Electronic supplementary Information:

Single-source mediated electrosynthesis of *p*-Cu_2S thin films on TCO with enhanced photocatalytic activities

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Contents:

Table S1: Crystal data and structure refinement parameters for the crystal

Empirical formula	$C_{14}\ H_{20}\ Cl_2\ Cu_2\ N_4\ S_4$
Formula weight	570.56
Crystal system	Triclinic
Space group	P-1
a/Å	10.5271(9) Å
b/Å	10.7784(9) Å
c/Å	10.9396(9) Å
α/°	68.855(4)°
β/°	65.795(4)°
γ/°	78.787(5)°
V/Å^3	1054.33(15)
Z	2
$D_{calc.}$/mg.m^{-3}	1.797
Absorption coefficient/mm^{-1}	2.674
F(000)	576
Reflections collected	17096
Independent reflections	5169 [R(int) = 0.0613]
Theta(deg)	28.30°(98.6 %)
R1, wR2 [I>2σ(I)]	0.0526, 0.1342
R1, wR2 (all data)	0.0599, 0.1420
Largest diff. peak and hole/ e. Å^{-3}	1.490, -2.156

Table S2: Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for Crystal. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Atom	x	y	z	U(eq)	Atom	x	y	z	U(eq)
Cu(1)	7013(1)	799(1)	6811(1)	19(1)	Cu(2)	17369(1)	-5262(1)	-2086(1)	24(1)
Cl(1)	15649(1)	-4663(1)	-2732(1)	27(1)	Cl(2)	19192(1)	-5799(1)	-1598(1)	27(1)
S(1)	7956(1)	-1131(1)	6341(1)	19(1)	S(2)	9637(1)	-1549(1)	3555(1)	20(1)
N(1)	8581(2)	805(2)	3872(2)	16(1)	N(2)	7949(3)	1662(2)	4682(3)	18(1)
C(1)	8705(3)	-541(3)	4592(3)	17(1)	C(2)	8949(3)	1531(3)	2429(3)	18(1)
C(3)	8537(3)	2817(3)	2373(3)	22(1)	C(4)	7917(3)	2866(3)	3778(3)	20(1)
C(5)	9474(4)	-3179(3)	4832(3)	26(1)	C(6)	9613(3)	980(3)	1228(3)	25(1)
C(7)	7285(4)	4035(3)	4276(4)	27(1)	S(11)	7010(1)	1207(1)	8707(1)	21(1)
S(12)	4732(1)	2461(1)	10687(1)	22(1)	N(11)	4511(2)	2028(2)	8555(3)	16(1)
N(12)	5003(3)	1517(2)	7427(3)	17(1)	C(11)	5397(3)	1885(3)	9257(3)	17(1)
C(12)	3177(3)	2635(3)	8713(3)	18(1)	C(13)	2843(3)	2475(3)	7700(3)	20(1)
C(14)	4011(3)	1791(3)	6925(3)	19(1)	C(15)	6121(3)	1996(3)	11353(3)	25(1)
C(16)	2337(3)	3370(3)	9736(4)	24(1)	C(17)	4212(3)	1409(3)	5670(3)	24(1)

Table S3: Selected bond lengths (in Å unit) for the crystal.

Selected bonds	values(Å)	Selected bonds	values(Å)	Selected bonds	values(Å)
C(5)-H(5A)	0.9800	C(5)-H(5B)	0.9800	C(5)-H(5C)	0.9800
C(6)-H(6A)	0.9800	C(6)-H(6B)	0.9800	C(6)-H(6C)	0.9800
S(11)-C(11)	1.666(3)	S(12)-C(11)	1.719	(3)S(12)-C(15)	1.801(3)
N(11)-C(11)	1.390(4)	N(11)-N(12)	1.396(3)	N(11)-C(12)	1.398(3)
N(12)-C(14)	1.308(4)	C(12)-C(13)	1.364(4)	C(12)-C(16)	1.489(4)
C(13)-C(14)	1.420(4)	C(13)-H(13A)	0.9500	C(14)-C(17)	1.495(4)

Table S4: Selected bond angles in degree (°) for the crystal.

Selected angles	values(°)	Selected angles	values(°)	Selected angles	values(°)
N(12)-Cu(1)-N(2)	108.30(10)	N(12)-Cu(1)-S(1)	130.53(7)	N(2)-Cu(1)-S(1)	84.52(7)
N(12)-Cu(1)-S(11)	84.39(7)	N(2)-Cu(1)-S(11)	133.25(7)	S(1)-Cu(1)-S(11)	121.61(3)
Cl(1)-Cu(2)-Cl(2)	175.70(4)	C(1)-S(1)-Cu(1)	99.51(10)	C(1)-S(2)-C(5)	102.46(14)
C(1)-N(1)-N(2)	117.2(2)	C(1)-N(1)-C(2)	132.8(2)	N(2)-N(1)-C(2)	109.9(2)
C(4)-N(2)-N(1)	106.2(2)	C(4)-N(2)-Cu(1)	135.6(2)	N(1)-N(2)-Cu(1)	116.89(19)
N(1)-C(1)-S(1)	121.2(2)	N(1)-C(1)-S(2)	115.9(2)	S(1)-C(1)-S(2)	122.89(18)
C(3)-C(2)-N(1)	105.7(2)	C(3)-C(2)-C(6)	127.7(3)	N(1)-C(2)-C(6)	126.6(3)
C(2)-C(3)-C(4)	107.9(3)	C(2)-C(3)-H(3A)	126.0	C(4)-C(3)-H(3A)	126.0
N(2)-C(4)-C(3)	110.3(3)	N(2)-C(4)-C(7)	121.1(3)	C(3)-C(4)-C(7)	128.6(3)
S(2)-C(5)-H(5A)	109.5	S(2)-C(5)-H(5B)	109.5	H(5A)-C(5)-H(5B)	109.5
C(11)-S(11)-Cu(1)	99.56(10)	C(11)-S(12)-C(15)	102.24(14)	C(11)-N(11)-N(12)	117.2(2)
C(11)-N(11)-C(12)	132.9(2)	N(12)-N(11)-C(12)	109.9(2)	C(14)-N(12)-N(11)	106.0(2)
C(14)-N(12)-Cu(1)	135.7(2)	N(11)-N(12)-Cu(1)	117.69(17)	N(11)-C(11)-S(11)	120.8(2)
N(11)-C(11)-S(12)	116.0(2)	S(11)-C(11)-S(12)	123.14(18)	C(13)-C(12)-N(11)	106.2(2)
C(13)-C(12)-C(16)	127.5(3)	N(11)-C(12)-C(16)	126.2(3)	C(12)-C(13)-C(14)	106.6(3)
C(12)-C(13)-H(13A)	126.7	C(14)-C(13)-H(13A)	126.7	N(12)-C(14)-C(13)	111.3(3)
N(12)-C(14)-C(17)	120.1(3)	C(13)-C(14)-C(17)	128.6(3)	S(12)-C(15)-H(15A)	109.5

Figure S1:

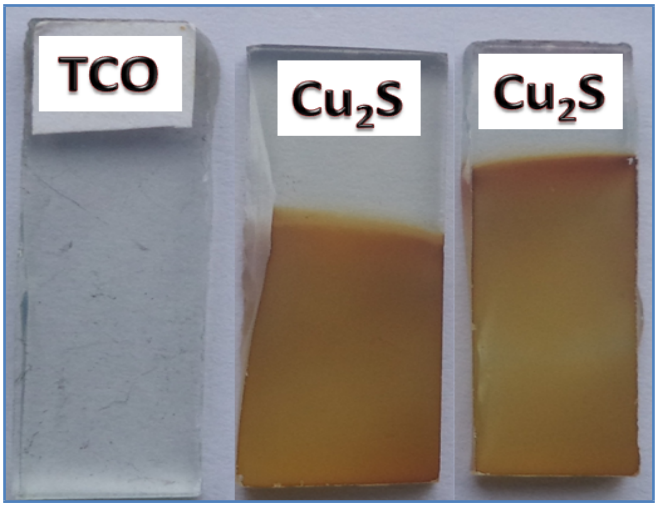

Fig. S1: Images of clean TCO and Cu_2S thin films.

Figure S2:

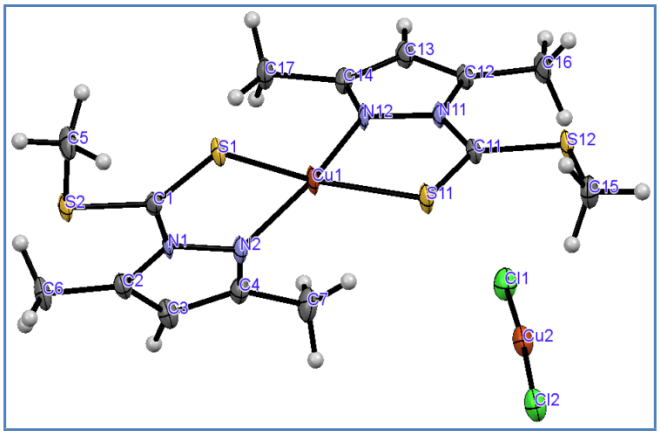

Figure S2: Crystal structure of SP showing atom numbering scheme (ORTEP diagram).

Figure S3:

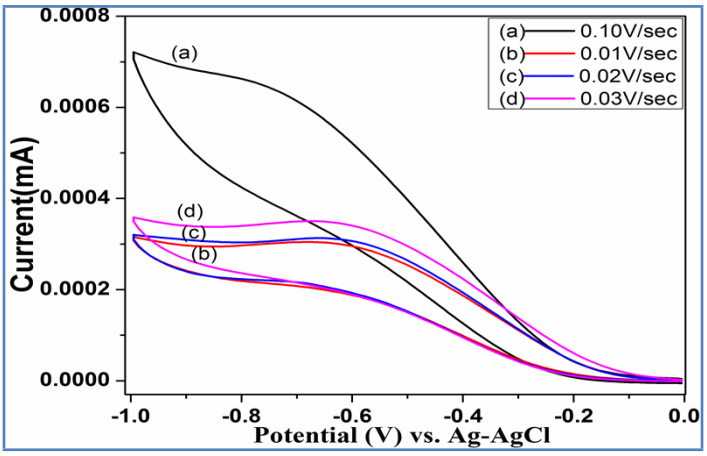

Fig.S3: CV study of 0.01M ligand solution at different applying voltages.

Figure S4:

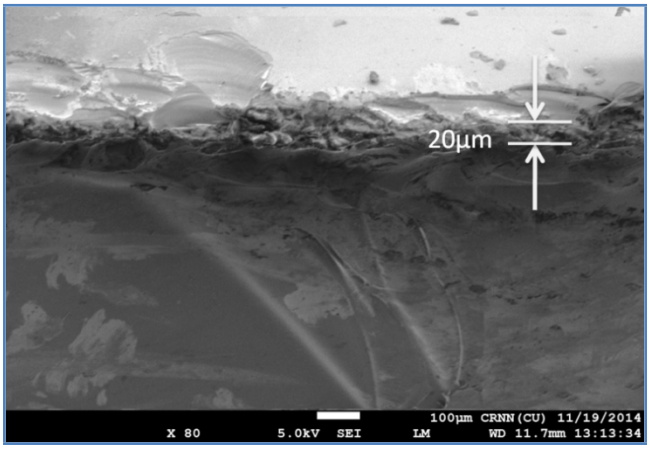

Fig.S4: Cross section picture of Cu_2S thin film on TCO glass.

Figure S5:

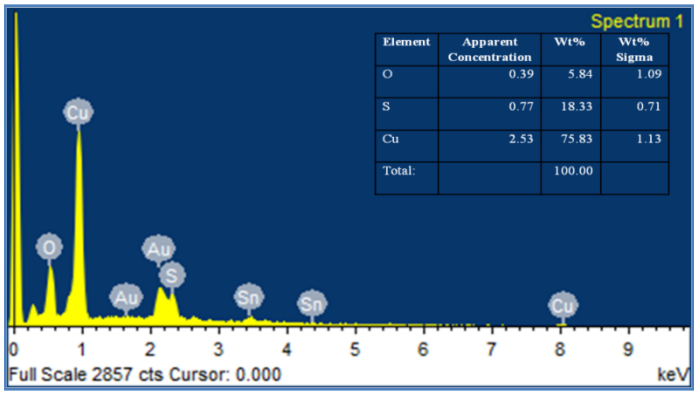

Fig.S5: EDX data of deposited Cu_2S thin film on TCO.

Figure S6:

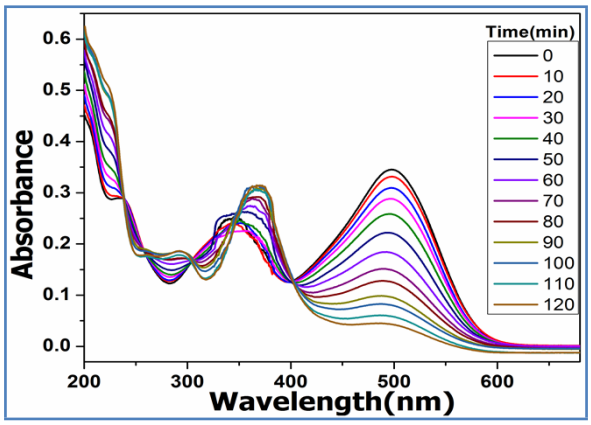

Fig. S6: Time dependant spectral changes of CR aqueous solution by Cu_2S/TCO.

Figure S7:

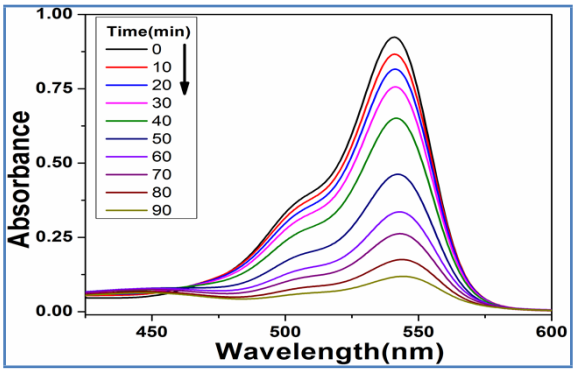

Fig. S7: Time dependant spectral changes of RB aqueous solution by Cu_2S/TCO with catalytic amount of H_2O_2.