

Supporting Information

Enhanced Near-Infrared to Visible Upconversion Nanoparticles of Ho^{3+} - Yb^{3+} - F^- Tri-Doped TiO_2 and Its Application in Dye-sensitized Solar Cells with 37% Improvement in Power Conversion Efficiency

Jia Yu, Yulin Yang,* Ruiqing Fan,* Danqing Liu, Liguo Wei, Shuo Chen, Liang Li, Bin Yang, and Wenwu Cao*

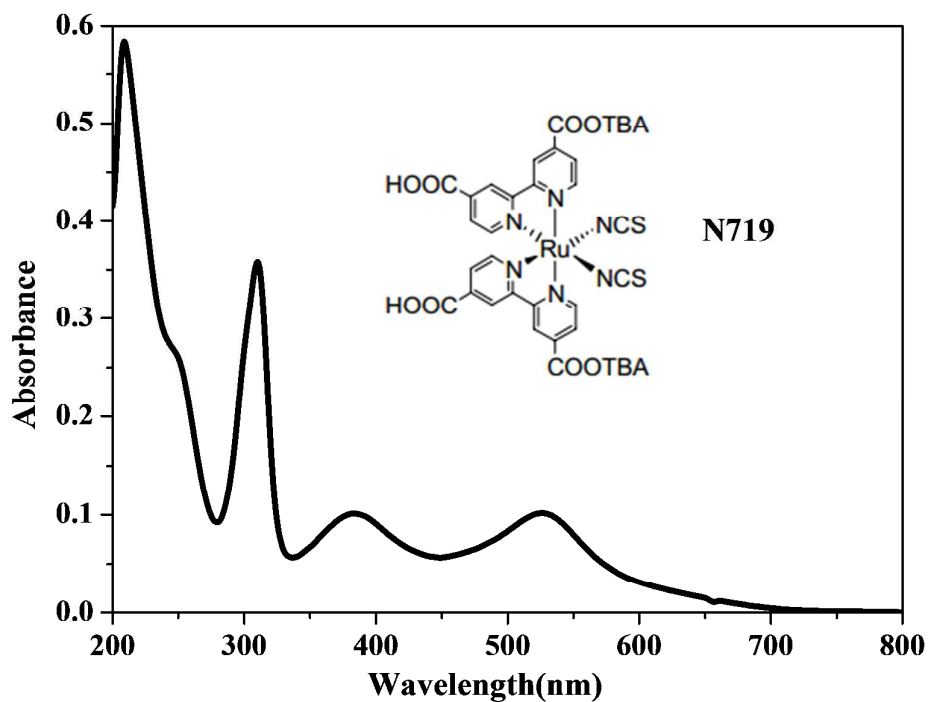


Figure S1. UV-vis absorption spectrum of N719 in ethanol solution and chemical structure is shown as inset.

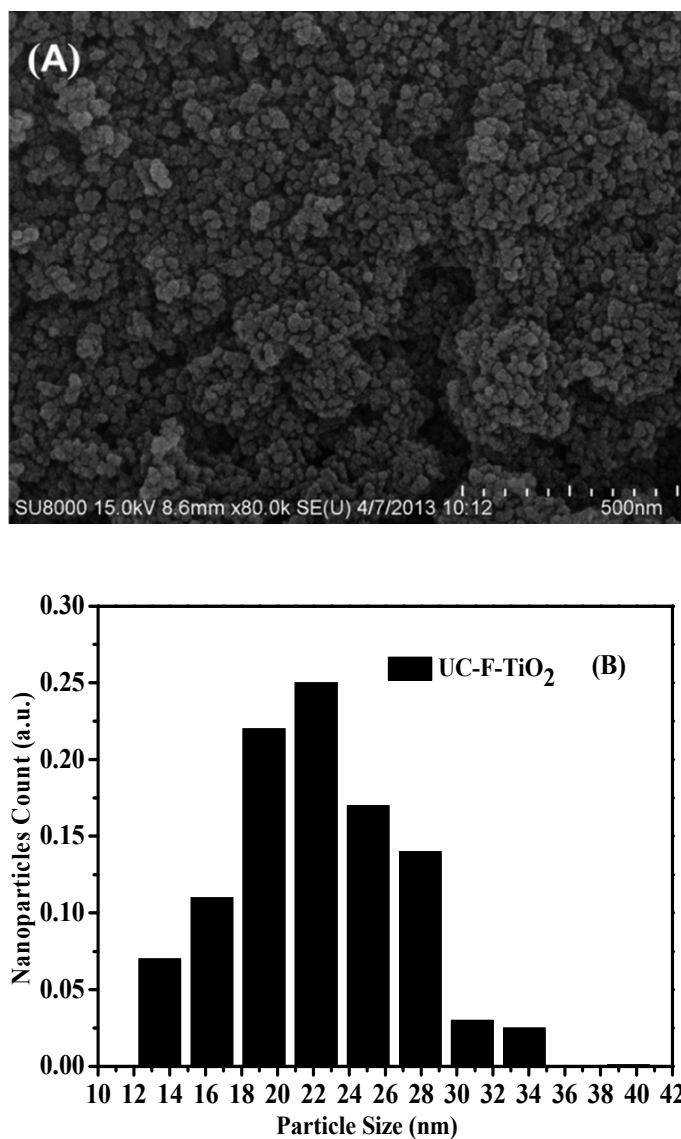


Figure S2. (A) SEM image of the synthesized TiO_2 . (B) Size distribution of the UC-F- TiO_2 . The amount of counted samples is 100 with maximal size of 39.55nm, minimal size of 13.45nm.

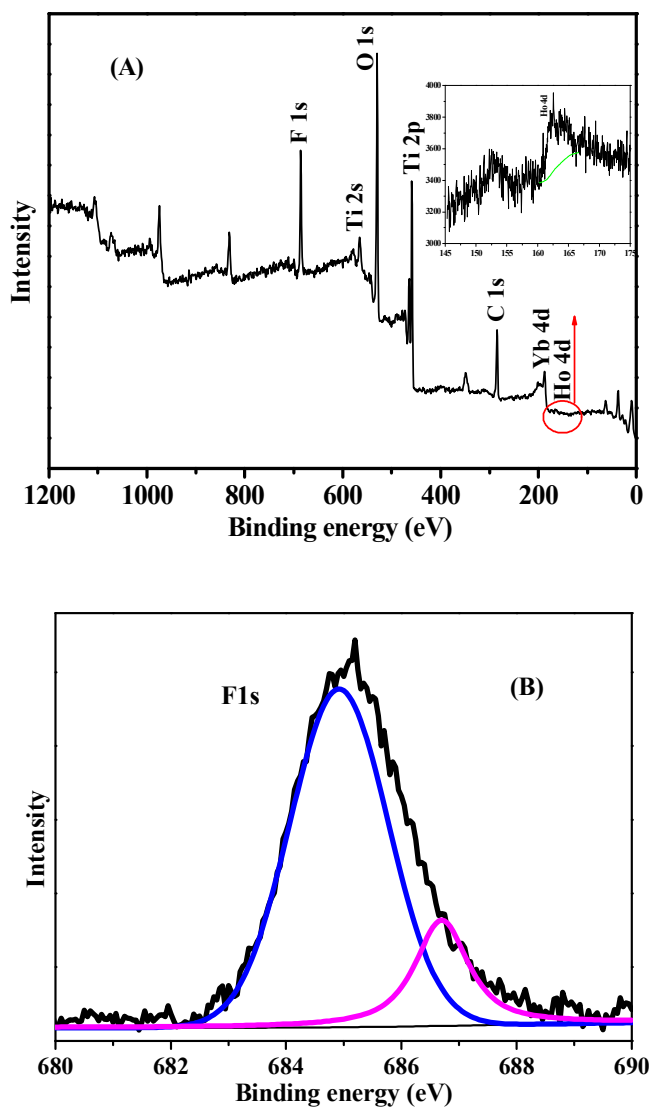


Figure S3. (A) XPS survey spectrum of UC-F-TiO₂ (inset: Ho 4d) and (B) F 1s region in UC-F-TiO₂.

Table S1. XPS measured the content of UC-F-TiO₂ products

sample	Ti	O	Ho	Yb	F
	content	content	content atomic	content	content atomic
	atomic	atomic	conc. (%)	atomic	conc. (%)
	conc. (%)	conc. (%)		conc. (%)	
UC-F-TiO ₂	21.93	57.23	0.13	1.52	19.19

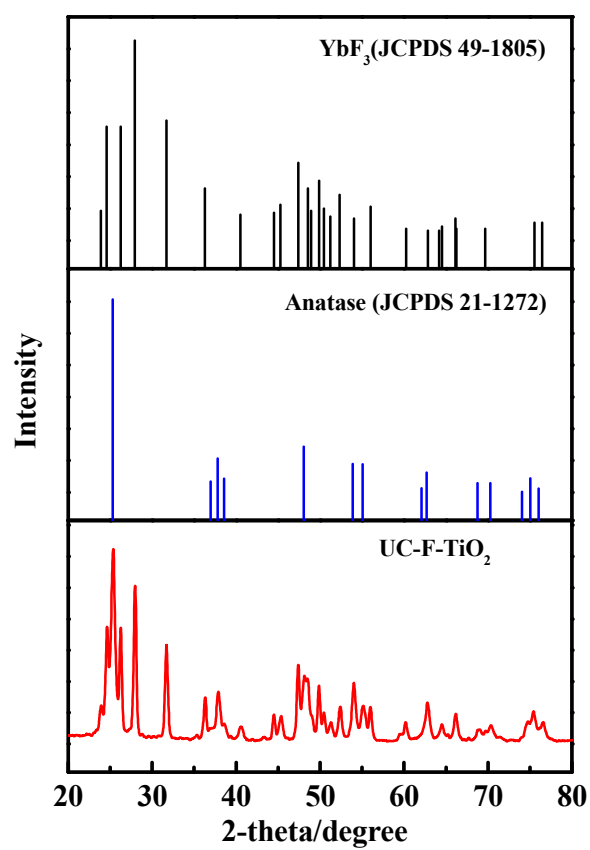


Figure S4. XRD pattern of the as-prepared UC-F-TiO₂.

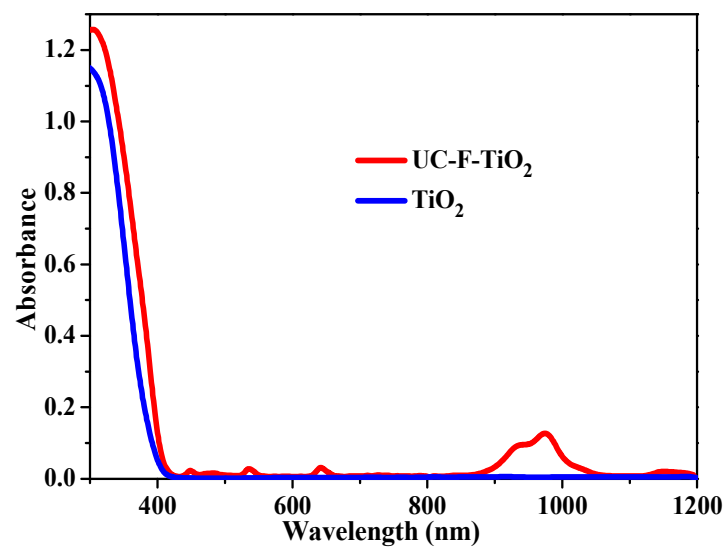


Figure S5. UV-vis-NIR absorption spectra for TiO_2 and UC-F-TiO_2

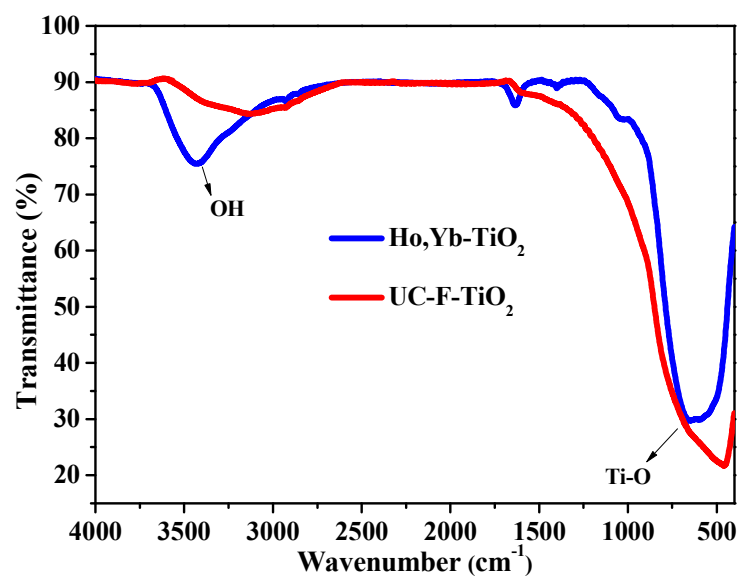


Figure S6. FT-IR spectra of $\text{Ho}^{3+}, \text{Yb}^{3+}$ - TiO_2 and UC-F- TiO_2 .

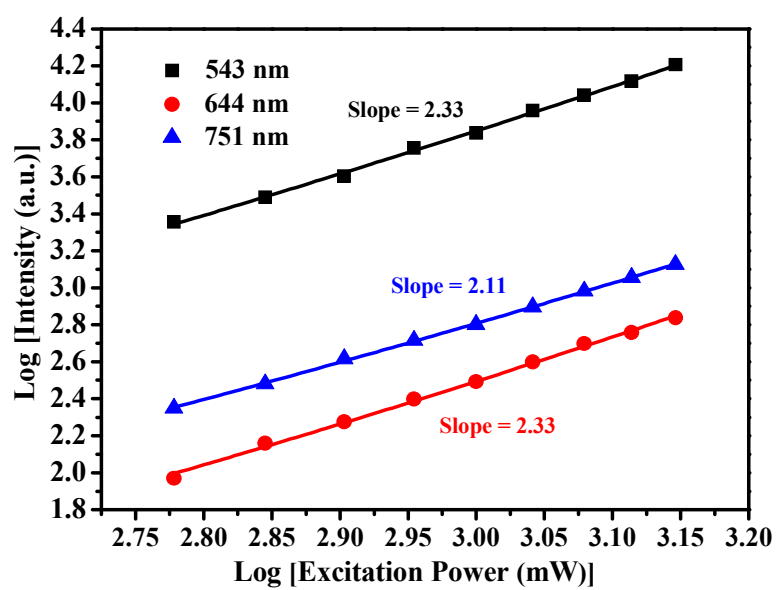


Figure S7. Dependence of UC-F-TiO₂ fluorescence intensity on the excitation power from a 980 nm laser at 543, 644 and 751 nm.

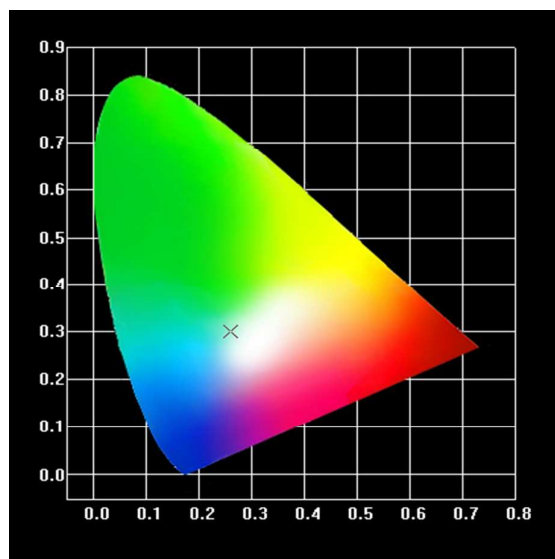


Figure S8. CIE coordinate of the upconversion emission from UC-F-TiO₂, upon 980 nm NIR excitation.

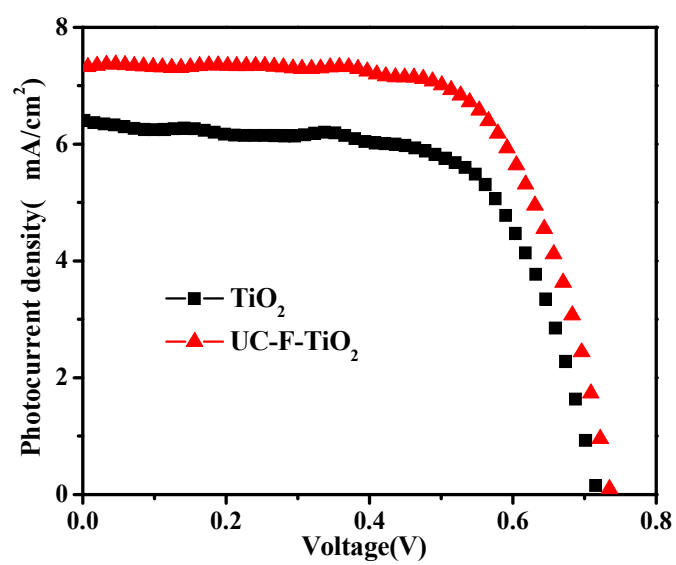


Figure S9. I-V curves of DSSC with a spectral filter of 645 nm under the simulated solar irradiation of 100 mW cm⁻² (AM1.5G).

Table S2. Summary of photovoltaic parameters of a series of DSSC based on UC-F-TiO₂

UC-F-TiO ₂ :TiO ₂	J _{sc} / mA cm ⁻²	V _{oc} / V	FF	η / %
1-1:0	7.83	0.78	0.62	3.74
2-1:0	8.06	0.77	0.60	3.75
3-1:0	8.26	0.77	0.59	3.73
4-1:0	8.30	0.76	0.63	3.97
5-1:0	8.42	0.75	0.62	3.93
1-4:6	19.53	0.73	0.55	7.83
2-4:6	18.01	0.74	0.55	7.34
3-4:6	18.14	0.76	0.54	7.37
4-4:6	18.49	0.76	0.57	8.06
5-4:6	18.01	0.75	0.56	7.66
1-3:7	21.99	0.73	0.56	8.97
2-3:7	20.74	0.74	0.58	8.90
3-3:7	21.94	0.73	0.56	8.86
4-3:7	21.41	0.74	0.57	8.97
5-3:7	21.92	0.73	0.56	8.94
1-2:8	17.86	0.71	0.59	7.50
2-2:8	18.77	0.71	0.57	7.58
3-2:8	17.68	0.71	0.6	7.51
4-2:8	17.94	0.72	0.57	7.39
5-2:8	17.86	0.71	0.59	7.50
1-0:1	15.29	0.69	0.55	5.84
2-0:1	15.29	0.71	0.58	6.34
3-0:1	15.60	0.71	0.57	6.37
4-0:1	16.06	0.70	0.56	6.28
5-0:1	15.71	0.71	0.57	6.36

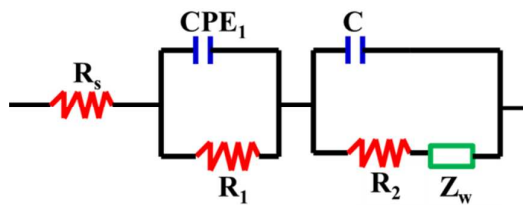


Figure S10. Equivalent circuit obtained by using ZSimpWin software:
 $R_s(C_1(R_1O_1))(R_2Q_2)$.

Table S3. Summary of the device performance of DSSC based on TiO₂ and UC-F-TiO₂ with TiCl₄ post-treatment

Sample	J _{sc} / mA cm ⁻²	V _{oc} / V	FF	η / %
1-TiO ₂ +TiCl ₄	16.66	0.701	0.61	7.11
2-TiO ₂ +TiCl ₄	16.56	0.734	0.60	7.28
3-TiO ₂ +TiCl ₄	16.30	0.725	0.60	7.08
4-TiO ₂ +TiCl ₄	16.89	0.714	0.59	7.16
5-TiO ₂ +TiCl ₄	17.53	0.703	0.60	7.34
1-UC-TiO ₂ +TiCl ₄	20.31	0.778	0.61	9.61
2-UC-TiO ₂ +TiCl ₄	20.63	0.770	0.62	9.77
3-UC-TiO ₂ +TiCl ₄	20.74	0.763	0.62	9.88
4-UC-TiO ₂ +TiCl ₄	22.32	0.764	0.62	10.48
5-UC-TiO ₂ +TiCl ₄	20.80	0.769	0.61	9.83