Supporting Information

Ligand-induced synthesis of two Cu-based coordination polymers and derived carbon-coated metal oxide heterojunction for enhanced photocatalytic degradation

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Table S1 Crystallographic data for complexes **1** and **2**.

Complex	**1**	**2**
Formula	$C_{24}H_{28}CuN_4O_6$	$C_{13}H_{15}CuN_2O_5$
Formula wt	532.04	342.81
Crystal system	Triclinic	Triclinic
Space group	*P–1*	*P–1*
T (K)	296(2)	296(2)
a (Å)	8.273(3)	8.4346(7)
b (Å)	9.463(3)	8.6526(8)
c (Å)	16.205(5)	11.0134(10)
α (°)	98.044(9)	69.429(2)
β (°)	98.914(9)	67.606(2)
γ (°)	100.409(10)	74.800(2)
V (Å^3)	1214.1(7)	688.08(11)
Z	2	2
D_{calc} (g cm^{-3})	1.455	1.655
F(000)	554	352
θ_{max} (°)	25.14	28.05
R_{int}	0.0774	0.0186
R_1 [a] [$I > 2\sigma(I)$]	0.0599	0.0354
wR_2 [b] (all data)	0.1745	0.0845
GOF	1.002	1.043

[a] $R_1 = \Sigma||F_o|-|F_c||/\Sigma|F_o|$, [b] $wR_2 = \Sigma[w(F_o^2-F_c^2)^2]/\Sigma[w(F_o^2)^2]^{1/2}$.

Table S2 Selected bond distances (Å) and angles (°) for complex **1**.

Cu(1) – O(1)	1.953(4)	Cu(1) – O(3)#3	1.969(4)
Cu(1) – O(4)#1	1.958(4)	Cu(1) – N(1)	2.179(4)
Cu(1) – O(2)#2	1.969(4)	Cu(1) – Cu(1)#2	2.6379(14)
O(1) – Cu(1) – O(4)#1	89.17(18)	O(2)#2 – Cu(1) – N(1)	90.28(16)
O(1) – Cu(1) – O(2)#2	167.98(14)	O(3)#3 – Cu(1) – N(1)	89.97(16)
O(4)#1 – Cu(1) – O(2)#2	88.82(17)	O(1) – Cu(1) – Cu(1)#2	85.76(11)
O(1) – Cu(1) – O(3)#3	90.95(17)	O(4)#1 – Cu(1) – Cu(1)#2	86.19(11)
O(4)#1 – Cu(1) – O(3)#3	167.98(14)	O(2)#2 – Cu(1) – Cu(1)#2	82.28(11)
O(2)#2 – Cu(1) – O(3)#3	88.56(17)	O(3)#3 – Cu(1) – Cu(1)#2	81.83(11)
O(1) – Cu(1) – N(1)	101.73(16)	N(1) – Cu(1) – Cu(1)#2	169.03(12)
O(4)#1 – Cu(1) – N(1)	101.77(16)		

Symmetry codes: #1 $x - 1, y, z$; #2 $-x, -y + 1, -z + 2$; #3 $-x + 1, -y + 1, -z + 2$.

Table S3 Selected bond distances (Å) and angles (°) for complex **2**.

Cu(1) – O(1)	1.9641(18)	Cu(1) – O(2)#3	1.9841(18)
Cu(1) – O(4)#1	1.9676(16)	Cu(1) – N(1)	2.2059(19)
Cu(1) – O(3)#2	1.9696(16)	Cu(1) – Cu(1)#3	2.6433(6)
O(1) – Cu(1) – O(4)#1	90.09(8)	O(3)#2 – Cu(1) – N(1)	100.02(7)
O(1) – Cu(1) – O(3)#2	89.63(8)	O(2)#3 – Cu(1) – N(1)	95.78(7)
O(4)#1 – Cu(1) – O(3)#2	167.74(7)	O(1) – Cu(1) – Cu(1)#3	82.25(5)
O(1) – Cu(1) – O(2)#3	167.99(7)	O(4)#1 – Cu(1) – Cu(1)#3	77.64(5)

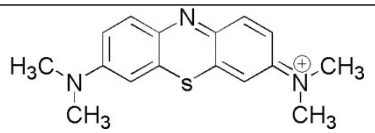
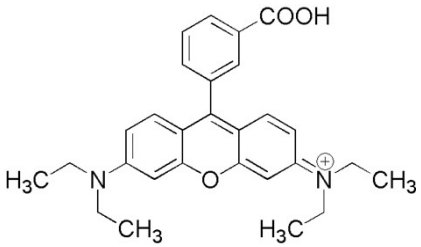
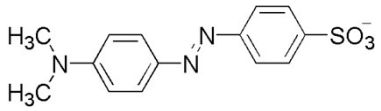
O(4)#1 – Cu(1) – O(2)#3	88.33(8)	O(3)#2 – Cu(1) – Cu(1)#3	90.18(5)
O(3)#2 – Cu(1) – O(2)#3	89.40(8)	O(2)#3 – Cu(1) – Cu(1)#3	85.78(5)
O(1) – Cu(1) – N(1)	96.17(7)	N(1) – Cu(1) – Cu(1)#3	169.68(6)
O(4)#1 – Cu(1) – N(1)	92.19(7)		

Symmetry codes: #1 $x + 1, y, z$; #2 $–x, –y + 1, –z + 1$; #3 $–x + 1, –y + 1, –z + 1$.

Table S4 BET surface area and adsorption average pore width for complexes **1** and **2** and the carbon-coated metal oxide heterojunctions.

Marterial	BET surface area (m^2 g^{-1})	Adsorption average pore width (nm)
Complex **1**	0.323	55.35
Cu@V-1	3.755	105.65
Cu@Mo-1	4.454	26.66
Cu@W-1	4.465	7.85
Complex **2**	1.908	552.08
Cu@V-2	18.394	6.53
Cu@Mo-2	84.181	15.36
Cu@W-2	58.415	19.44

Table S5 Organic dyes with different charge types and sizes.

Dye	Formula	Charge type	Size (nm × nm × nm)
Methylene Blue (MB)		Cationic	0.40 × 0.79 × 1.63
Rhodamine B (RhB)		Cationic	0.68 × 1.18 × 1.57
Methyl Orange (MO)		Anionic	0.53 × 0.73 × 1.74

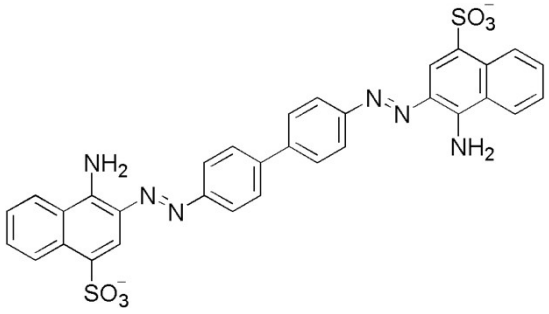
Congo Red (CR)		Anionic	0.39 × 0.86 × 2.61

Table S6 Pseudo-first-order and pseudo-second-order kinetic parameters for the photodegradation of dyes by **Cu@Mo-2**.

Dye	Concentration (mg L^{-1})	Rate constant (K min^{-1})	Half-life $t_{1/2}$ (min)	R^2
MB	10	0.0115	60.27	0.8563
RhB	10	0.0057	121.60	0.9692
MO	40	0.0029	239.02	0.9891
CR	80	0.0081	85.57	0.9892

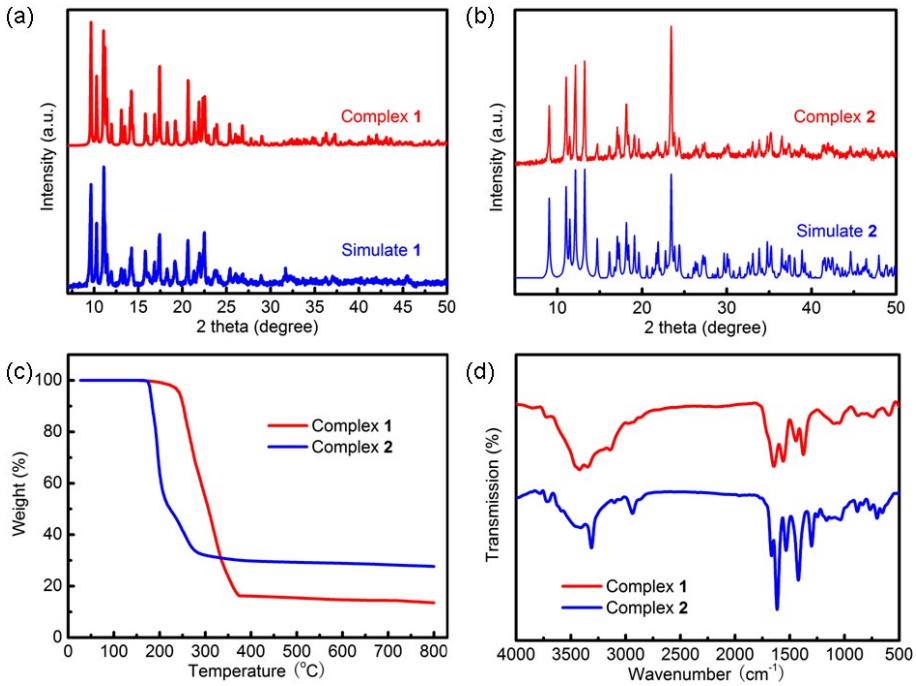


Fig. S1 (a) The PXRD patterns of simulated and fresh sample for complex **1**; (b) The PXRD patterns of simulated and fresh sample for complex **2**; (c) The TG curve of complexes **1** and **2**; (d)The IR spectra of complexes **1** and **2**.

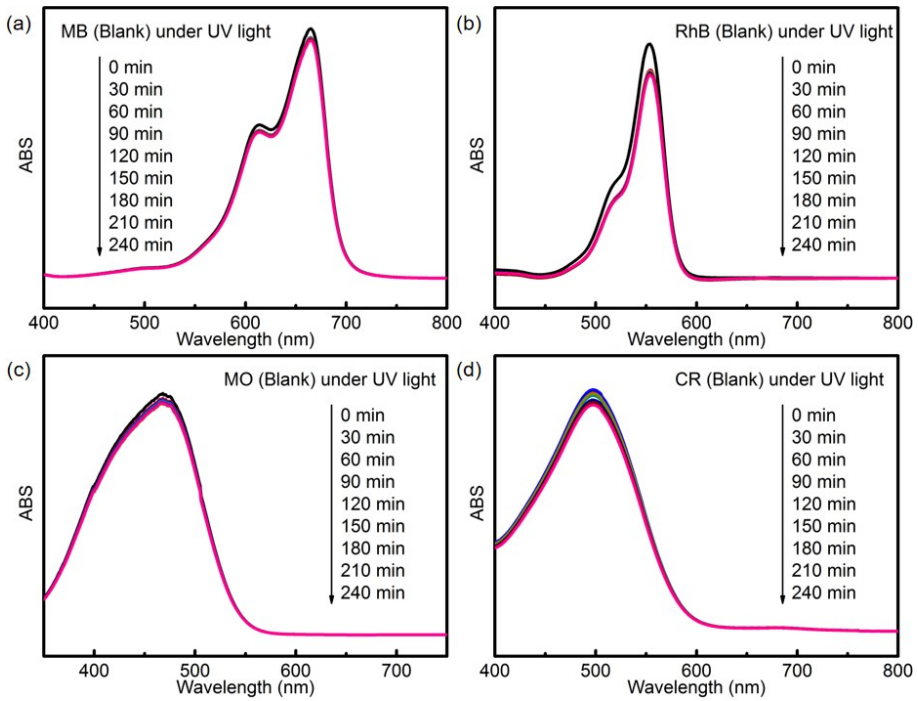


Fig. S2 UV-vis spectra of blank experiment for dye photocatalysis (performed in the absence of any catalyst).

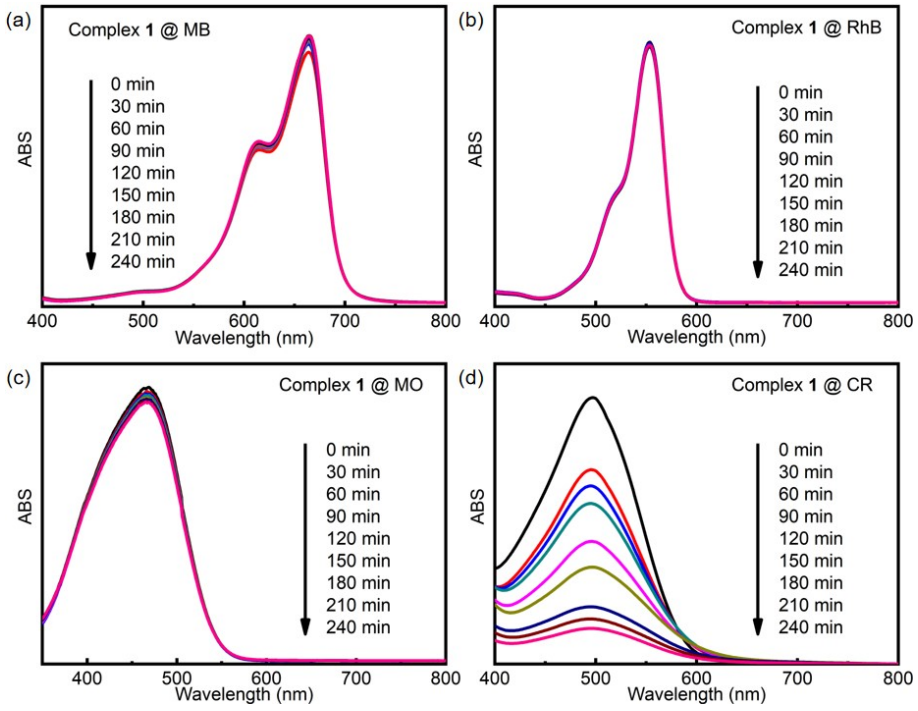


Fig. S3 UV-vis spectra of MB (a), RhB (b), MO (c) and CR (d) solutions recorded after different adsorption times with complex **1**.

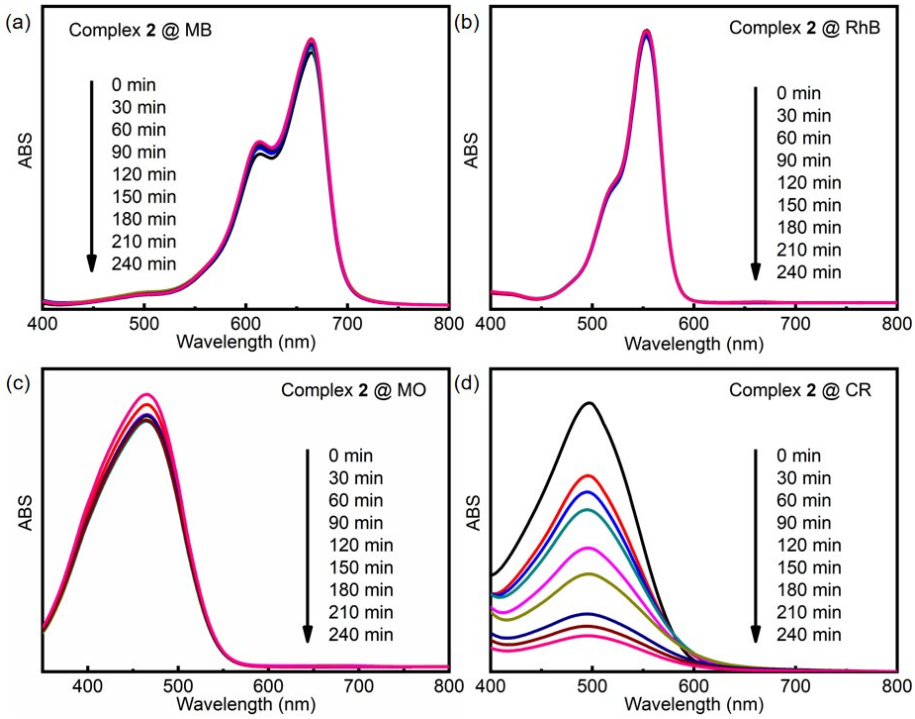


Fig. S4 UV-vis spectra of MB (a), RhB (b), MO (c) and CR (d) solutions recorded after different adsorption times with complex **2**.

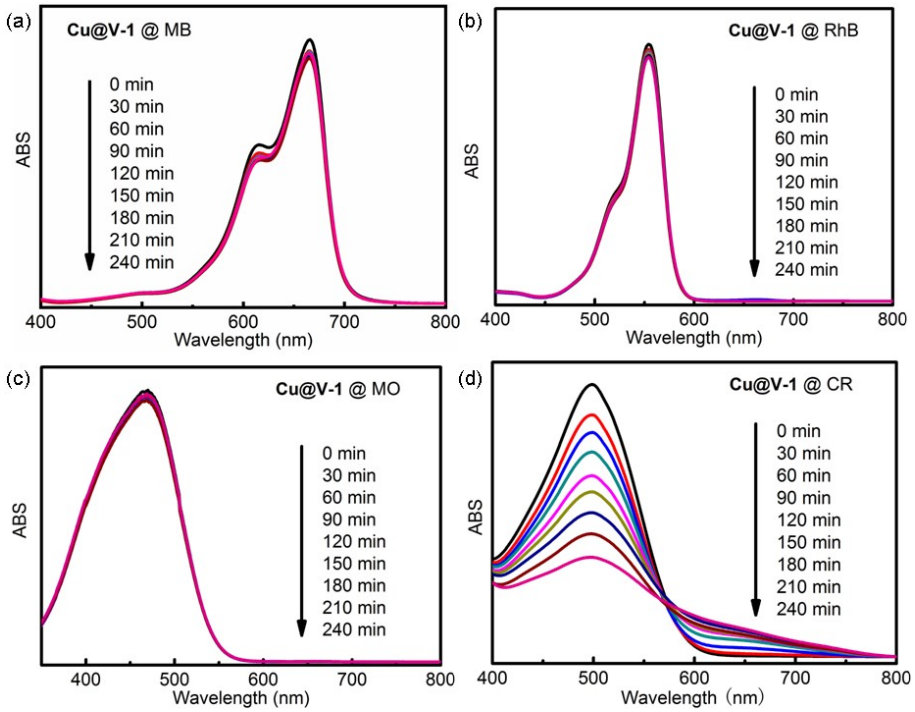


Fig. S5 UV-vis spectra of MB (a), RhB (b), MO (c) and CR (d) solutions recorded after different adsorption times with **Cu@V-1**.

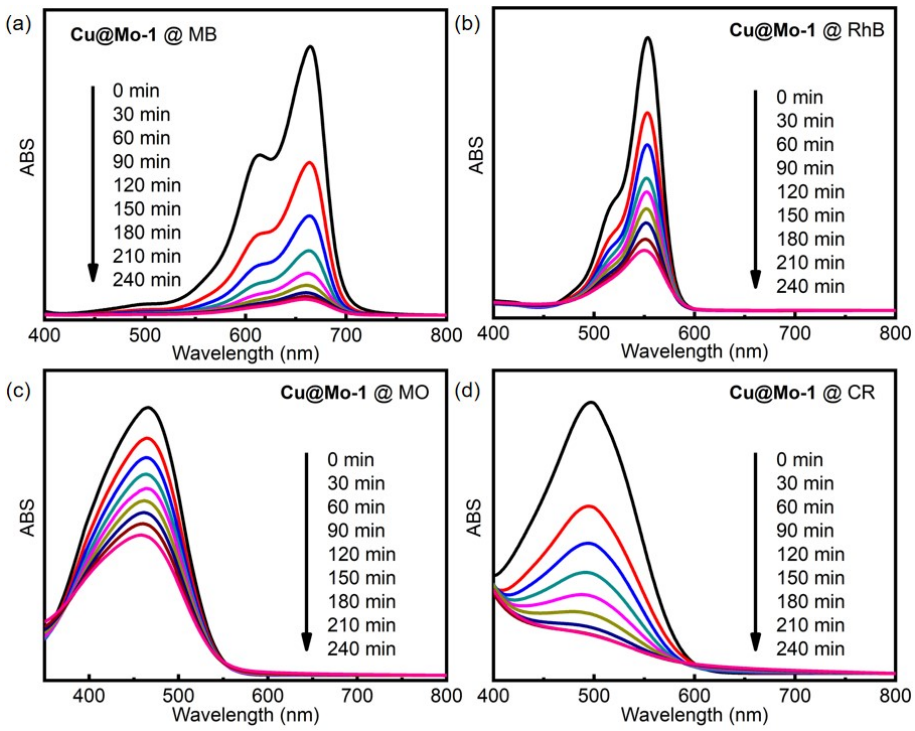


Fig. S6 UV-vis spectra of MB (a), RhB (b), MO (c) and CR (d) solutions recorded after different adsorption times with **Cu@Mo-1**.

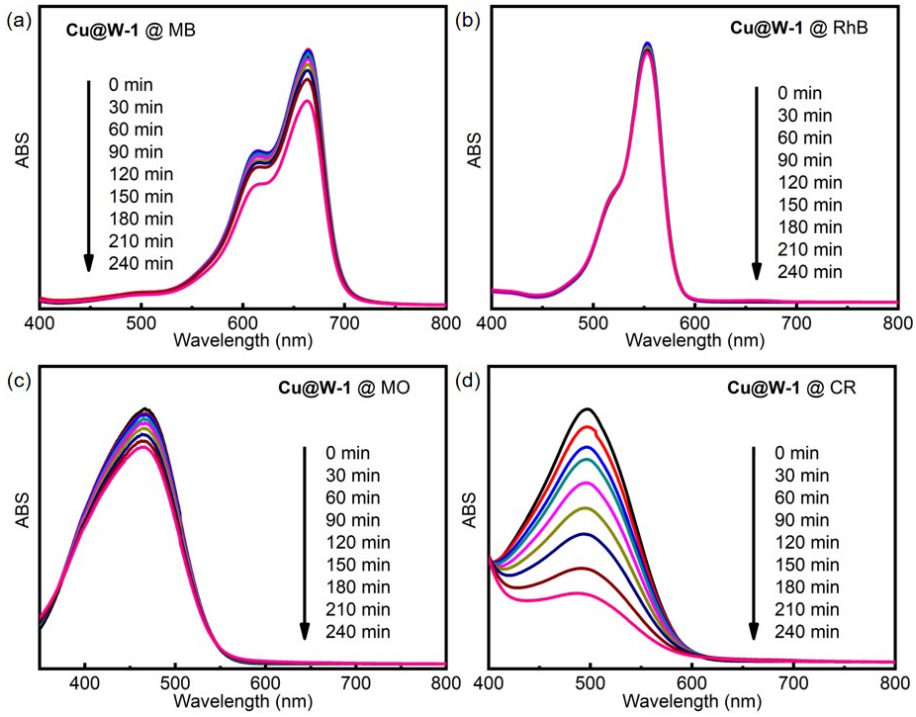


Fig. S7 UV-vis spectra of MB (a), RhB (b), MO (c) and CR (d) solutions recorded after different adsorption times with **Cu@W-1**.

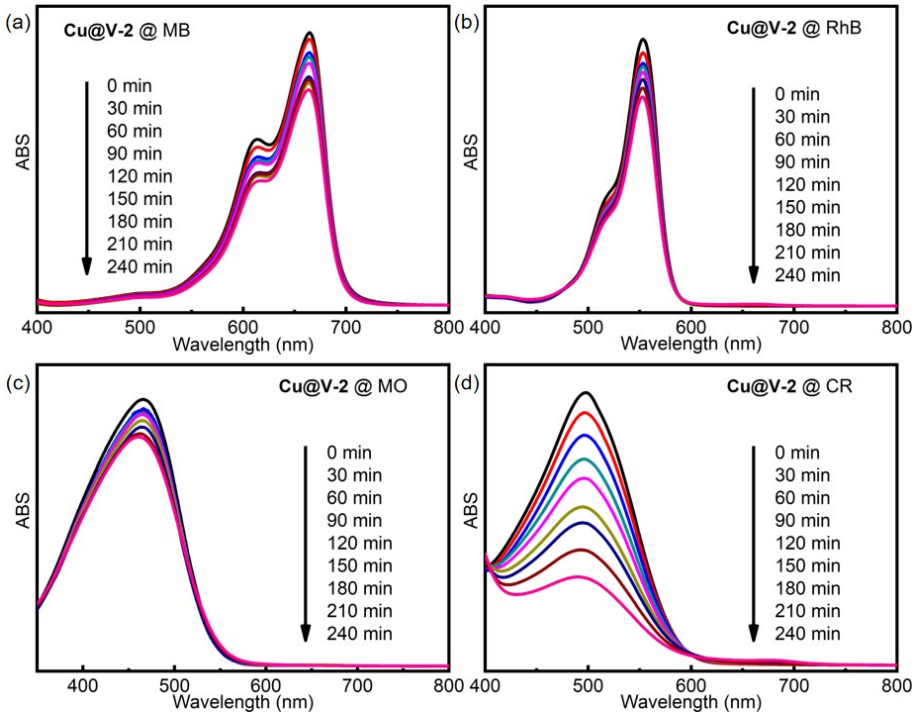


Fig. S8 UV-vis spectra of MB (a), RhB (b), MO (c) and CR (d) solutions recorded after different adsorption times with **Cu@V-2**.

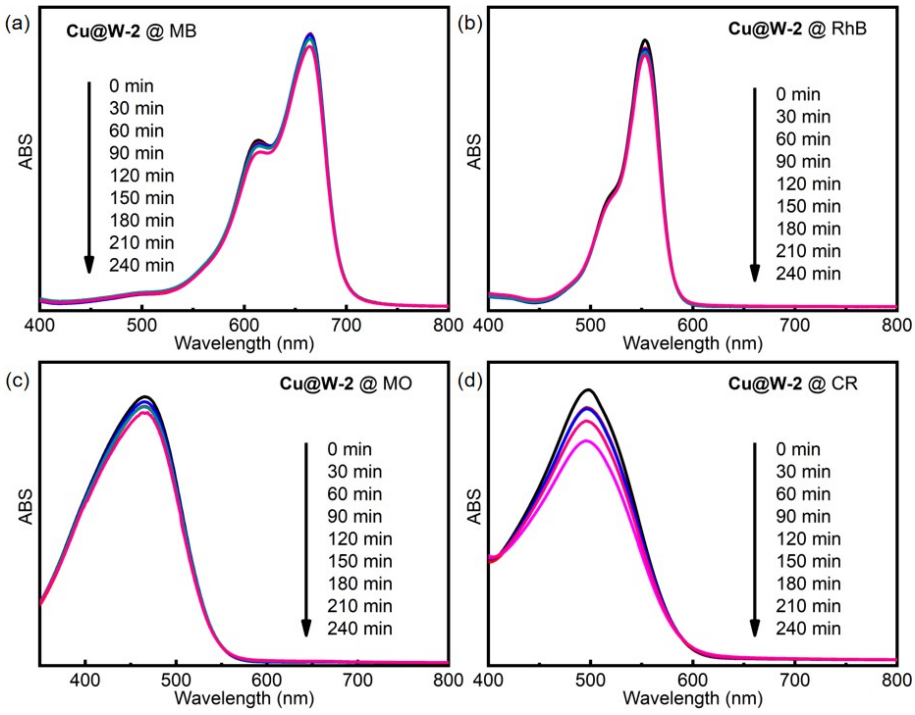


Fig. S9 UV-vis spectra of MB (a), RhB (b), MO (c) and CR (d) solutions recorded after different adsorption times with **Cu@W-2**.

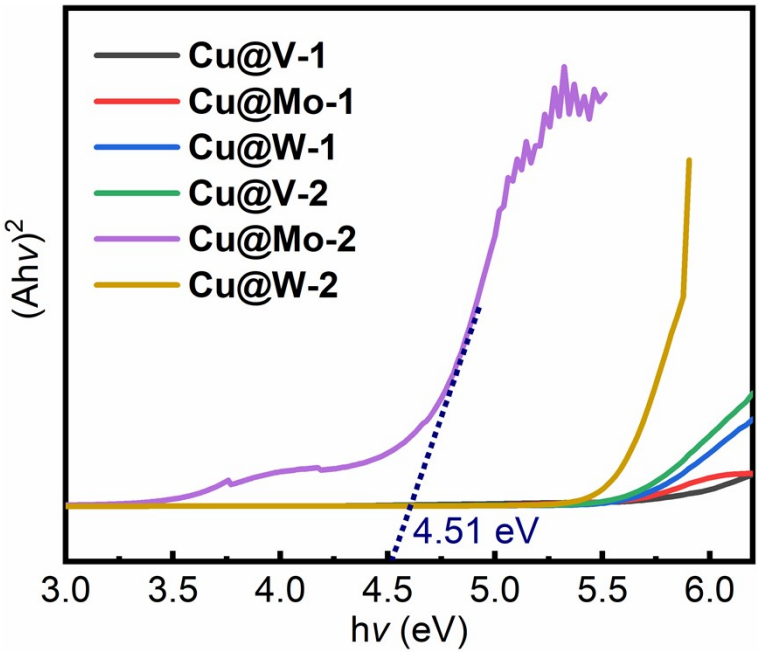


Fig. S10 Tauc's plots of the carbon-coated metal oxide heterojunctions.

S1. Pseudo-first-order kinetics.

These calculations were performed via equations (S1) and (S2):

$$\ln\left(C_0/C_t\right) = kt \quad \text{(S1)}$$

$$t_{1/2} = \frac{ln2}{k} \quad \text{(S2)}$$

where C_0 represents the initial concentration of dye (mg L^{-1}), C_t is the residual concentration of dye at time t (min), k denotes the pseudo-first-order rate constant (min^{-1}), and $t_{1/2}$(min) represents the half-life period of the reaction.

S2. Pseudo-second-order kinetics.

These calculations were performed via equations (S3):

$$t/C_t = 1/(kC_t^2) + t/C_0 \quad \text{(S3)}$$

where C_0 represents the initial concentration of dye, C_t is the residual concentration of dye at time t (min), and k denotes the pseudo-second-order rate constant (L mg^{-1} min^{-1}).

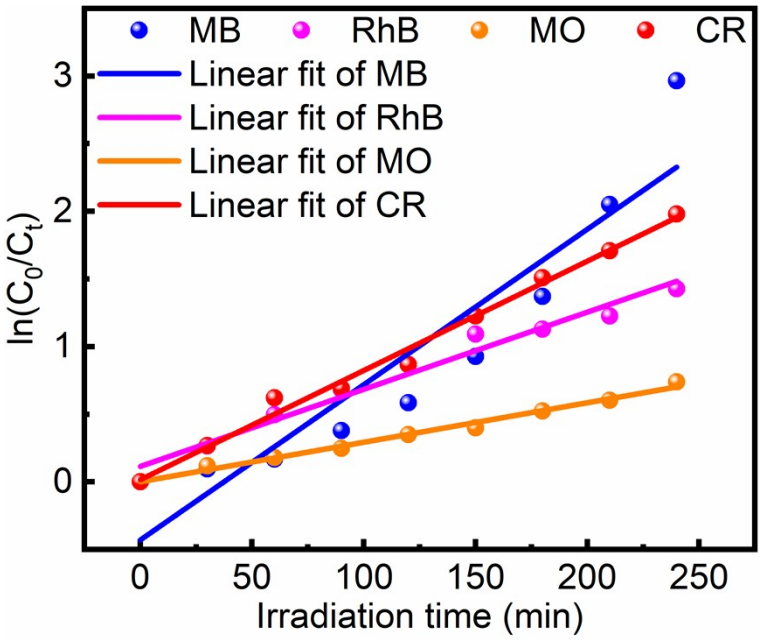


Fig. S11 Pseudo-first-order plots with respect to time for **Cu@Mo-2** in aqueous dye solutions.

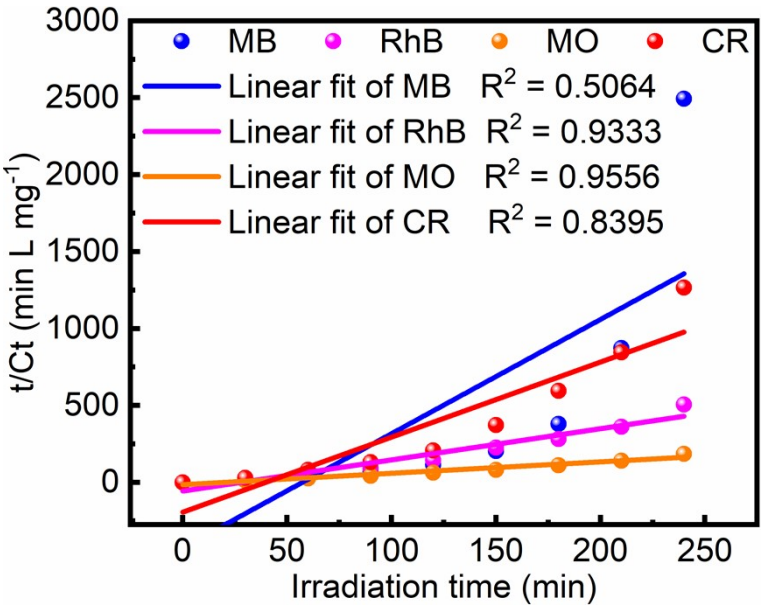


Fig. S12 Pseudo-second-order plots with respect to time for **Cu@Mo-2** in aqueous dye solutions.

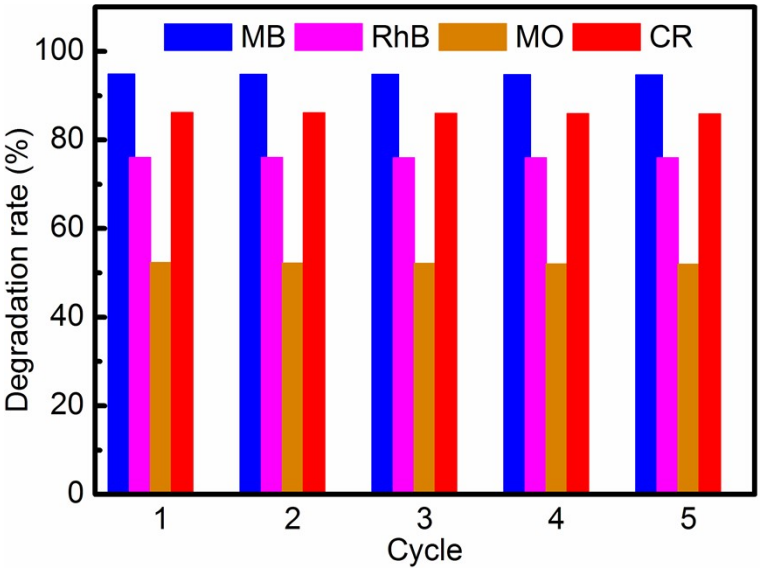


Fig. S13 The reproducibility of the photocatalyst **Cu@Mo-2** for dyes.