Electronic Supplementary Information for

Effects of co-coordinated auxiliary ligands on photoelectrochemical behaviours of titanium-alkoxide-dyes

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Figures

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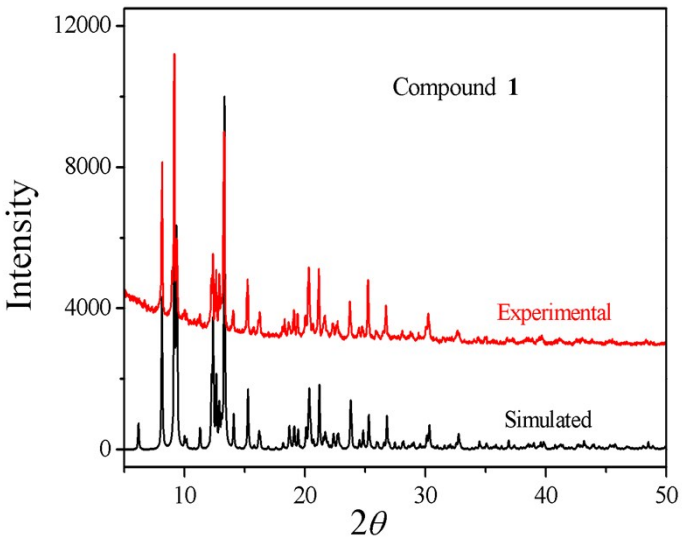
FIGURES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Experimental
Simulated
Intensity
2θ
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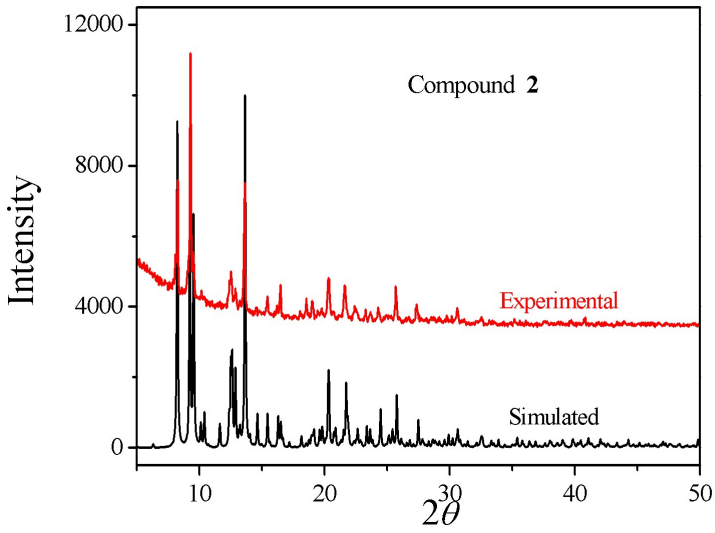
8000
4000
0
10
20
30
40
50

(a)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Intensity
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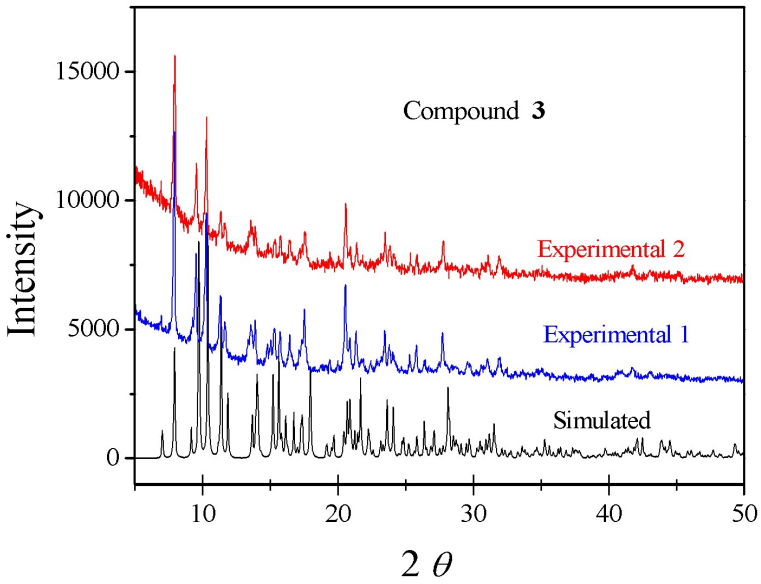
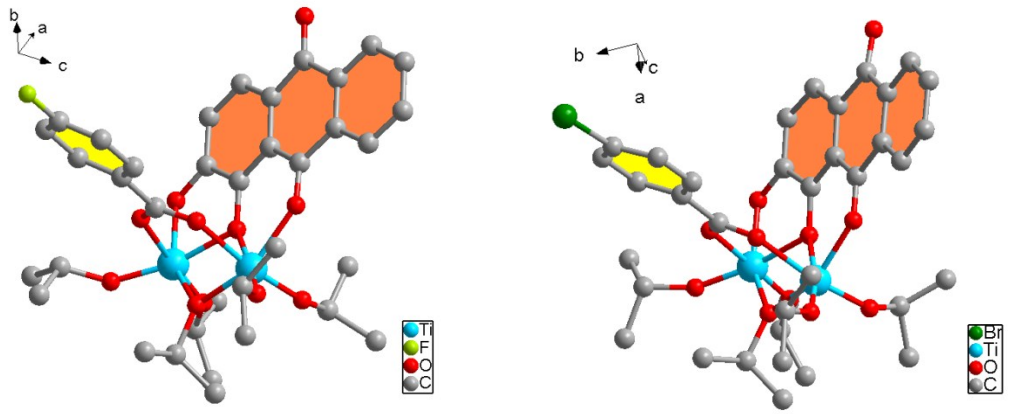
(b)



(c)

Fig. S1. Experimental XRD patterns of **1** (a), **2** (b) and **3** (c) along with the calculated patterns from the crystal data.



(a) (b)

Fig. S2. Ball-stick plots of compound **2** (a), **3** (b), showing the molecular structuure.

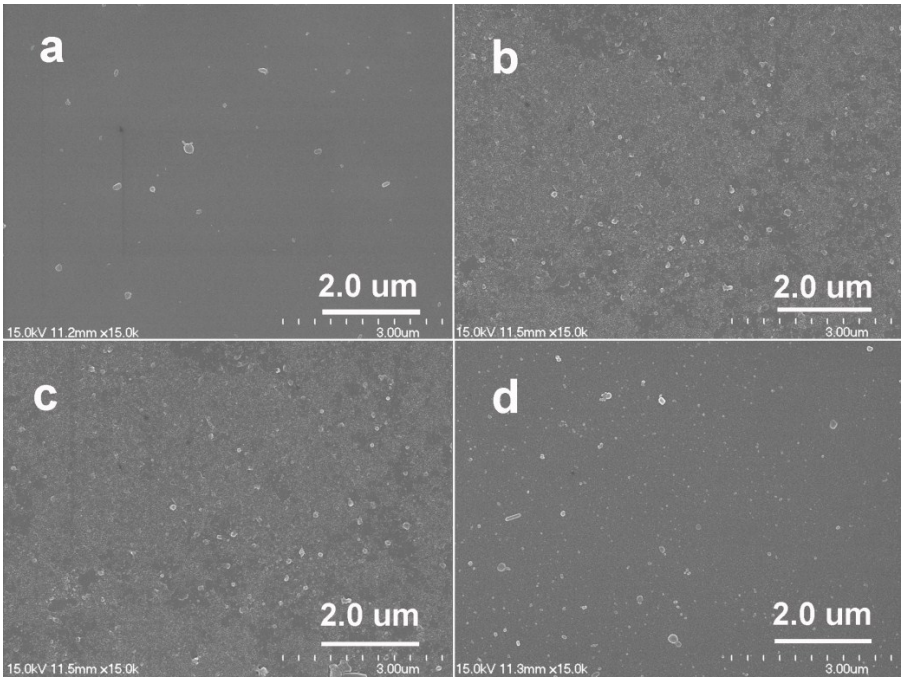


Fig. S3. The surface morphologies of the nano TiO_2 film (a) and films of **1** (b), **2** (c), **3** (d), showing the smooth and uniform surfaces.

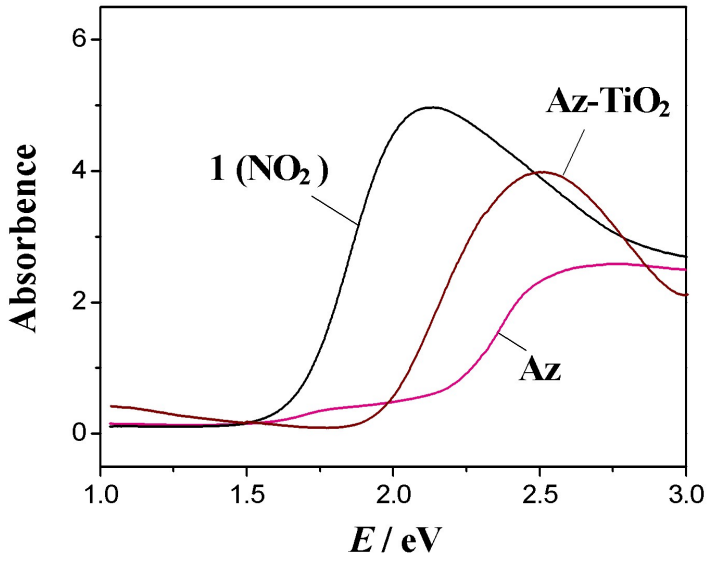


Fig. S4. The absorption spectra of **1**, dye Az and Az treated TiO_2 substrate.

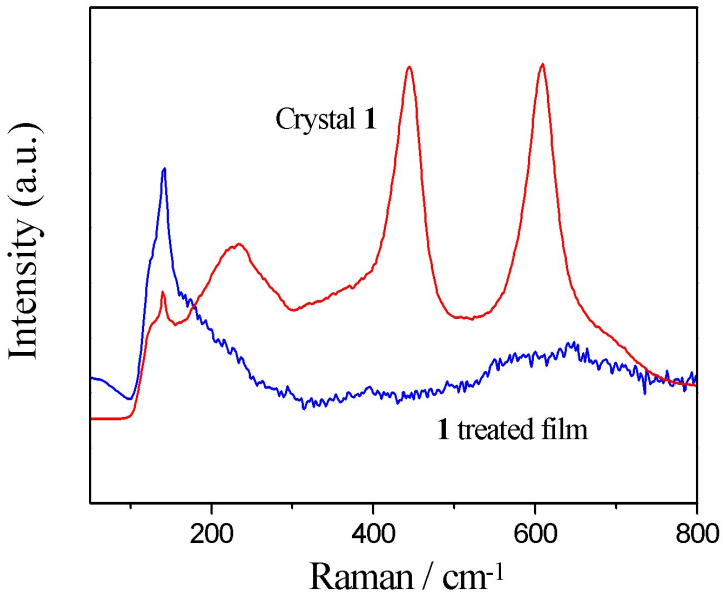


Fig. S5. Raman spectra of the crystal **1** and **1** treated TiO2 electrode.

T Table S1 Crystal data and structural refinement parameters for **1**–**3**.

	1	**2**	**3**
formula	$C_{36}H_{45}NO_{13}Ti_2$	$C_{36}H_{45}FO_{11}Ti_2$	$C_{36}H_{45}BrO_{11}Ti_2$
fw	795.51	768.51	829.41
cryst size (mm^3)	0.35 × 0.20 × 0.10	0.50 × 0.40 × 0.30	0.26 × 0.24× 0.20
cryst syst	monoclinic	monoclinic	monoclinic
space group	$P2_1/c$	$P2_1/c$	$P2_1/c$
a (Å)	9.6859(3)	9.6424(13)	12.9644 (12)
b (Å)	21.7550(6)	21.475(3)	13.1630(12)
c (Å)	19.0222(5)	18.640(2)	23.030(2)
α (deg)	90.00	90.00	90.00
β (deg)	93.686(3)	96.6066(4)	104.724(3)
γ (deg)	90.00	90.00	90.00
V ($Å^3$)	4000.0(2)	3834.2(9)	3801.0(6)
Z	4	4	4
ρ_{calcd} (g cm^{-3})	1.321	1.331	1.449
F(000)	1664	1608	1712
μ (mm^{-1})	0.460	0.477	1.528
T (K)	293(2)	293(2)	120(2)
reflns collected	31104	20324	60996
unique reflns	10589	6748	8698
observed reflns	6508	3688	5888
no. params	479	468	461
GOF on F^2	1.065	1.084	1.165
R_1 [I>2σ(I)]	0.0665	0.0902	0.0543
$_wR_2$	0.1442	0.1731	0.1345

Table S2 Results of TD-DFT calculation for compunds for **1**, **2** and **3**.

	1	**2**	**3**
Gap Energy (eV)	2.127	2.120	2.112
Absorption (nm)	583	585	587
f	0.0996	0.1045	0.1024
Transition	198A →199A	204A →205A	191A→192A
	198B →199B	204B →205B	191B→192B
Coefficient	0.69933	0.69924	0.69942