Supporting information

Experimental section

All reagents and solvents used were analytical grade. A Bruker D8 diffractometer with monochromatic radiation, a scanning rate of 6°/min, and a step size of 0.02° was used to capture the powder X-ray diffraction (PXRD) spectra. Direct methods were used to solve the structures, then full-matrix least-squares on F^2 were used to refine them. The SHELXTL program was used for structure solving, refinement, and data output. Anisotropic refinement was used on non-hydrogen atoms. DIAMOND-4.6 and MERCURY were used to form pictures and hydrogen bonding associations. Nicolet Impact 750 FTIR was used to record the Fourier transform infrared (FT-IR) spectrum in KBr disc between 400-4000 cm^{-1}. TGA was carried out in nitrogen environment from ambient temperature to 900 °C at a heating rate of 10 °C min^{-1}.

X-ray crystallographic data collection and structural determination

The crystallographic diffraction data for **1–3** were collected on a Bruker SMART APEX II CCD diffractometer with graphite-monochromated Mo Ka radiation (k = 0.71073 Å) at 296(2) K using the u/x scanning technique. All the structures were solved using direct methods and successive Fourier difference synthesis, and refined using the full-matrix least-squares method on F^2 with anisotropic thermal parameters for all non-hydrogen atoms by SHELXS-97. An empirical absorption correction was applied using the SADABS program. Basic information pertaining to crystal parameters and structure refinements are summarized in Table S1. Selected bond lengths and angles for 1–3 are listed in Table S2. Hydrogen bonding distance and angle data are listed in Table S3, shown in Supplementary data. CCDC: 2244699-2244701.

Table 1. Crystallographic data and structure refinement details for 1-3

Parameter	**1**	**2**	**3**

Formula weight	882.72	1188.91	929.64
Crystal system	Triclinic	Orthorhombic	Triclinic
Space group	*P-1*	*P21212*	*P-1*
Crystal Color	Pink	Pink	Pink
a, Å	9.9846(14)	18.3153(4)	11.1329(3)
b, Å	13.9514(18)	19.6079(6)	11.1958(3)
c, Å	15.528(2)	8.6585(2)	17.3063(4)
α, °	73.277(2)	90	84.085(2)
β, °	85.155(2)	90	78.096(2)
γ, °	75.511(3)	90	67.442(3)
V, Å ^{3}	2005.5(5)	3109.48(14)	1948.53(10)
Z	2	2	2
ρ_{calcd}, g/cm^3	1.462	1.270	1.584
μ, mm^{-1}	0.499	4.712	7.286
F(000)	914	1224	956
θ Range, deg	1.4-27.6	3.3-76.3	4.3-76.1
Reflection Collected	8703	6067	7616
Independent reflections (R_{int})	0.052	0.051	0.054
Reflections with $I > 2\sigma(I)$	4371	5217	6840
Number of parameters	527	351	561
R_1, wR_2 ($I > 2\sigma(I)$)*	0.1067, 0.2809	0.0779, 0.1876	0.0494, 0.1211
R_1, wR_2 (all data)**	0.2014, 0.3219	0.0878, 0.1946	0.0555, 0.1244

* $R = \sum(F_o - F_c)/\sum(F_o)$, ** $wR_2 = \{\sum[w(F_o^2 - F_c^2)^2]/\sum(F_o^2)^2\}^{1/2}$.

Table 2. Selected bond distances (Å) and angles (deg) for **1-3**

		1	
Co(1)-O(1)	2.025(7)	Co(1)-N(1)	2.118(8)
Co(1)-N(4)#1	2.117(8)	Co(1)-O(3)#2	2.123(6)
Co(1)-O(2)#3	2.042(7)		
		2	
Co(1)-O(1)	2.020(5)	Co(1)-O(6)	2.110(6)

Co(1)-N(1)	2.069(7)	Co(1)-O(4)#1	2.045(6)
Co(1)-N(4)#2	2.020(4)		
	3		
Co(1)-O(2)	2.134(2)	Co(1)-O(11)	2.0249(19)
Co(1)-N(1)	2.144(2)	Co(1)-O(10)#1	2.080(2)
Co(1)-O(4)#2	2.159(2)	Co(1)-O(8)#2	2.086(2)
Co(2)-O(1)	2.073(2)	Co(2)-O(11)	2.067(2)
Co(2)-O(9)#1	2.232(2)	Co(2)-N(4)#3	2.168(3)
Co(2)-O(30#4	2.181(2)	Co(2)-O(11)#5	2.0688(19)

	1		
O(1)-Co(1)-N(1)	86.2(3)	O(1)-Co(1)-N(4)#1	90.0(3)
O(1)-Co(1)-O(3)#2	100.8(3)	O(1)-Co(1)-C(8)#2	129.9(3)
O(1)-Co(1)-O(2)#3	112.7(3)	N(1)-Co(1)-N(4)#1	176.2(4)
O(3)#2-Co(1)-N(1)	93.3(3)	N(1)-Co(1)-C(8)#2	93.0(3)
O(2)#3-Co(1)-N(1)	88.2(3)	O(3)#2-Co(1)-N(4)#1	86.7(3)
N(4)#1-Co(1)-C(8)#2	88.9(3)	O(2)#3-Co(1)-N(4)#1	93.9(3)
O(3)#2-Co(1)-C(8)#2	29.2(3)	O(2)#3-Co(1)-O(3)#2	146.5(3)
O(2)#3-Co(1)-C(8)#2	117.4(3)		
	2		
O(1)-Co(1)-O(6)	90.3(2)	O(1) -Co(1)-N(1)	91.3(2)
O(1)-Co(1)-O(4)#1	142.2(2)	O(1)-Co(1)-N(4)#2	104.3(3)
O(6)-Co(1)-N(1)	174.4(3)	O(4))#1-Co(1)-O(6)	87.5(2)
O(6)-Co(1)-N(4)#2	89.7(3)	O(4))#1-Co(1)-N(1)	88.0(3)
N(1)-Co(1)-N(4)#2	95.1(3)	O(4))#1-Co(1)-N(4)#2	113.4(3)
	3		
O(2)-Co(1)-O(11)	95.56(8)	O(2)-Co(1)-N(1)	86.63(8)
O(2)-Co(1)-O(10)#1	94.59(9)	O(2)-Co(1)-O(4)#2	171.02(8)
O(2)-Co(1)-O(8)#2	92.14(9)	O(11)-Co(1)-N(1)	172.19(11)
O(10)#1-Co(1)-O(11)	90.75(9)	O(4)#2-Co(1)-O(11)	92.32(8)
O(8)#2-Co(1)-O(11)	96.59(9)	O(10)#1-Co(1)-N(1)	81.59(11)
O(4)#2-Co(1)-N(1)	86.13(8)	O(8)#2-Co(1)-N(1)	90.81(11)
O(4)#2-Co(1)-O(10)#1	89.59(9)	O(8)#2-Co(1)-O(10)#1	169.53(8)
O(4)#2-Co(1)-O(8)#2	82.67(9)	O(1)-Co(2)-O(11)	103.34(8)
O(1)-Co(2)-O(9)#1	83.35(8)	O(1)-Co(2)-N(4)#3	85.31(9)
O(1)-Co(2)-O(3)#4	84.94(8)	O(1)-Co(2)-O(11)#5	165.80(9)
O(9)#1-Co(2)-O(11)	94.96(8)	O(11)-Co(2)-N(4)#3	88.99(10)
O(3)#4-Co(2)-O(11)	170.93(8)	O(11)-Co(2)-O(11)#5	83.09(8)
O(9)#1-Co(2)-N(4)#3	168.58(8)	O(3)#4-Co(2)-O(9)#1	89.62(8)

O(9)#1-Co(2)-O(11)#5	83.49(8)	O(3)#4-Co(2)-N(4)#3	88.01(10)
O(11)#5-Co(2)-N(4)#3	107.66(9)	O(3)#4-Co(2)-O(11)#5	89.67(8)

Symmetry Codes: **For1**: #1=-1+x,y,1+z; #2=-x,-y,1-z; #3=1-x,-y,1-z; **For2**: #1=1/2+x,3/2-y,-z; #2=3/2-x,1/2+y,2-z; **For3**: #1=-1+x,1+y,z; #2=x,1+y,z; #3= 1+x,-1+y,-1+z; #4= 1-x,-y,-z; #5=1-x,1-y,-z.

Table 3. Hydrogen Bonds Distances (Å) and angles (deg) for **1-3**

Contact D-H···A	Distance, Å			Angle D-H···A, deg
	D-H	H···A	D···A	
		1		
O(8)-H(8)···O(4)	0.8200	1.9100	2.669(12)	153.00
O(10)-H(10)···O(11)	0.8200	1.7500	2.565(15)	170.00
C(25)-H(25)···O(2)	0.9300	2.5200	2.979(11)	110.00
C(30)-H(30)···O(6)	0.9300	2.5400	3.135(11)	122.00
C(44)-H(44C)···O(11)	0.9600	2.3700	2.761(17)	104.00
		2		
O(6)-H(6B)···O(2)	0.9200	1.7900	2.589(8)	144.00
		3		
N(5)-H(5A)···O(9)	0.9000	1.8500	2.702(5)	157.00
N(5)-H(5B)···O(3)	0.9000	1.9700	2.704(5)	138.00
O(11)-H(11)···O(7)	0.9900	2.1000	2.954(4)	143.00
O(11)-H(11)···O(9)	0.9900	2.4800	2.866(3)	103.00
C(25)-H(25)···O(4)	0.9400	2.4000	2.930(4)	115.00
C(30)-H(30)···O(8)	0.9400	2.4100	3.344(4)	172.00
C(35)-H(35)···O(2)	0.9400	2.5400	3.274(4)	135.00
C(35)-H(35)···O(8)	0.9400	2.5400	3.310(4)	139.00
C(40)-H(40)···O(4)	0.9400	2.2200	3.039(4)	145.00
C(44)-H(44A)···O(7)	0.9700	2.5100	3.433(8)	160.00
C(44)-H(44B)···O(7)	0.9700	2.5200	3.347(8)	143.00

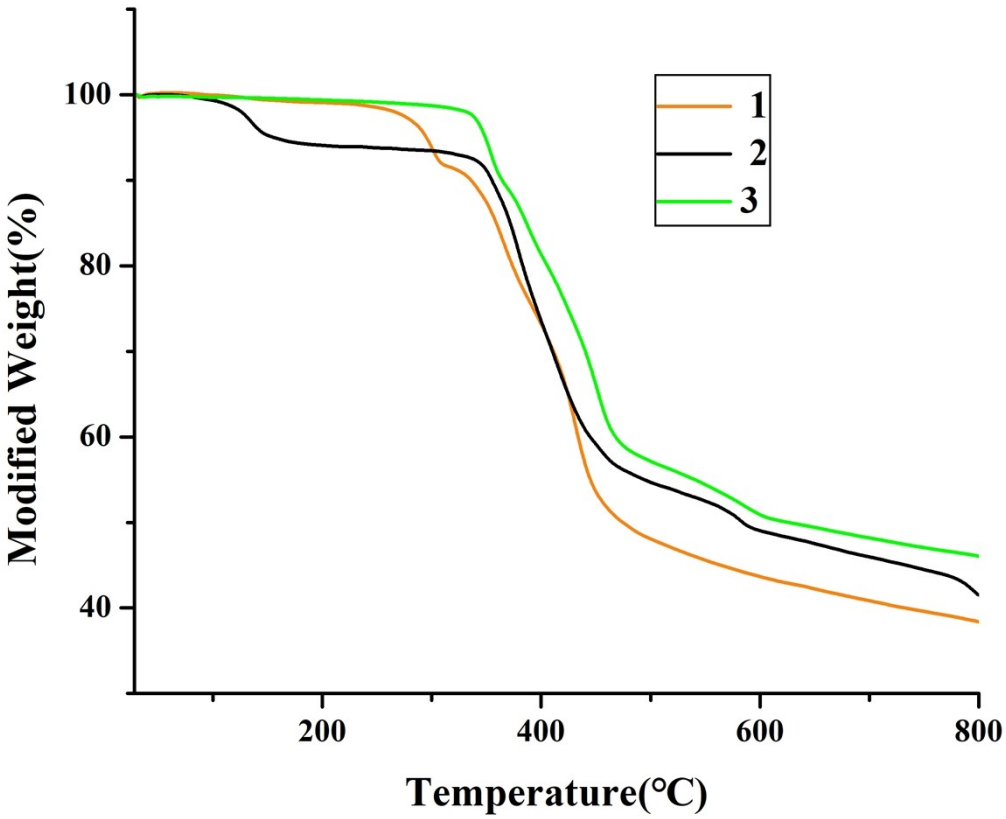

Figure S1. TGA of 1-3

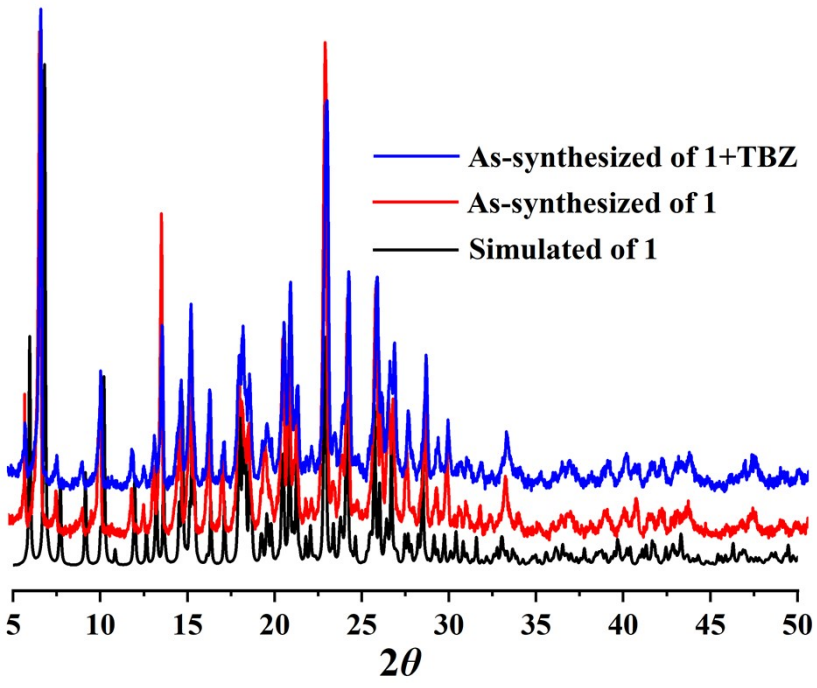

Figure S2. PXRD of **1**.

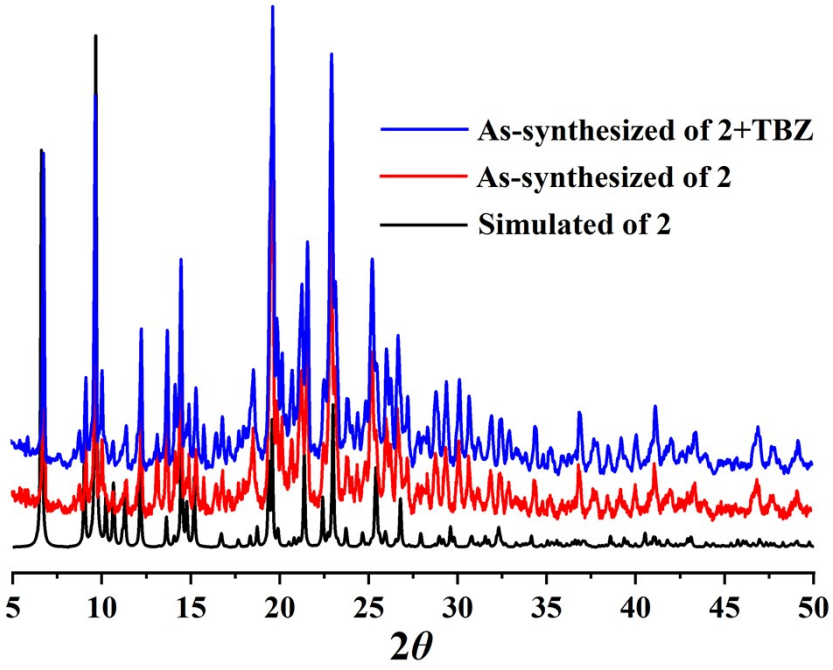

Figure S3. PXRD of **2**.

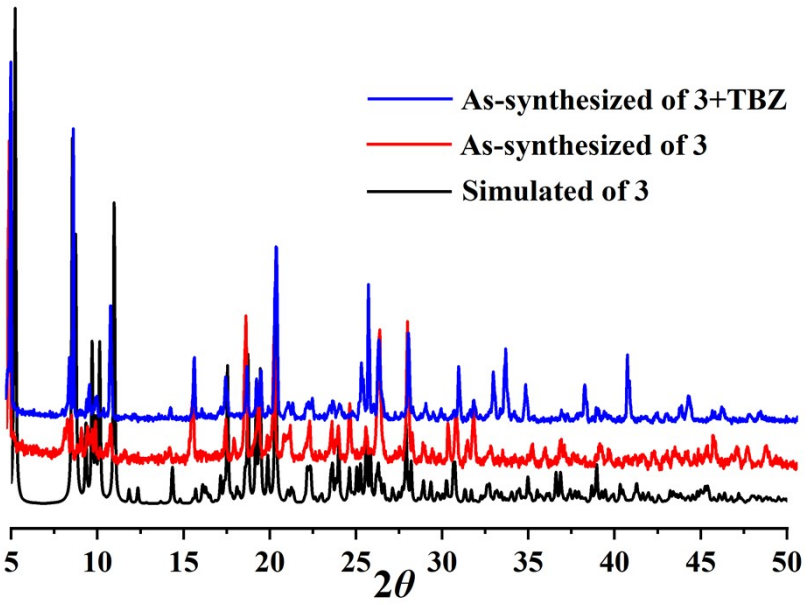

Figure S4. PXRD of **3**.

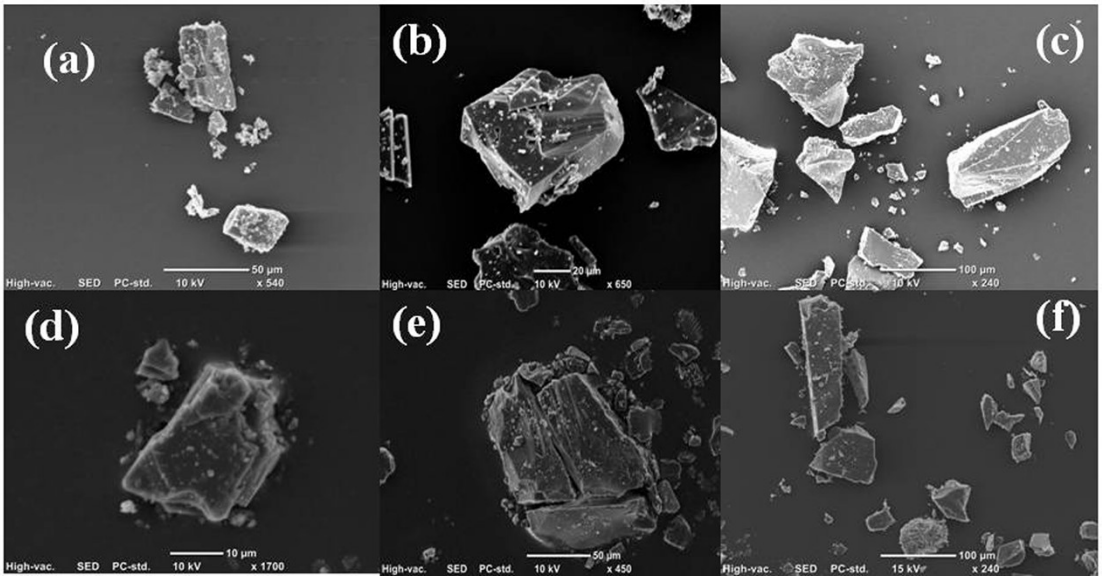

Fig. S5 SEM images of MOFs 1-3 before photocatalytic process (a)-(c); and after running photocatalysis (d)-(f).

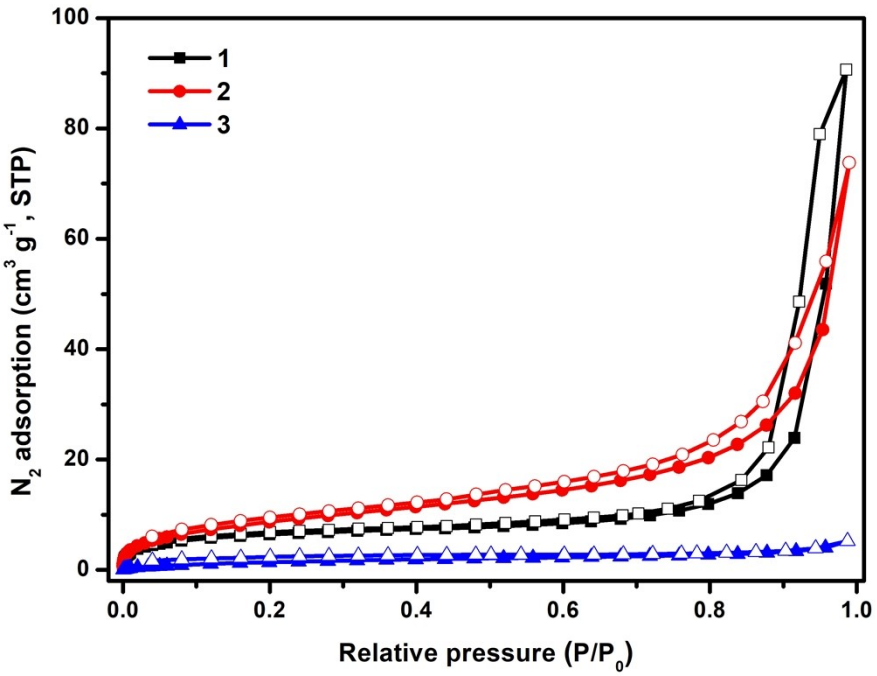

Fig. S6 N_2 adsorption–desorption isotherms of **1-3**. The adsorption and desorption isotherms are displayed with circular and square-shaped symbols.

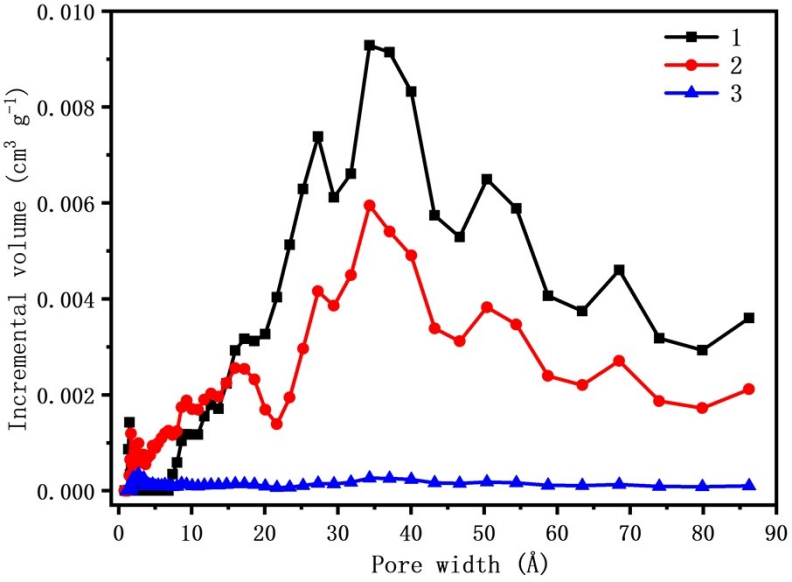

Fig. S7 pore size distribution of samples **1-3**.

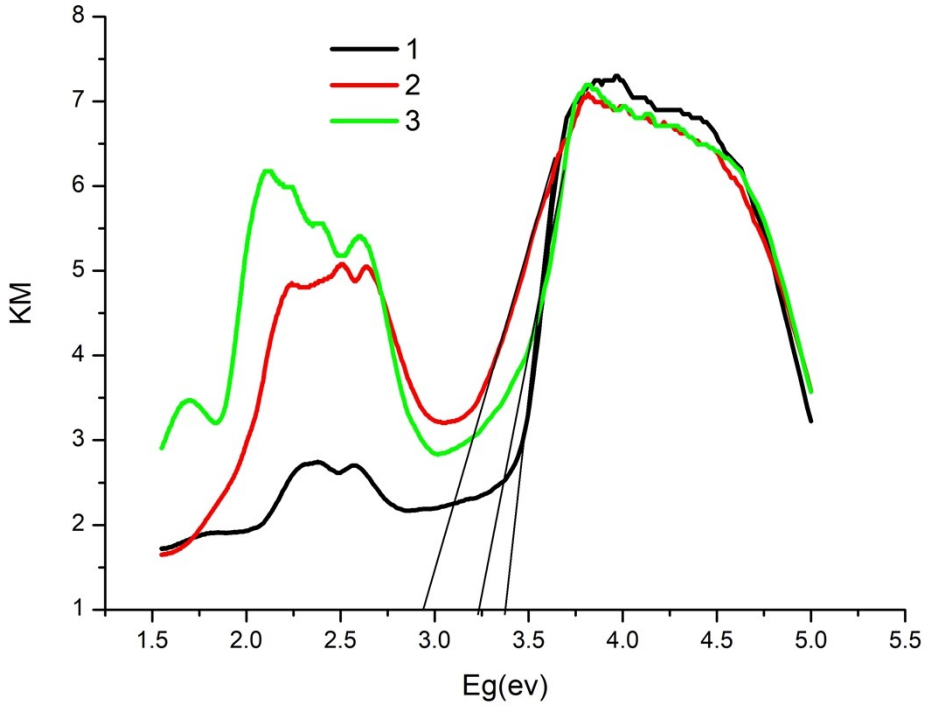

Figure S8. The diffuse reflectance (DR) UV-vis of **1-3**

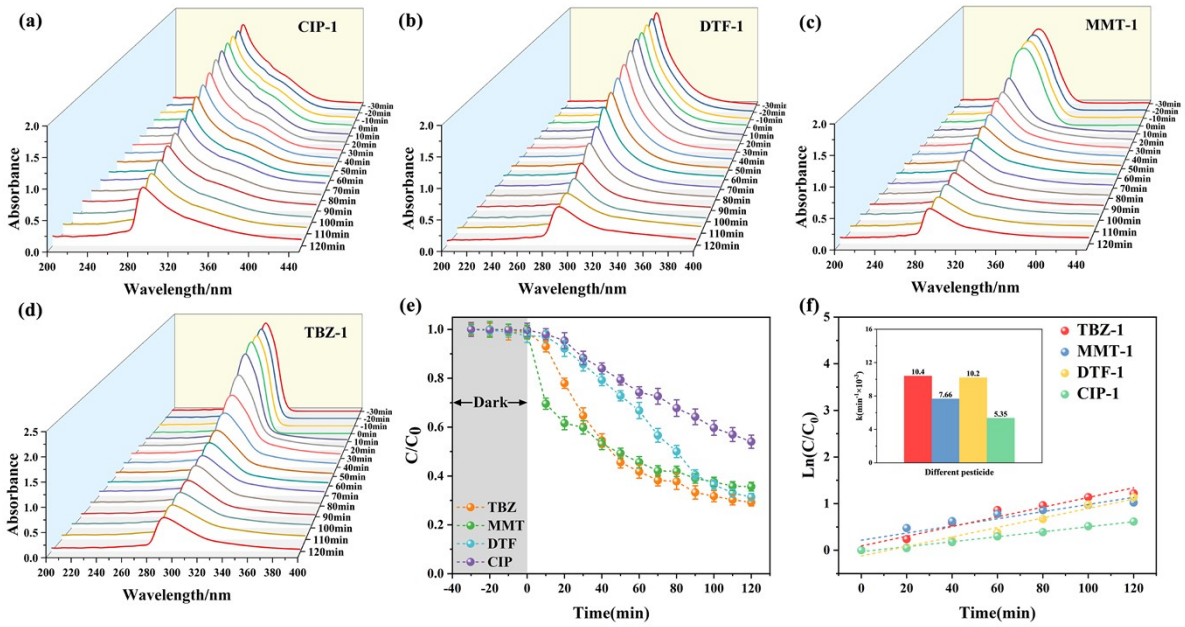

Figure S9. (a-d) time-dependent absorption of different Pesticide CIP, DTF, MMT, and TBZ using **1** (e,f) the concentration changes of the pesticide

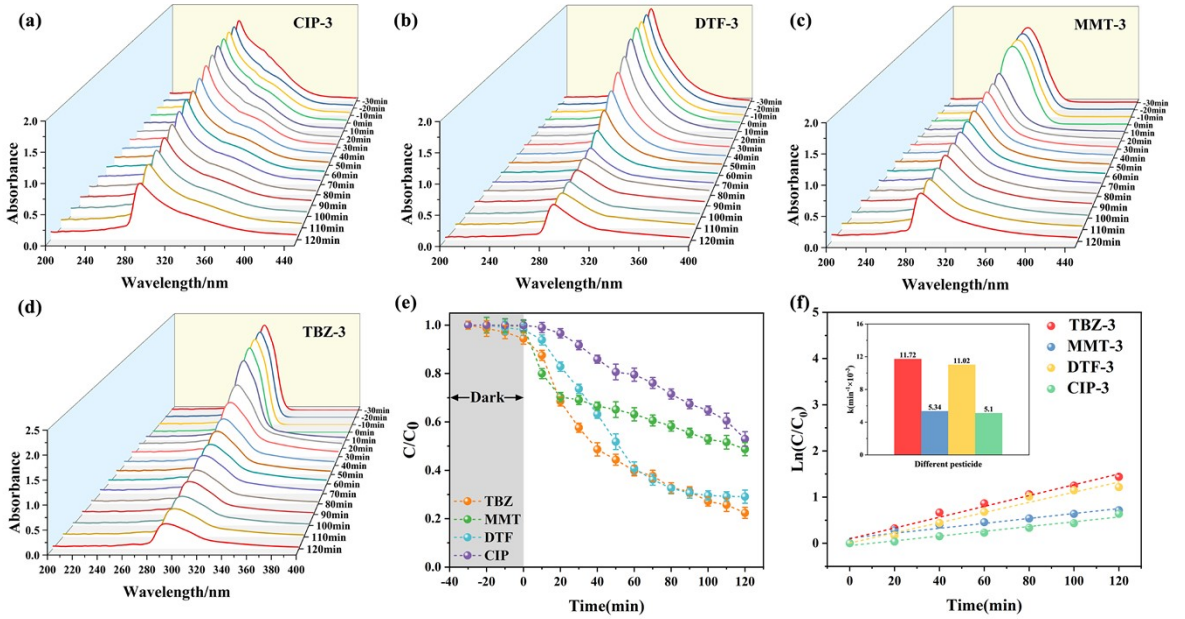

Figure S10. (a-d) time-dependent absorption of different Pesticide CIP, DTF, MMT, and TBZ using **3** (e,f) the concentration changes of the pesticide

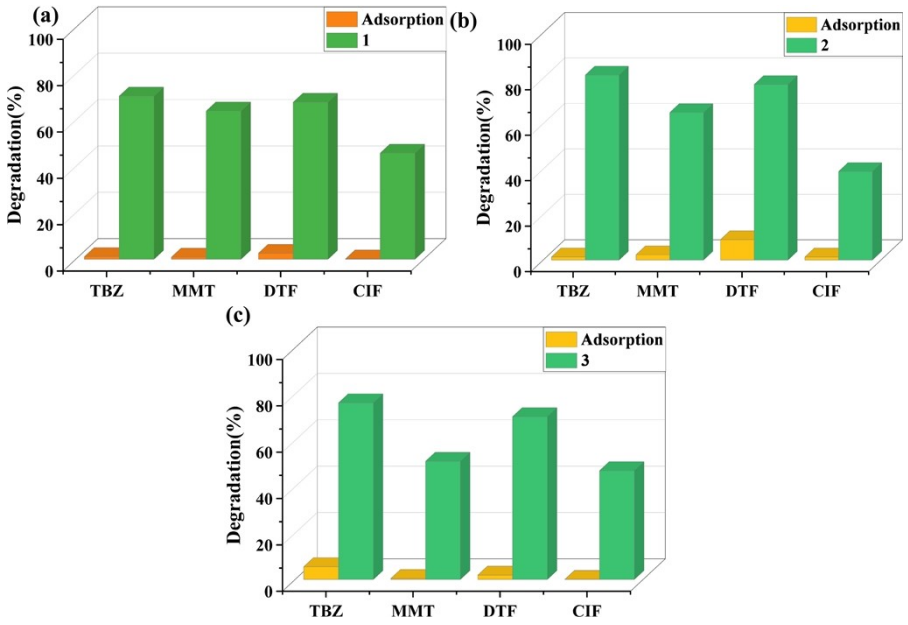

Figure S11. The degradation of **1, 2** and **3** at different pesticide

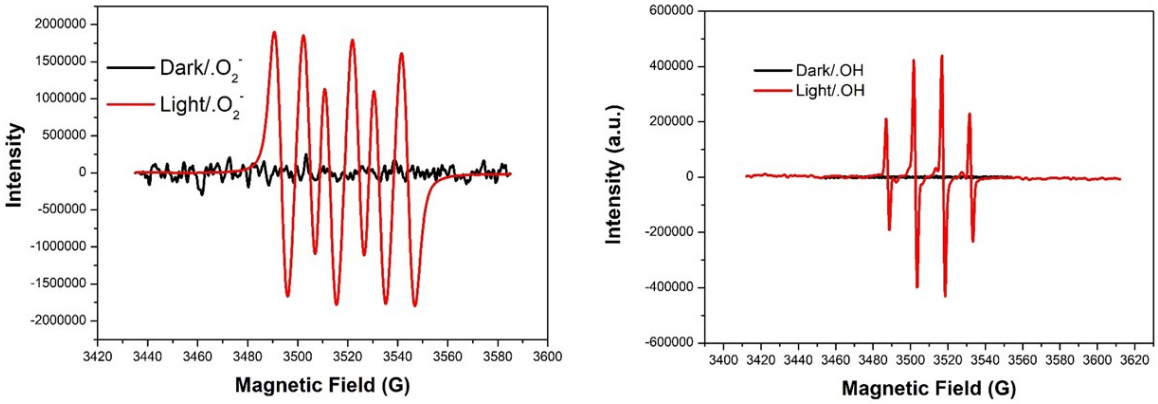

Figure S12. DMPO spin-trapping ESR spectra

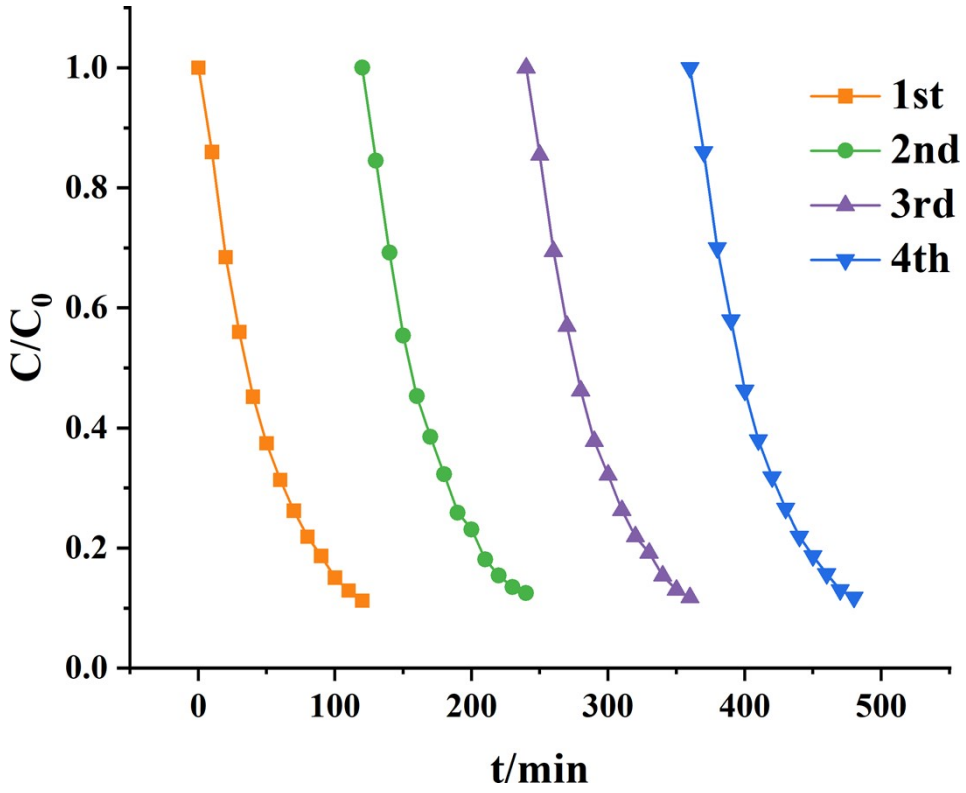

Figure S13. cycling runs of the photocatalytic degradation of TBZ for 2.