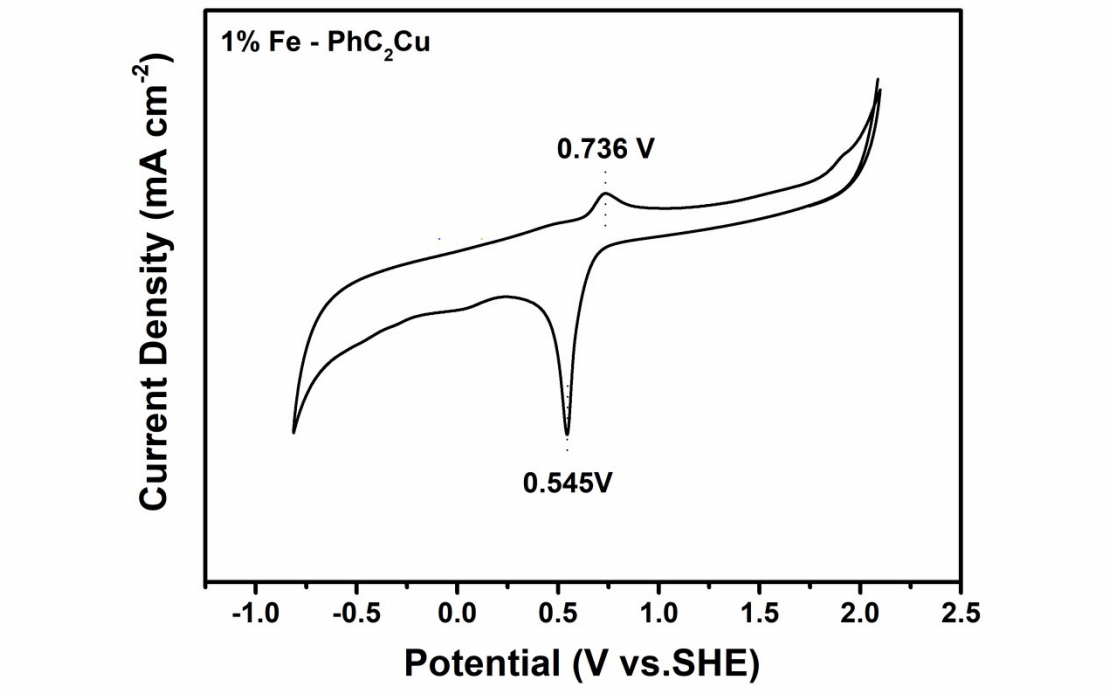

Figure S8 Cyclic voltammetry curve of 1% Fe-PhC_2Cu.

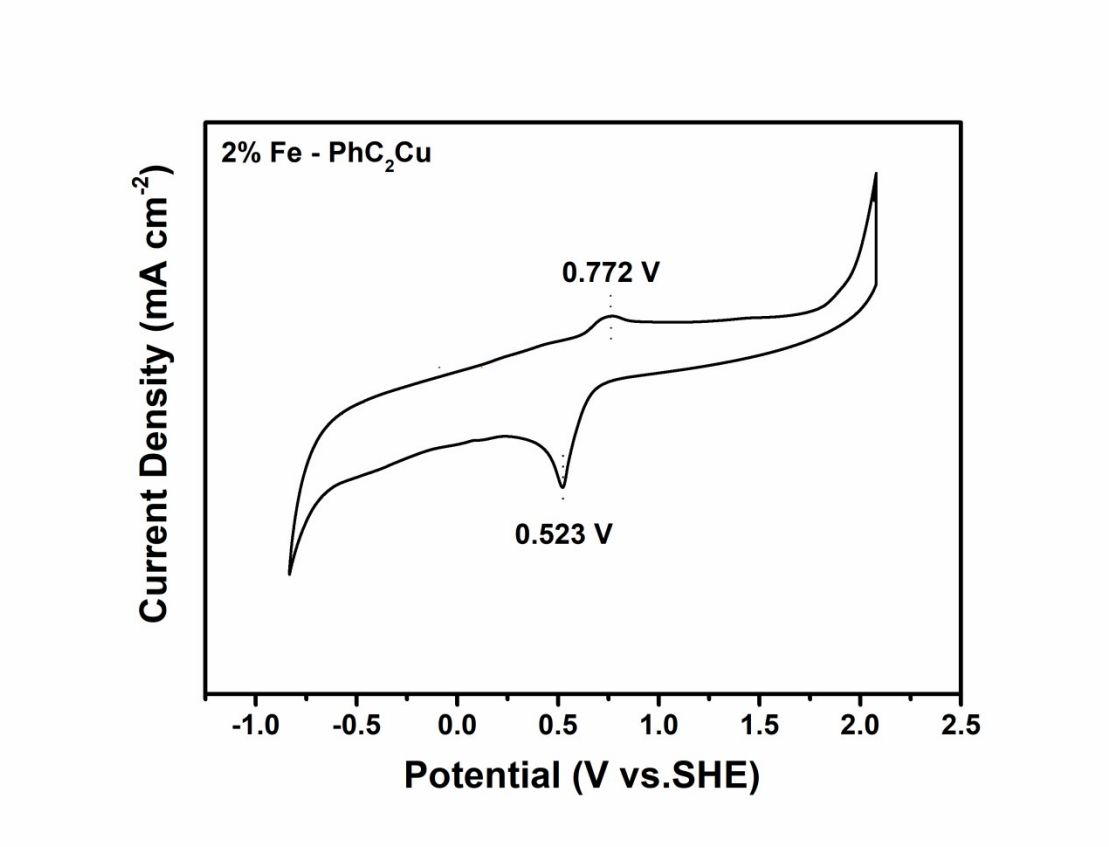

Figure S9 Cyclic voltammetry curve of 2% Fe-PhC_2Cu.

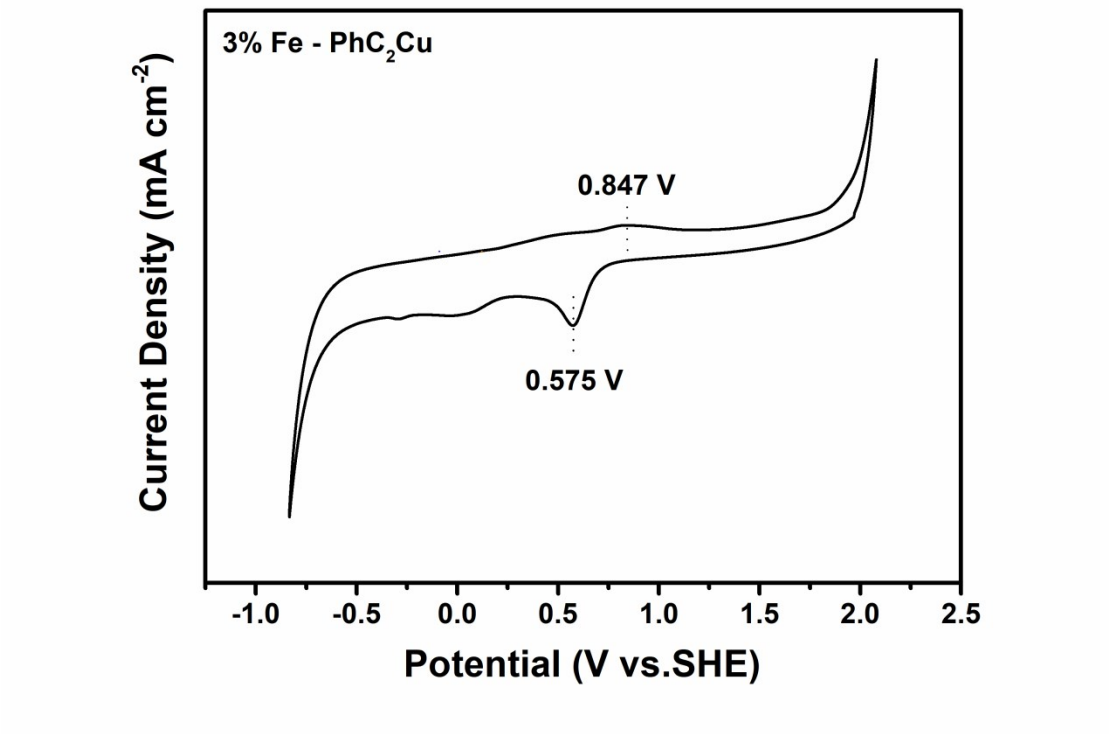

Figure S10 Cyclic voltammetry curve of 3% Fe-PhC_2Cu.

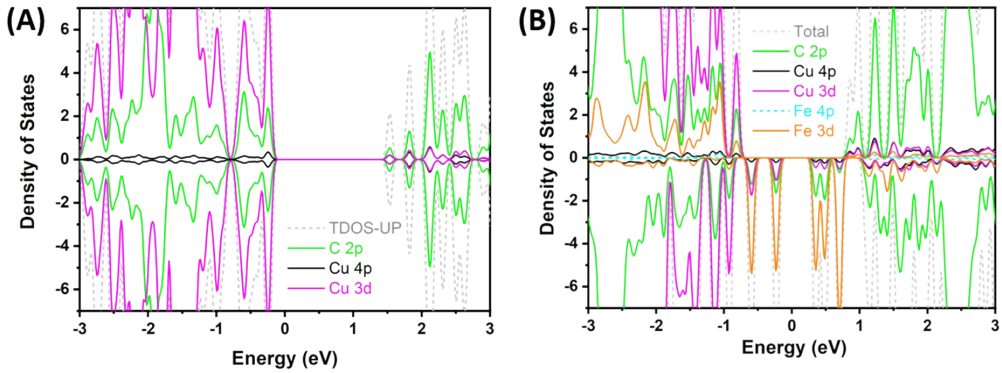

Figure S11 Calculated density of states (DOS) of PhC_2Cu (A) and Fe-PhC_2Cu (B).

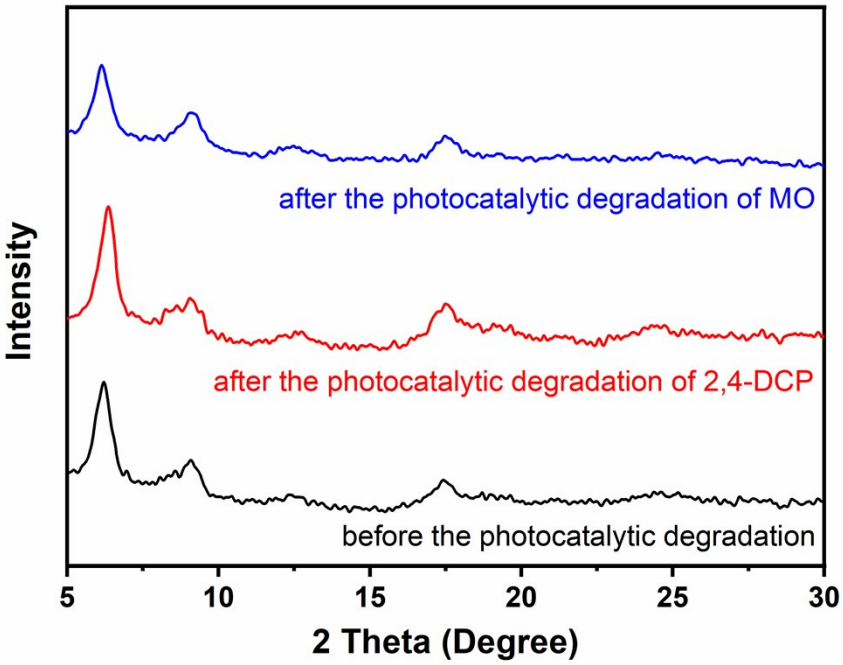

Figure S12 XRD patterns of 2% Fe/PhC_2Cu before and after the photocatalytic degradation of 2,4-DCP and MO.

Table S1 The mole ratios of Fe:Cu for the Fe-PhC_2Cu samples detected by ICP-OES

Sample	0% Fe-PhC_2Cu	1% Fe-PhC_2Cu	2% Fe-PhC_2Cu	3% Fe-PhC_2Cu
n_{Fe} : n_{Cu} (%)	0.25	1.48	2.01	3.46

Table S2 The energy band structures of the Fe-PhC_2Cu samples

Sample	0% Fe-PhC_2Cu	1% Fe-PhC_2Cu	2% Fe-PhC_2Cu	3% Fe-PhC_2Cu
Band Gap (eV)	2.388	2.372	2.365	2.318
Valence Band (V vs. SHE)	0.638	0.641	0.648	0.711
Conduction Band (V vs. SHE)	-1.750	-1.731	-1.717	-1.607

1. P. Hohenberg and W. Kohn, *Phys. Rev.* 1964, **136**, B864
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