Electronic Supplementary Information

Ferrocenecarboxylate-functionalized titanium-oxo-cluster: ferrocene wheel as sensitizer for photocurrent response

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Table S1. Crystal data and structure refinements summary for **C1**, **C2** and **C3**.

	C1	**C2**	**C3**
Empirical formula	$C_{84}H_{96}O_{24}Ti_6Fe_6$	$C_{84}H_{84}O_{24}Ti_6$	$C_{90}H_{96}O_{24}Ti_6$
Formula weight	2112.10	1764.91	1849.06
Crystal system	monoclinic	triclinic	triclinic
Space group	$P2_1/n$	P-1	P-1
a (Å)	16.8249(7)	13.3081(10)	13.4769(14)
b (Å)	13.8268(4)	13.8105(12)	13.9496(15)
c (Å)	19.4260(7)	14.5437(11)	14.1303(13)
α (°)	90	63.018(8)	65.816(10)
β (°)	90.638(4)	66.477(7)	83.373(9)
γ (°)	90	62.871(8)	62.506(11)
V (Å^3)	4518.9(3)	2056.8(4)	2140.7(4)
Z	2	1	1
ρ_{calcd} (g cm^{-3})	1.552	1.425	1.434
μ (mm^{-1})	1.501	0.630	0.609
F(000)	2160	912	960
T (K)	295(2)	295(2)	295(2)
Measured refls.	19561	14685	16003
Independent refls.	8852	7251	8402
R_{int}	0.0391	0.0717	0.0248
GOF	1.022	1.036	1.034
R_1 [$I > 2\sigma(I)$][a]	0.0501	0.0805	0.0442
wR_2 [$I > 2\sigma(I)$][b]	0.1070	0.1310	0.1129

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

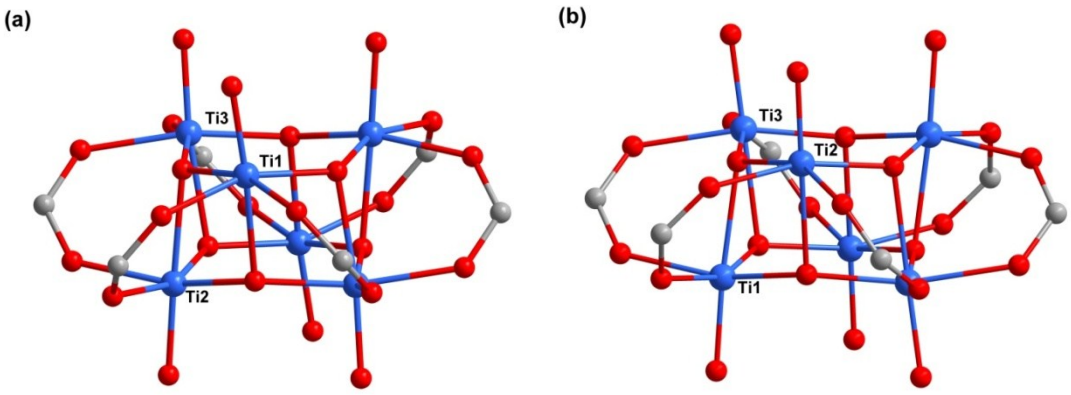

Fig. S1 (a) Coordination mode of $\{Ti_6\}$ in **C2**. (b) Coordination mode of $\{Ti_6\}$ in **C3**.

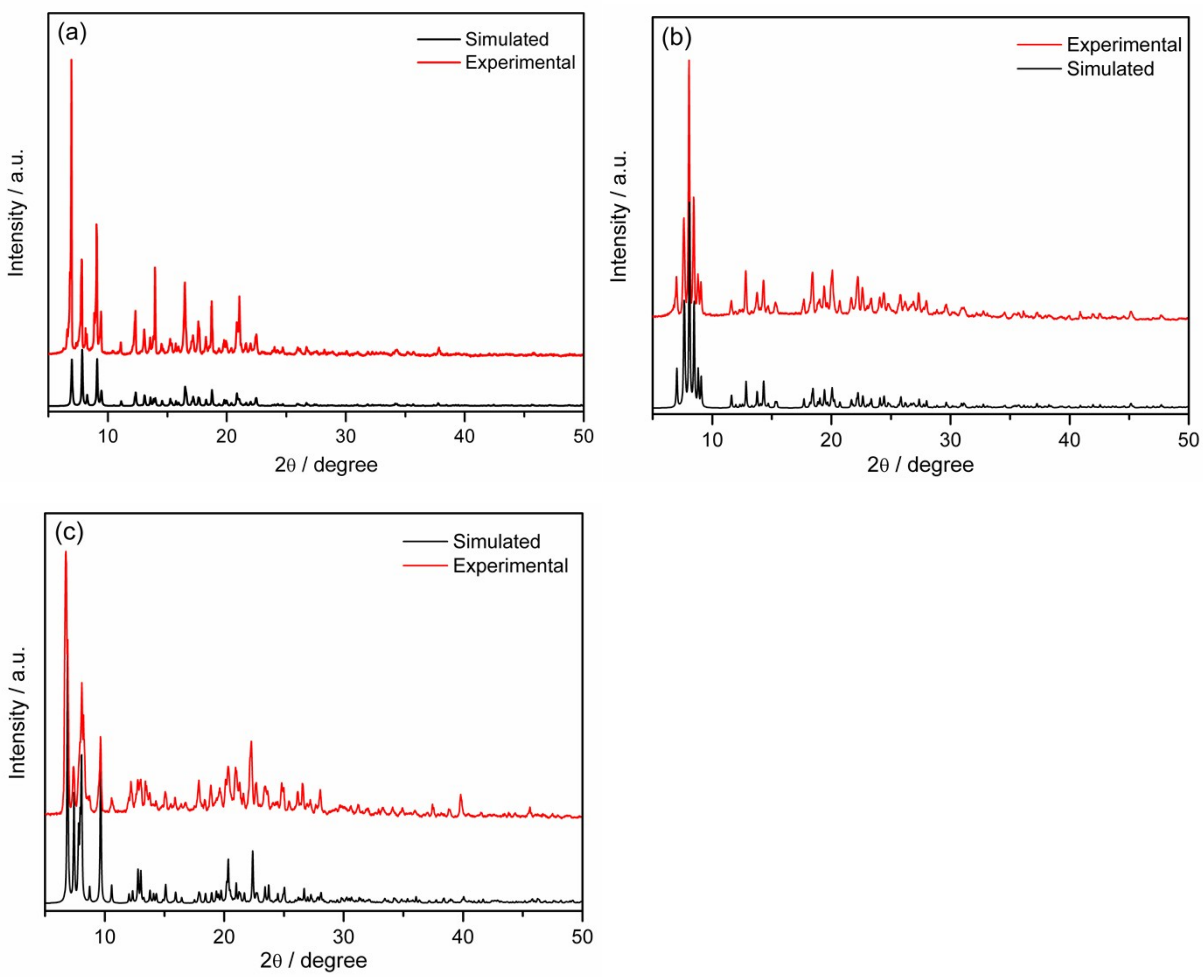

Fig. S2 XRD patterns of (a) **C1**, (b) **C2** and (c) **C3**.

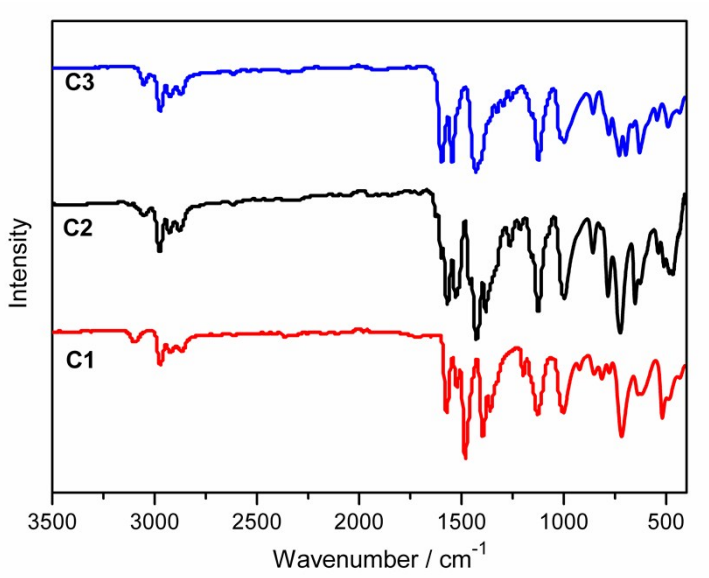

Fig. S3 FT-IR spectra of **C1**, **C2** and **C3**.

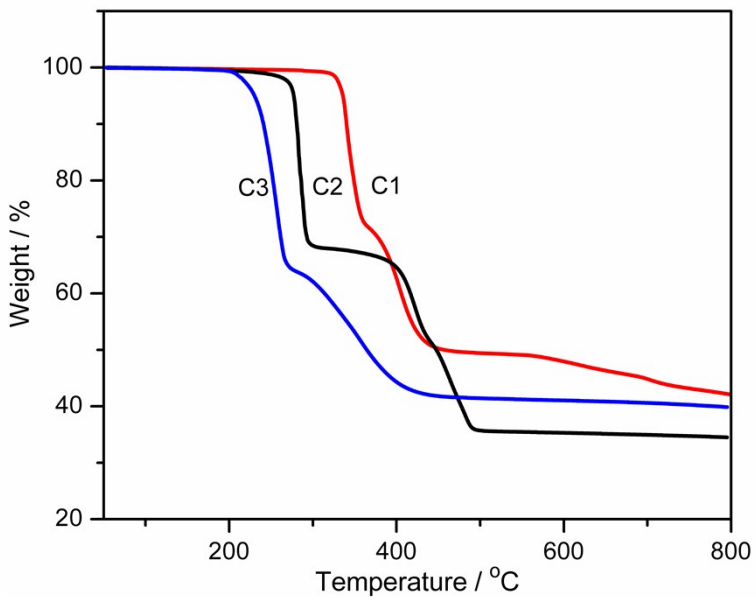

Fig. S4 The TGA curves of **C1**, **C2** and **C3**.

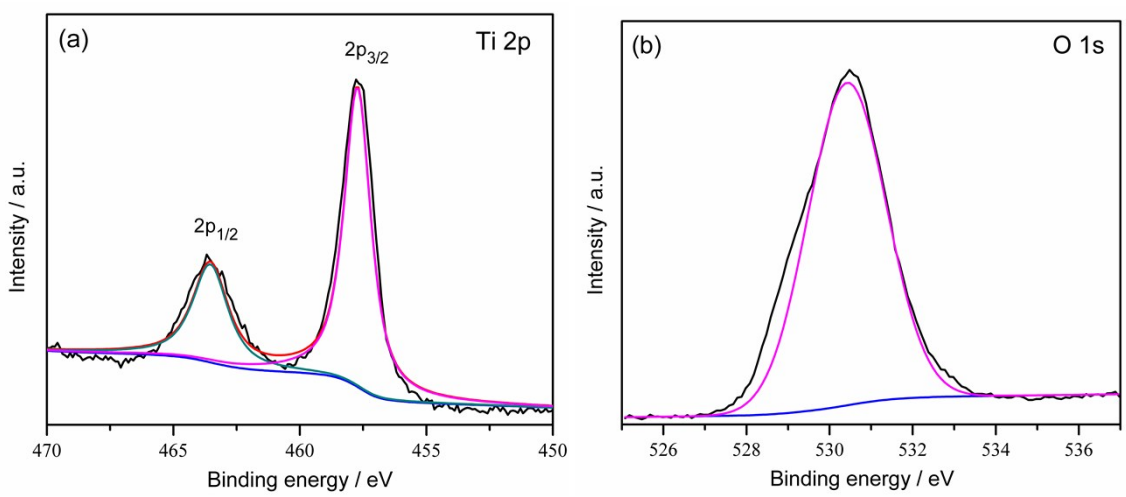

Fig. S5 XPS spectra of (a) Ti 2p peaks and (b) O 1s peaks for **C2**.

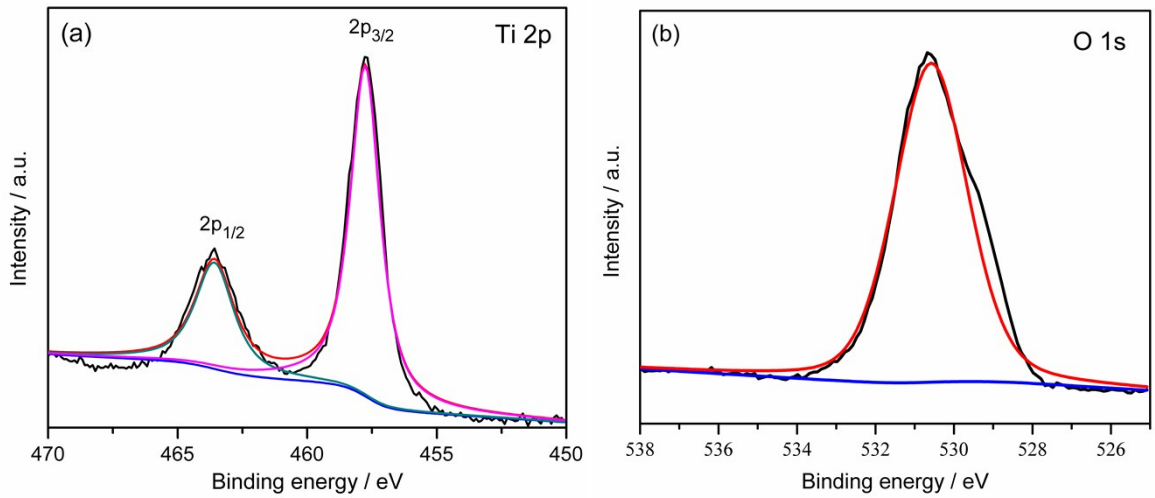

Fig. S6 XPS spectra of (a) Ti 2p peaks and (b) O 1s peaks for **C3**.

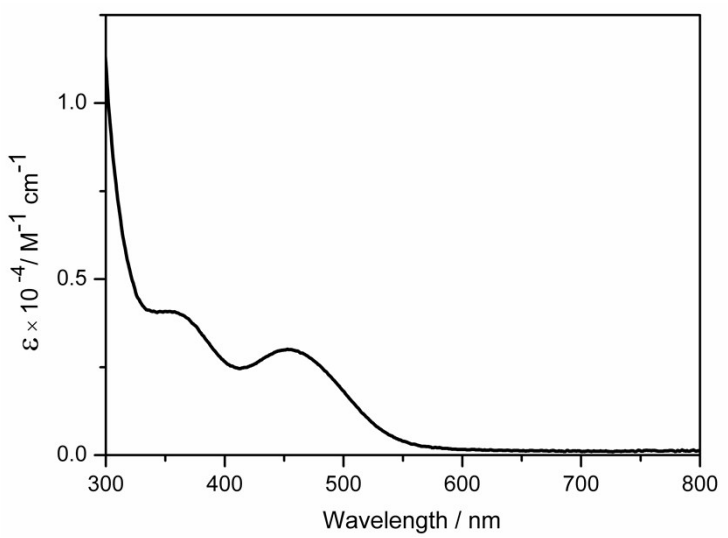

Fig. S7 UV-vis spectra of 1×10^{-4} M solution of **C1** in dichloromethane.

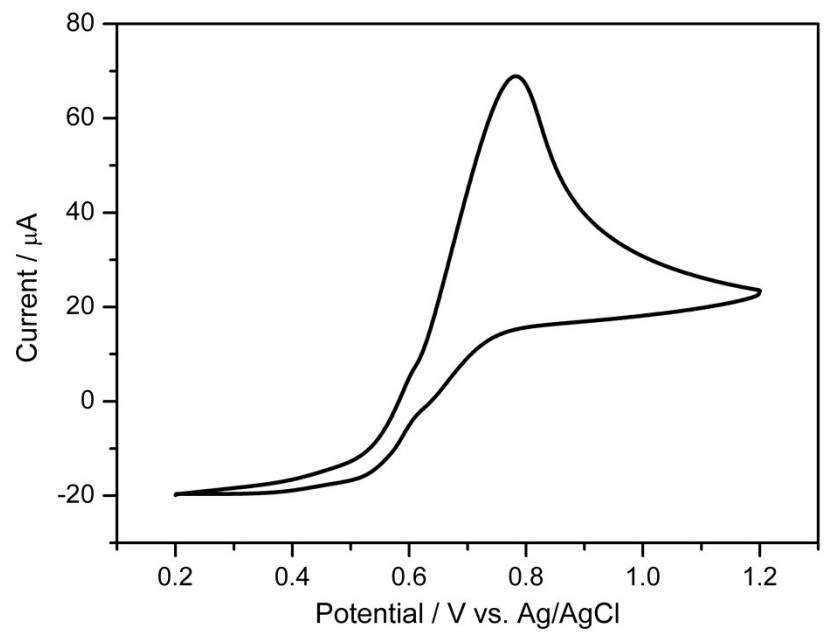

Fig. S8 CV curves of ferrocenecarboxylic acid in dichloromethane solution containing 0.1 M n-Bu_4NPF_6 as the supporting electrolyte, scan rate = 100 mV s^{-1}.

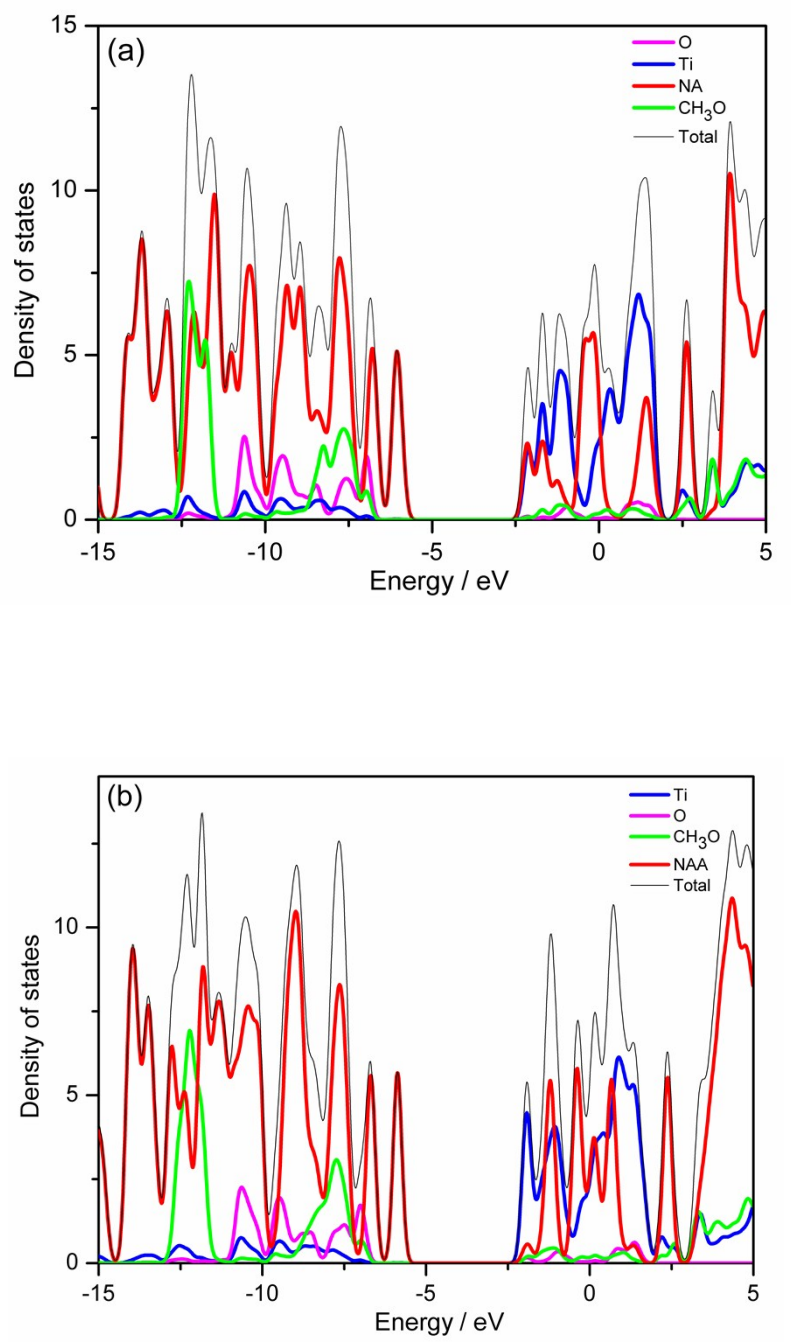

Fig. S9 Density of states (DOS) plots for (a) **C2** and (b) **C3**.

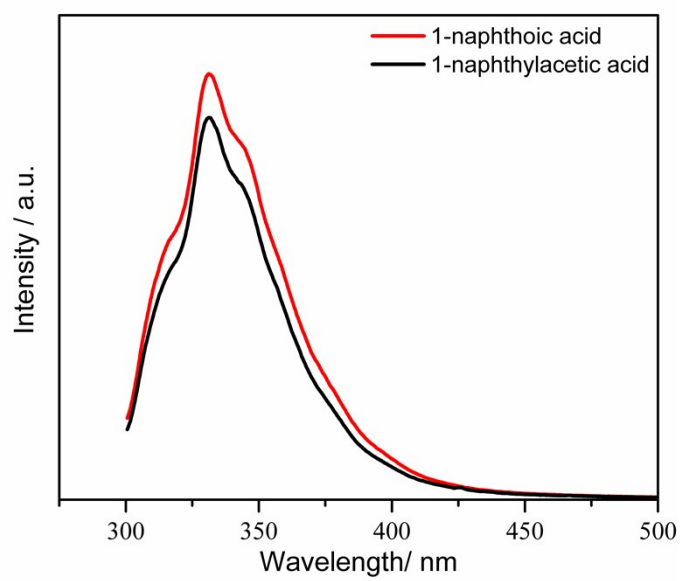

Figure S10 Room-temperature emission spectra of 1-naphthoic acid and 1-naphthylacetic acid in dichloromethane solutions (1×10^{-6} M) with 280 nm excitation.