Electronic Supplementary Material (ESI) for RSC Advances.

Ag^{+}, Fe^{3+} and Zn^{2+} Intercalated Cadmium (II)-Metal-Organic Frameworks for enhanced Day Light Photocatalysis

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Table S1 Crystal data for Cd-MOF

	Cd-MOF
Empirical formula	$H_7O_7CdC_5$
Formula weight	291.51
Temperature/K	100.01(10)
Crystal system	triclinic
Space group	$P\bar{1}$
a/Å	5.5108(7)
b/Å	7.8194(10)
c/Å	9.6854(11)
α/°	109.785(11)
β/°	104.283(11)
γ/°	98.964(10)
Volume/Å^3	367.24(8)
Z	2
ϱ_{calc}mg/mm^3	2.636
m/mm^{-1}	2.979
F(000)	282
2Θ range for data collection	5.74 to 55°
Index ranges	$-7 \le h \le 7$, $-10 \le k \le 10$, $-12 \le l \le 10$
Reflections collected	2913
Independent reflections	1682[R(int) = 0.0331]
Data/restraints/parameters	1682/0/122
Goodness-of-fit on F^2	1.206
Final R indexes [I>=2σ (I)]	$R_1 = 0.0304$, $wR_2 = 0.0785$
Final R indexes [all data]	$R_1 = 0.0317$, $wR_2 = 0.0794$
Largest diff. peak/hole / e Å^{-3}	0.72/-1.24

Table S2 Selected bond and angles in Cd-MOF

Bond	**Distance (Å)**	**Bond**	**Distance (Å)**
Cd(1)-O(1)	2.324(3)	O(3)-C(5^{2})	1.275(6)
Cd(1)-O(1^{1})	2.340(3)	O(4)-C(5)	1.251(5)
Cd(1)-O(3)	2.236(3)	C(1)-C(2)	1.410(6)
Cd(1)-O(5)	2.371(4)	C(1)-C(3)	1.388(6)
Cd(1)-O(6)	2.280(3)	C(1)-C(4)	1.508(6)
Cd(1)-O(7)	2.346(3)	C(2)-C(3^{3})	1.399(6)
O(1)-Cd(1^{1})	2.340(3)	C(2)-C(5)	1.494(6)
O(1)-C(4)	1.271(5)	C(3)-C(2^{3})	1.399(6)
O(2)-C(4)	1.253(5)	C(5)-O(3^{2})	1.275(6)
Angle	(°)	Angle	(°)
O(1)-Cd(1)-O(1^{1})	73.94(12)	C(4)-O(1)-Cd(1^{1})	136.4(3)
O(1)-Cd(1)-O(5)	76.18(13)	C(4)-O(1)-Cd(1)	109.3(3)
O(1^{1})-Cd(1)-O(5)	86.59(14)	C(5^{2})-O(3)-Cd(1)	112.0(3)
O(1^{1})-Cd(1)-O(7)	171.36(11)	C(2)-C(1)-C(4)	123.8(4)
O(1)-Cd(1)-O(7)	112.80(11)	C(3)-C(1)-(C2)	119.5(4)
O(3)-Cd(1)-O(1)	87.11(11)	C(3)-C(1)-C(4)	116.7(4)
O(3)-Cd(1)-O(1^{1})	84.52(12)	C(1)-C(2)-C(5)	121.8(4)
O(3)-Cd(1)-O(5)	162.71(14)	C(3^{3})-C(2)-C(1)	118.5(4)
O(3)-Cd(1)-O(6)	114.07(13)	C(3^{3})-C(2)-C(5)	119.7(4)
O(3)-Cd(1)-O(7)	90.33(12)	C(1)-C(3)-C(2^{3})	122.0(4)
O(6)-Cd(1)-O(1)	151.68(12)	O(1)-C(4)-C(1)	119.6(4)
O(6)-Cd(1)-O(1^{1})	88.96(11)	O(2)-C(4)-O(1)	121.9(4)
O(6)-Cd(1)-O(5)	80.50(13)	O(2)-C(4)-C(1)	118.1(4)
O(6)-Cd(1)-O(7)	86.81(12)	O(3^{2})-C(5)-C(2)	116.8(4)
O(7)-Cd(1)-O(5)	100.12(15)	O(4)-C(5)-O(3^{2})	123.8(4)
Cd(1)-O(1)-Cd(1^{1})	106.06(12)	O(4)-C(5)-C(2)	119.4(4)

Symmetry transformation ^{1}-X,1-Y,-Z; ^{2}-1-X,1-Y,-Z; ^{3}-X,1-Y,1-Z

Scherrer equation:

Eq. $$D = \frac{k\lambda}{\beta \cos\theta} \quad \text{(S1)}$$

Where D is the crystallite size in nm, K is the shape constant (0.9), λ is the wavelength of Cu Kα radiation (1.5406 Å), β is full width at half maximum and θ is the diffraction angle (°)[34].

The energy gap (E_g) was calculated by using Kubelka–Munk function.

Eq. $$F(R\infty) = \frac{(1 - R\infty)2}{2R\infty} \quad \text{(S2)}$$

$$E(eV) = \frac{hC}{\lambda} \quad \text{(S3)}$$

Where R^{∞} is the diffused reflectance of at the given wavelength, where h is the Planck's constant (6.626×10^{-34} J s), C is the speed of light (3.0×10^{8} ms^{-1}) and λ is the wavelength[49,50].

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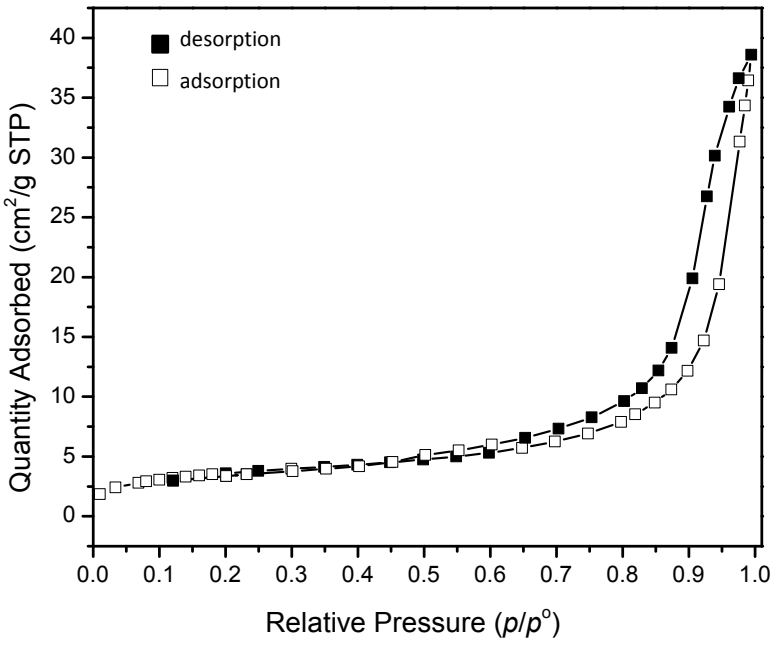


Fig. S1 The N_2 adsorption-desorption isotherms of pure Cd-MOF

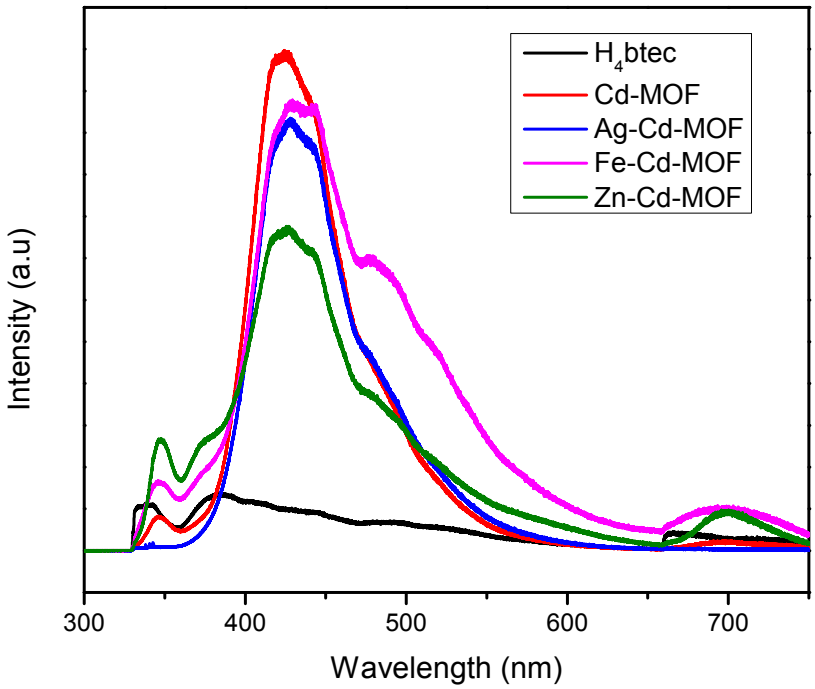


Fig. S2 Photoluminescence spectra of free H_4btec linker, complex Cd-MOF, metal ions intercalated Cd-MOF at room temperature (λ_{ex}= 325nm)

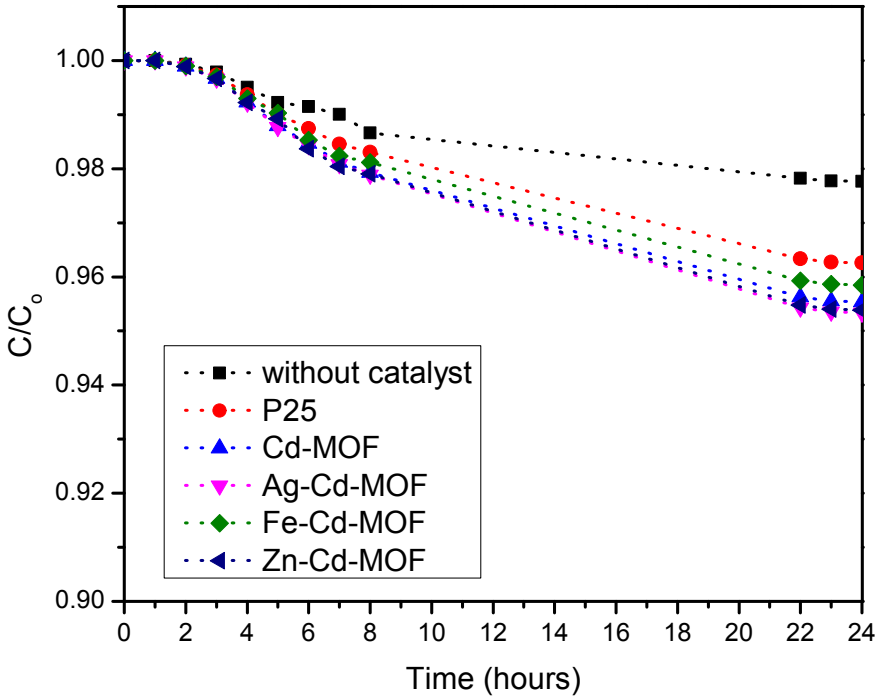
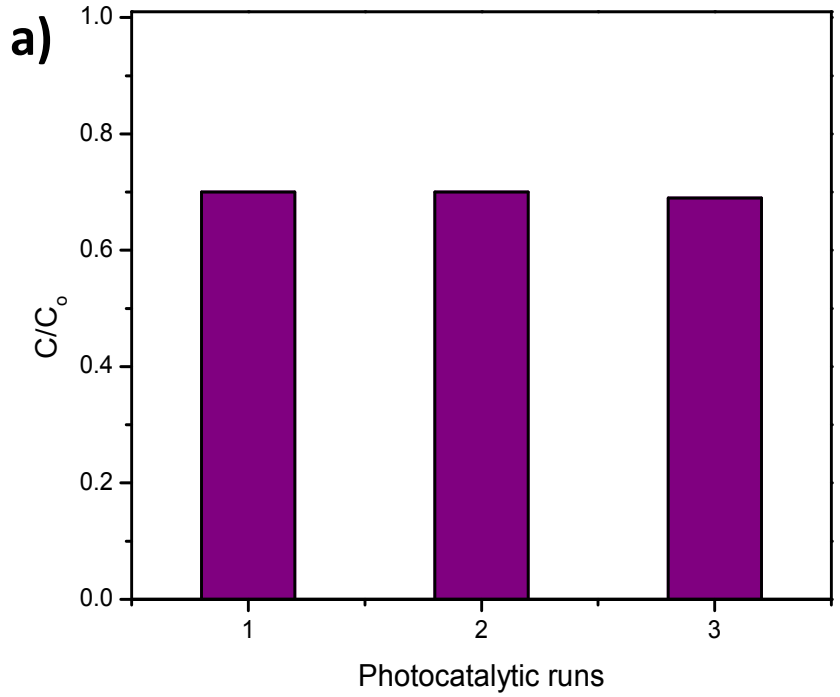
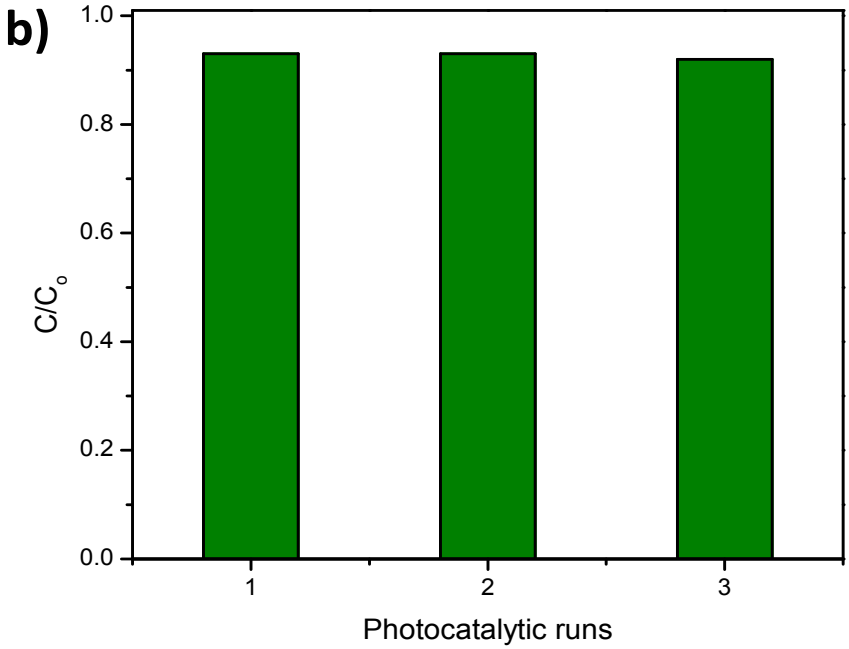


Fig. S3 Adsorption performance of the studied MOFs under dark condition


a)
1.0
0.8
0.6
0.4
0.2
0.0
C/C$_o$
1
2
3
Photocatalytic runs


b)
1.0
0.8
0.6
0.4
0.2
0.0
C/C$_o$
1
2
3
Photocatalytic runs

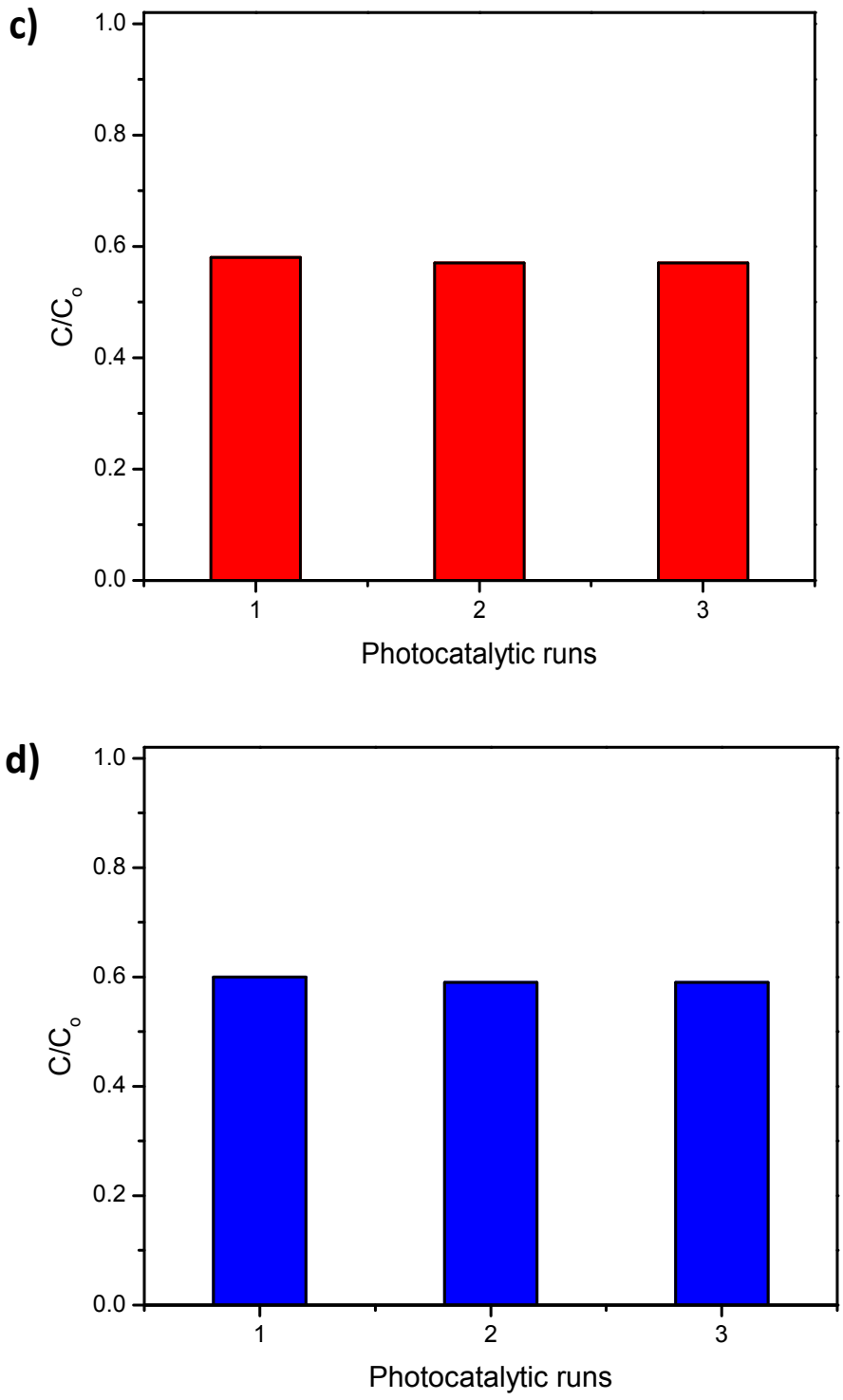
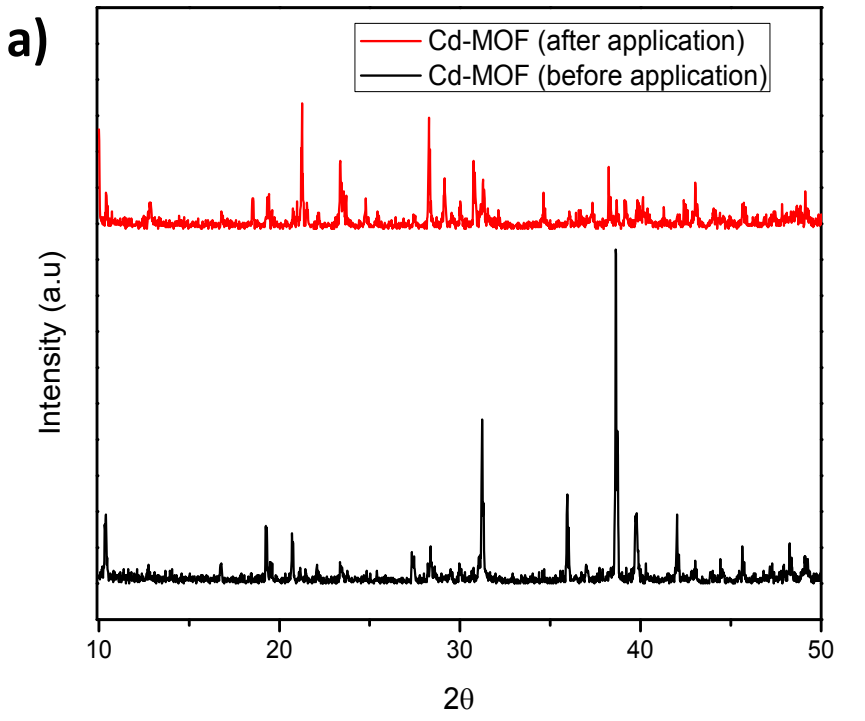
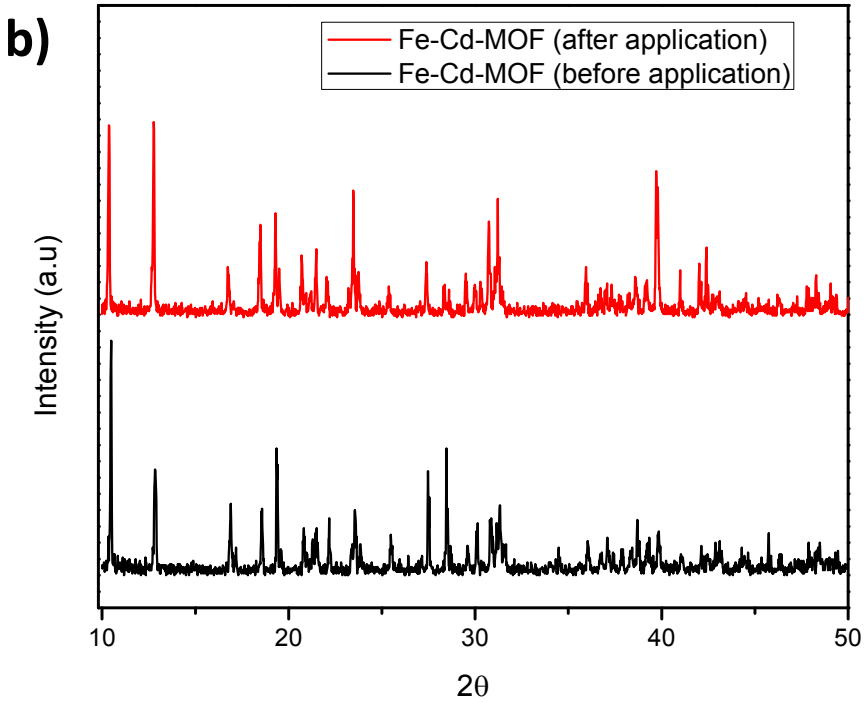


Fig. S4 Reusability study (a) Cd-MOF and (b) Fe-Cd-MOF (c) Ag-Cd-MOF (d) Zn-Cd-MOF on 2-CP degradation


a)
Cd-MOF (after application)
Cd-MOF (before application)
Intensity (a.u)
10
20
30
40
50
2θ


b)
Fe-Cd-MOF (after application)
Fe-Cd-MOF (before application)
Intensity (a.u)
10
20
30
40
50
2θ

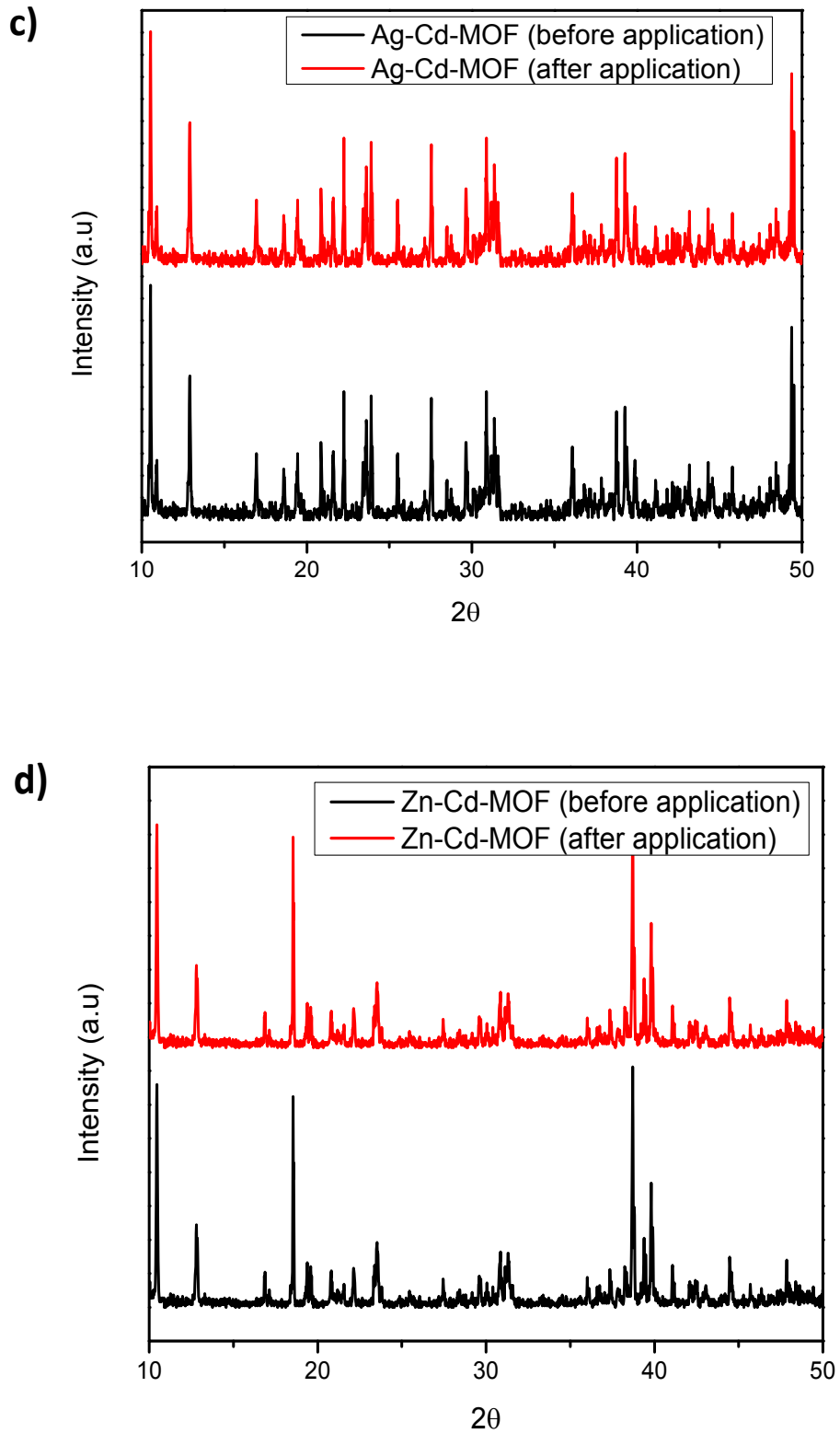


Fig. S5 Diffraction obtained before and after day light photocatalysis application

Eq. $$\ln \frac{C}{Co} = - kt \quad \text{(S4)}$$

Wherein C_0 is the initial 2-CP concentration, C is the 2-CP concentration at a certain time, t is the reaction time, and k is the kinetic rate constant. The values of k can be calculated from the slope and the intercept of the linear plot[9].

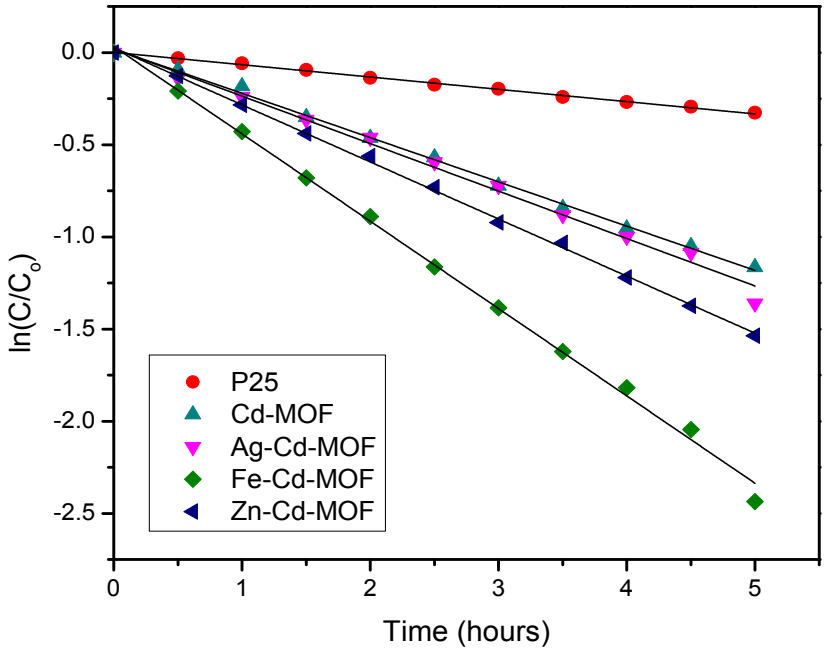


Fig. S6 The kinetics of 2-CP photodegradation under solar light irradiation