

SI materials for manuscript:

Two Ti_{13} -oxo-clusters showing non-compact structures, film electrode preparation and photocurrent property

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Fig. S1 The experimental and simulated XRD results of **1** and **2**.

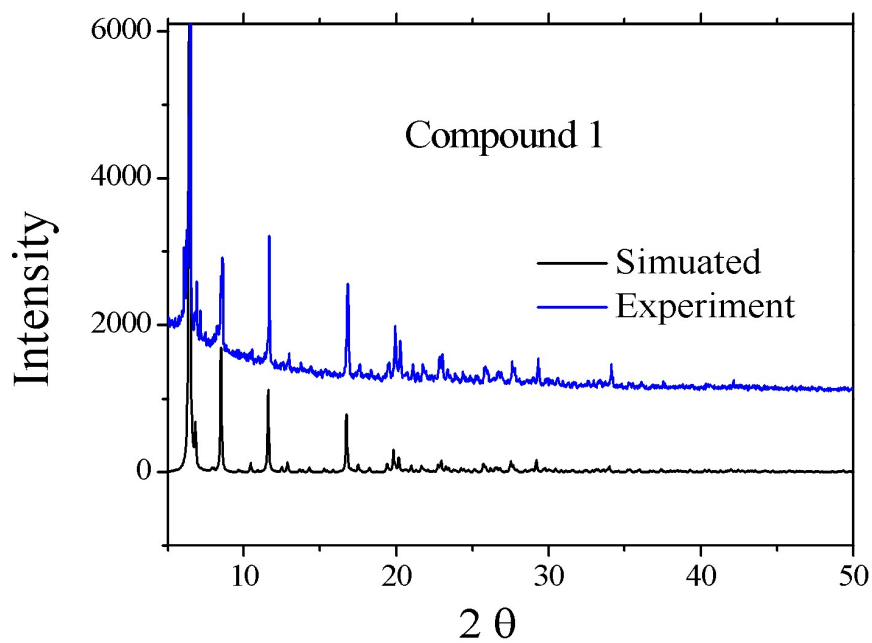
Fig. S2 The IR spectra of **1** and **2**.

Fig. S3 (a) The UV-vis absorption spectra of **1** and **2**. (b) Thermogravimetric measurements of **1** and **2**.

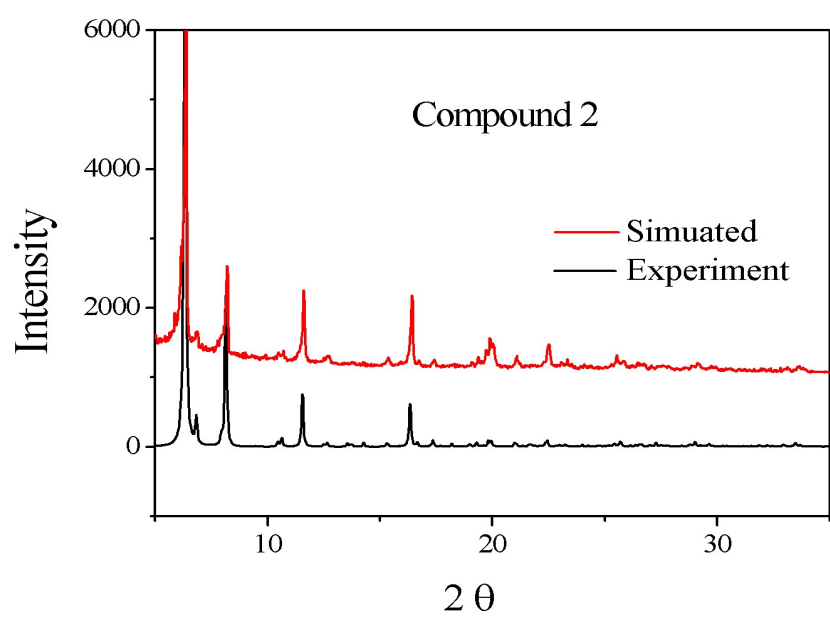
Fig. S4 The IR spectra of the films **1** (a) and **2** (b), before heated (black line), after 280 °C annealing (red line) and after 500 °C annealing (blue line).

Fig. S5 The XRD measurement of the 500 °C treated films **1** and **2**, showing that they are nanostructural anatase with weak peaks at 25.5 and 47.8.

Table S1 Important Ti-O bond lengths in **1** and **2**.

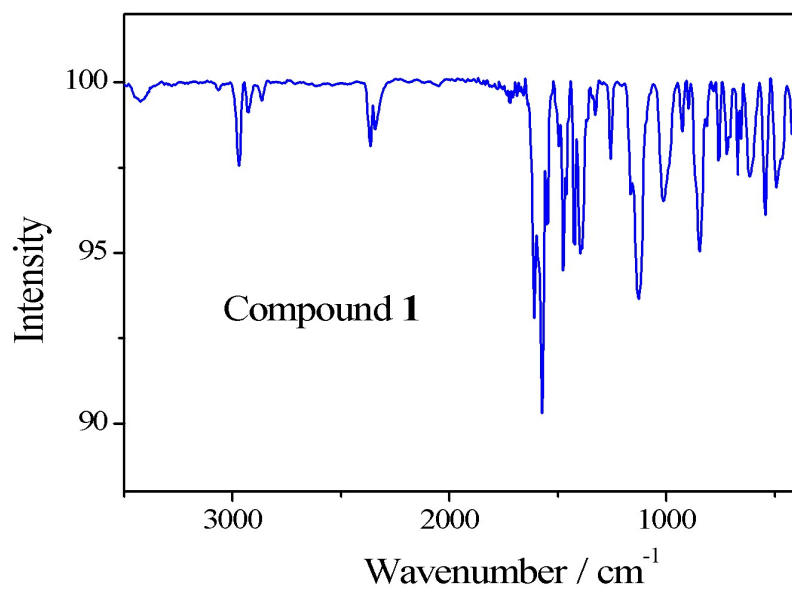


(a)

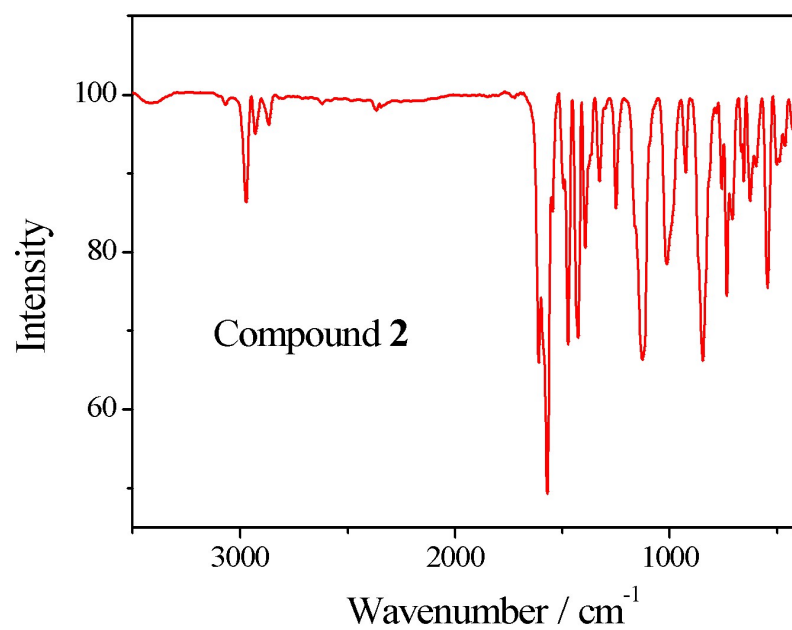


(b)

Fig. S1 The experimental and simulated XRD results of **1** and **2**.

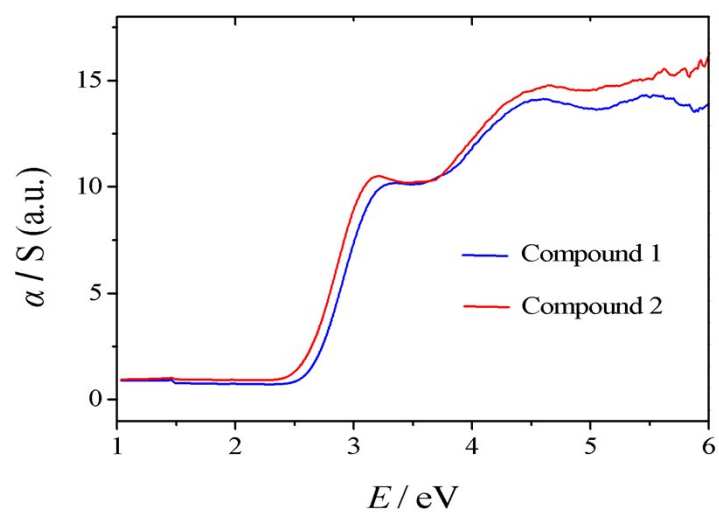


(a)

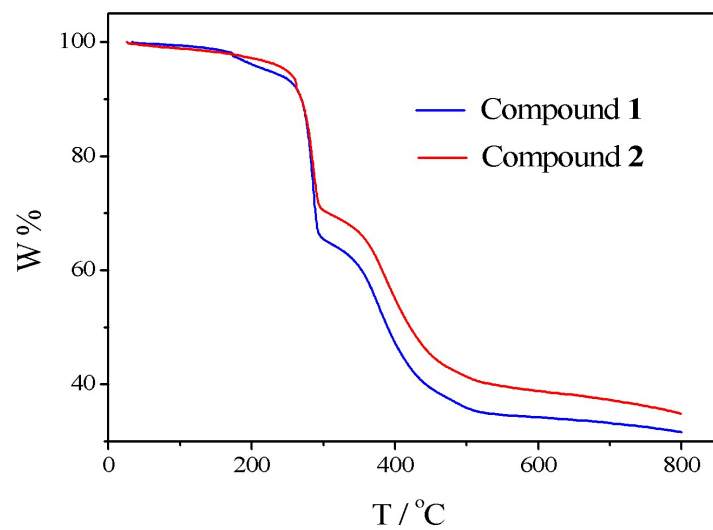


(b)

Fig. S2 The IR spectra of **1** and **2**.

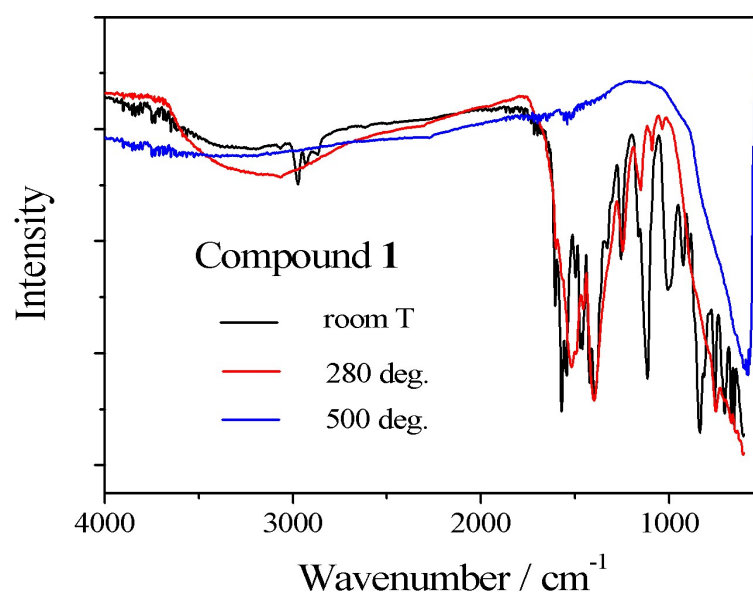


(a)

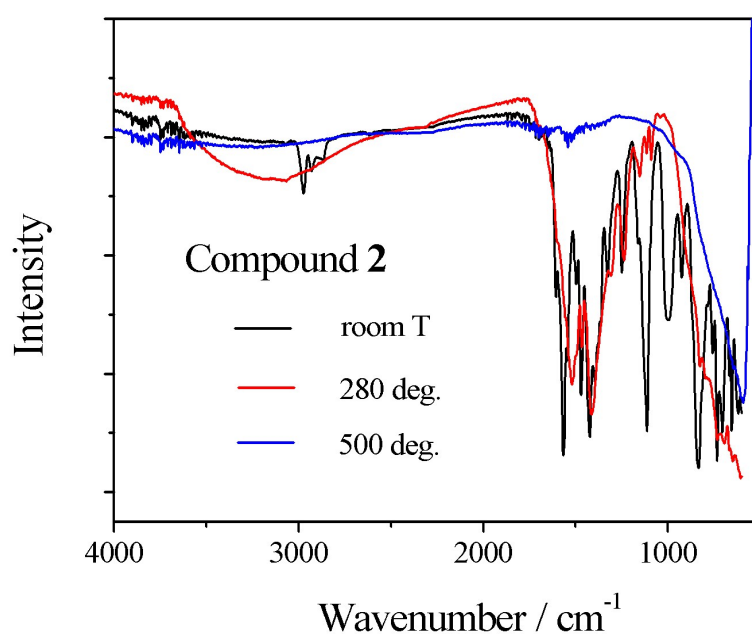


(b)

Fig. S3 (a) The UV-vis absorption spectra of **1** and **2**. (b) Thermogravimetric measurements of **1** and **2**.



(a)



(b)

Fig. S4 The IR spectra of the films of **1** (a) and **2** (b), before heated (black line), after 280 °C annealing (red line) and after 500 °C annealing (blue line).

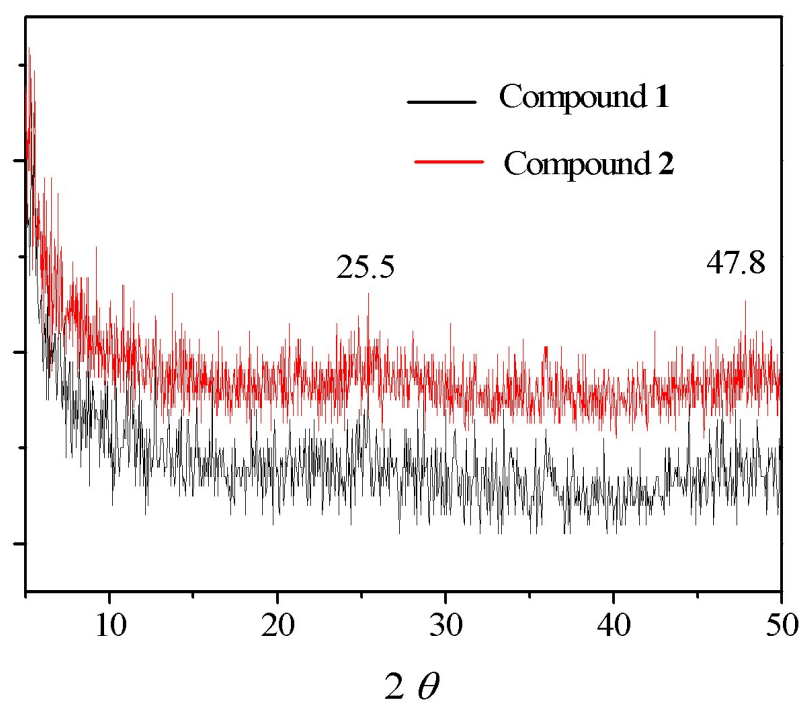


Fig. S5 The XRD measurement of the 500 °C treated films **1** and **2**, showing that they are nanostructural anatase with weak peaks at 25.5 and 47.8.

Table S1 Important Ti-O bond lengths in **1** and **2**.

1		2	
Bond	Distance (Å)	Bond	Distance (Å)
Ti1–O10	1.780(6)	Ti1–O8	1.756(6)
Ti1–O9	1.787(7)	Ti1–O9	1.762(8)
Ti1–O7	1.903(6)	Ti1–O5	1.917(7)
Ti1–O8	2.032(5)	Ti1–O10	2.016(5)
Ti1–O6	2.164(5)	Ti1–O6	2.166(5)
Ti1–O1	2.174(6)	Ti1–O4	2.209(6)
Ti2–O11	1.725(5)	Ti2–O12	1.721(5)
Ti2–O12	1.892(4)	Ti2–O11	1.892(5)
Ti2–O8	2.000(5)	Ti2–O3	1.988(5)
Ti2–O2	2.009(5)	Ti2–O10	2.014(5)
Ti2–O3	2.039(5)	Ti2–O2	2.028(5)
Ti2–O6	2.271(5)	Ti2–O6	2.286(6)
Ti3–O13	1.758(5)	Ti3–O13	1.737(6)
Ti3–O14	1.9202(19)	Ti3–O14	1.904(2)
Ti3–O11	1.930(5)	Ti3–O12	1.931(5)
Ti3–O5	2.016(5)	Ti3–O7	2.013(5)
Ti3–O4	2.033(5)	Ti3–O1	2.046(5)
Ti3–O12	2.075(4)	Ti3–O11	2.073(5)
Ti4–O12	1.953(4)	Ti4–O11	1.958(4)
Ti4–O14	1.987(6)	Ti4–O14	1.991(7)