Electronic Supporting Information for

The effects of transition-metal doping and chromophor anchoring on photocurrent response of titanium-oxo-clusters

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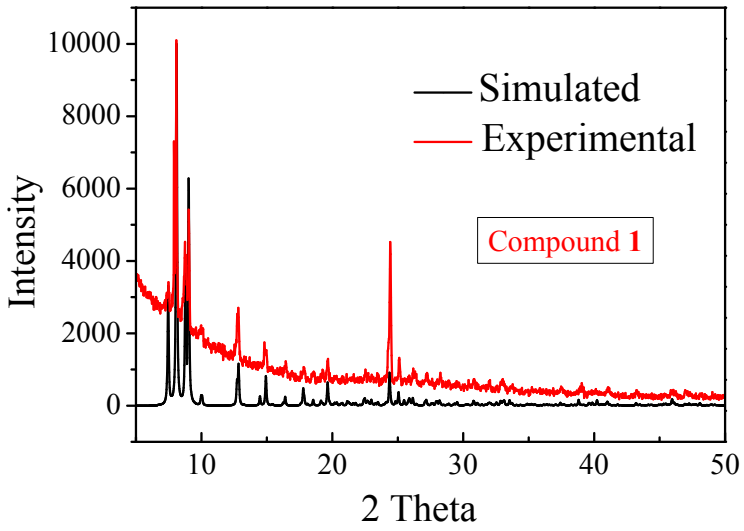
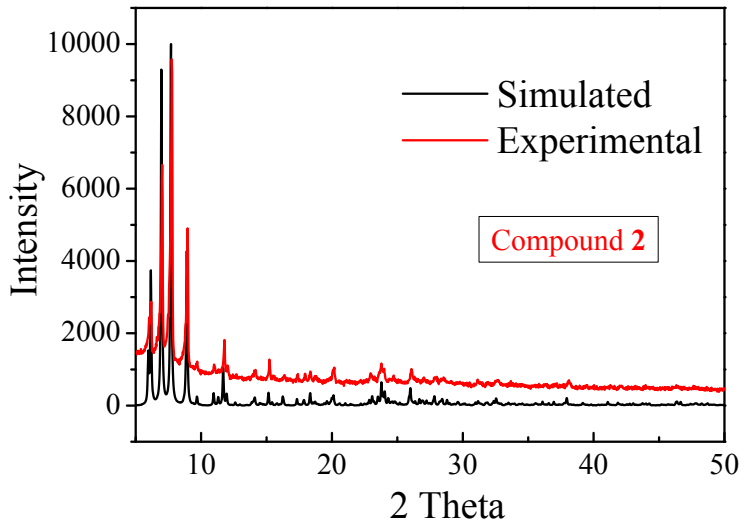

Simulated
Experimental
Compound 1
Intensity
2 Theta
0
2000
4000
6000
8000
10000
10
20
30
40
50


Simulated
Experimental
Compound 2
Intensity
2 Theta
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8000
10000
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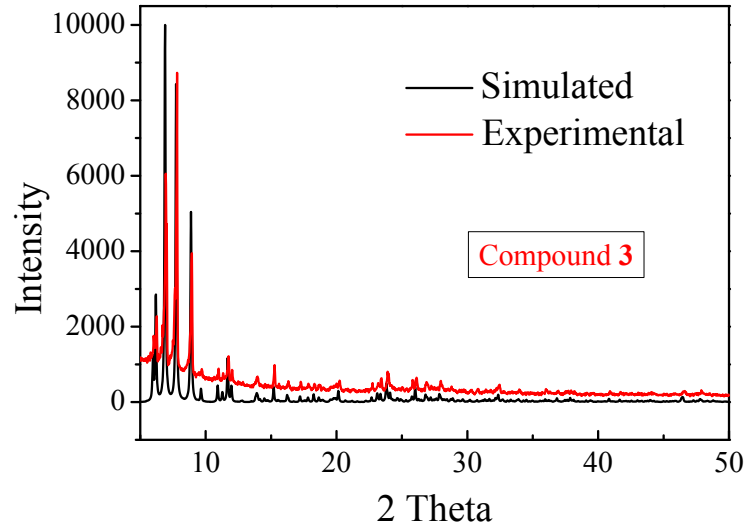


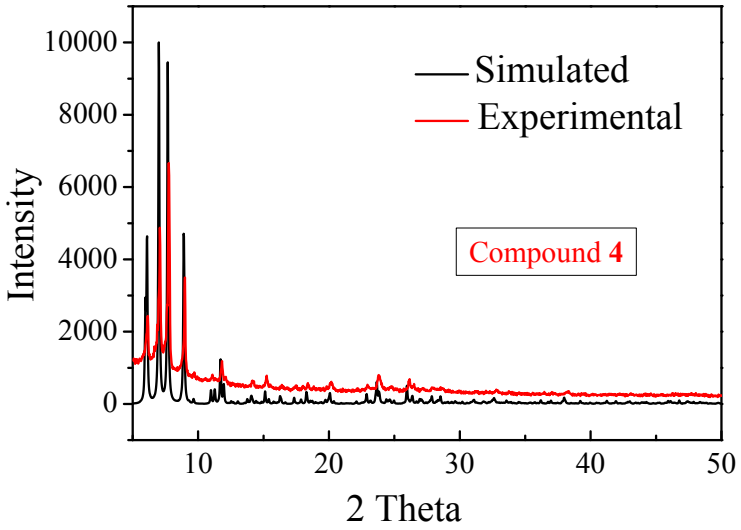


Fig. S1. Comparing of the experimental XRD patterns of the bulky samples with the calculated patterns from the crystal data of compounds **1-4**.

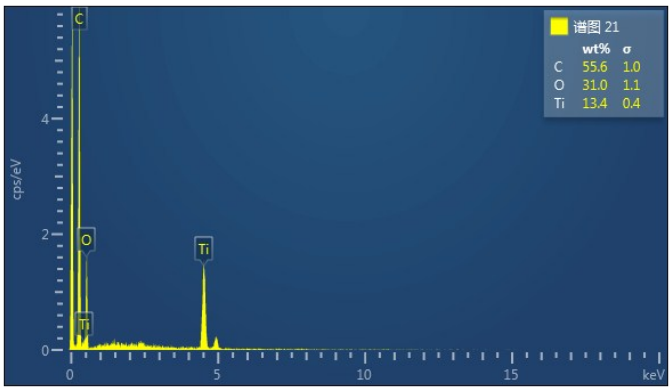


Fig. S2. EDS result of compound **1**.

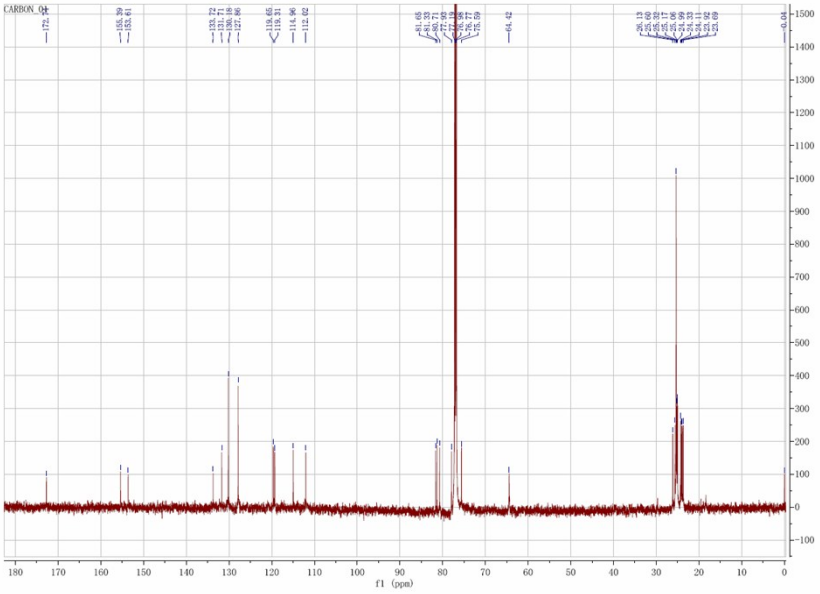
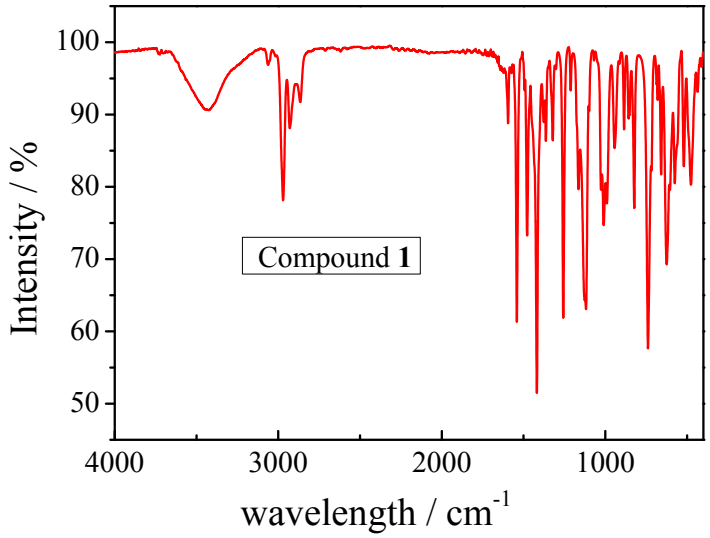
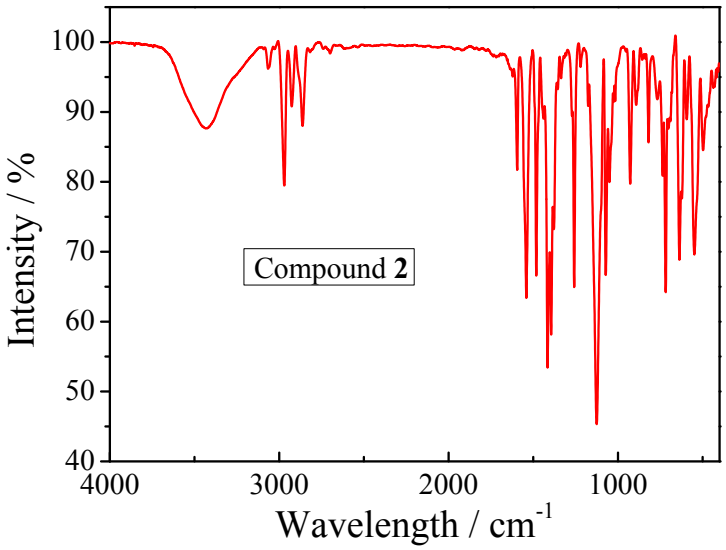


Fig. S3. ^{13}C NMR spectrum of compound **1** in $CDCl_3$.


Intensity / %
100
90
80
70
60
50
Compound 1
4000
3000
2000
1000
wavelength / cm-1


Intensity / %
100
90
80
70
60
50
40
Compound 2
4000
3000
2000
1000
Wavelength / cm-1

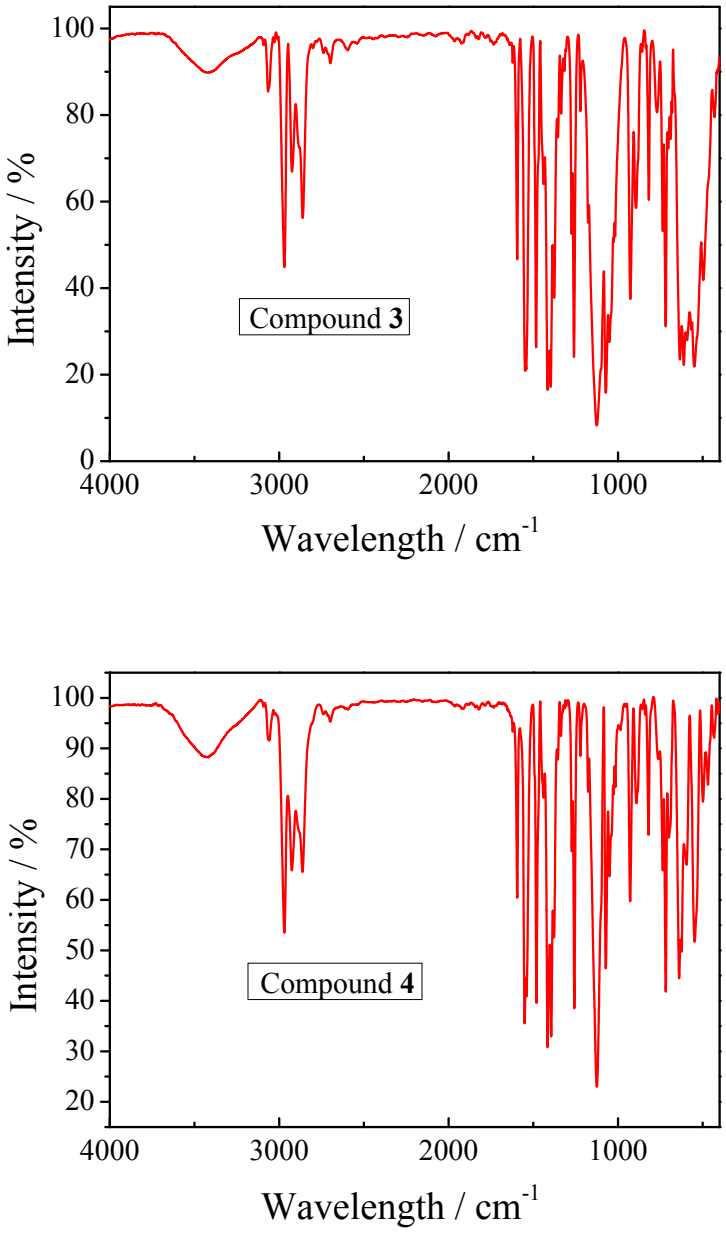


Figure S4. The IR spectra of the clusters **1**, **2**, **3** and **4**.

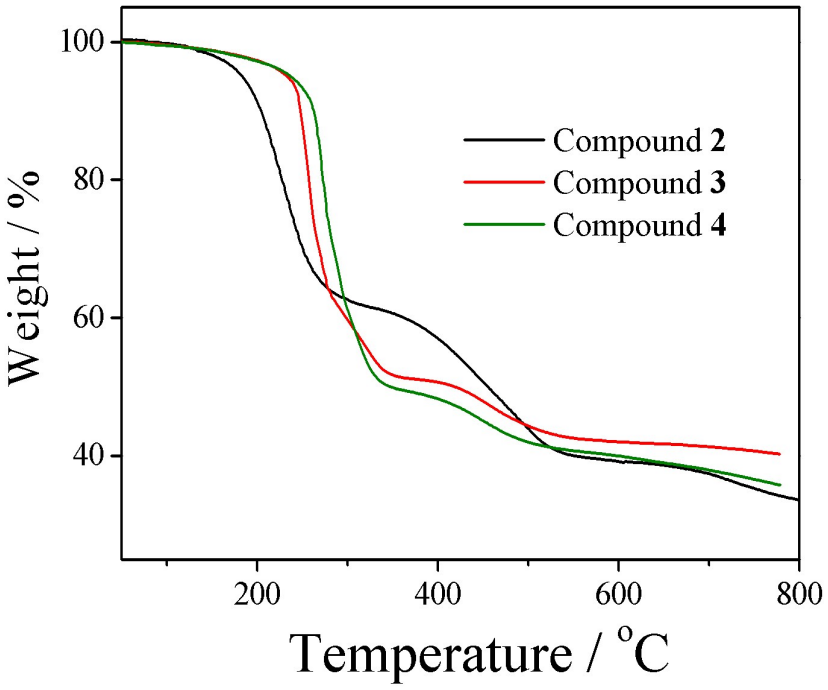


Fig. S5. TG curves of clusters **2**, **3** and **4**.

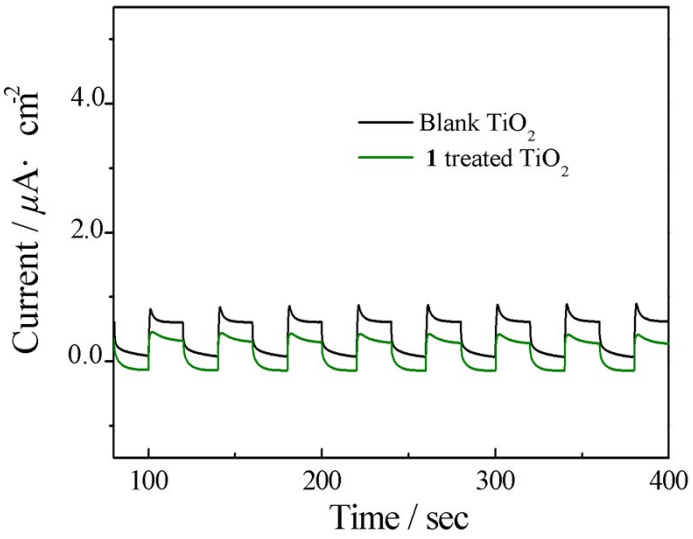


Fig. S6. Photocurrent densities of **1** treated electrode and the blank porous TiO_2 electrode.

Table S1. Crystal Data and Structural Refinement Parameters for **1**-**4**.

	1	**2**	**3**	**4**
formula	$C_{56}H_{88}O_{22}Ti_6$	$C_{88}H_{148}Co_2O_{46}Ti_{12}$	$C_{88}H_{148}Mn_2O_{46}Ti_{12}$	$C_{88}H_{148}Ni_2O_{46}Ti_{12}$
Fw	1400.58	2634.54	2626.55	2634.06
cryst size (mm^3)	0.40 × 0.30 × 0.20	0.55 × 0.30 × 0.25	0.40 × 0.35 × 0.20	0.35 × 0.35 × 0.25
cryst syst	monoclinic	monoclinic	monoclinic	monoclinic
space group	*C*2/*c*	*P* 2_1/*c*	*P* 2_1/*c*	*P* 2_1/*c*
a (Å)	20.749(4)	14.622(3)	14.530(3)	14.6941(10)
b (Å)	13.908(3)	14.022(3)	14.214(3)	13.8919(9)
c (Å)	24.407(5)	30.184(6)	30.116(6)	29.990(2)
α (deg)	90.00	90.00	90.0	90.00
β (deg)	104.01(3)	101.25(3)	101.00(3)	100.884(2)
γ (deg)	90.00	90.00	90.0	90.00
V ($Å^3$)	6834(2)	6069(2)	6105(2)	6011.7(7)
Z	4	2	2	2
ρ_{calcd} (g cm^{-3})	1.361	1.442	1.429	1.413
F(000)	2928	2724	2716	2576
μ (mm^{-1})	0.736	1.085	1.014	1.132
T (K)	293(2)	293(2)	293(2)	293(2)
reflns collected	27161	23377	4469	63572
unique reflns	6001	10520	10735	10586
observed reflns	5119	6360	8841	5266
no. params	406	706	713	675
GOF on F^2	1.163	1.178	1.164	1.096
R_1[I>2σ(*I*)]	0.0633	0.0969	0.0971	0.0896
$_wR_2$	0.1540	0.1730	0.1741	0.1923