

Electronic supplementary information (ESI) for New Journal of Chemistry.

Supporting Information (SI)

Probing the Formation and Optical Property of Ti^{3+} - TiO_2 with (001) Exposed Crystal Facet by Ethanol-Assisted Fluorination

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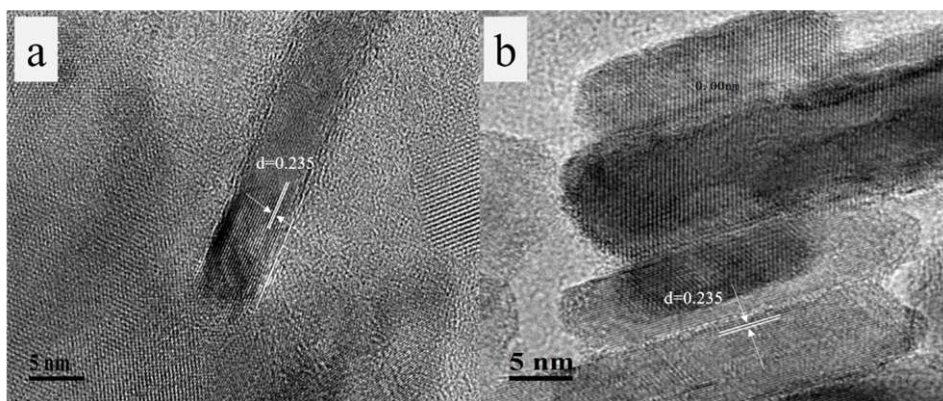


Figure S1. HRTEM images of the sample F_{1.2}-EA-0 (a) and F_{1.2}-EA-40 (b).



Figure S2. Color contrast picture of the as-prepared samples.

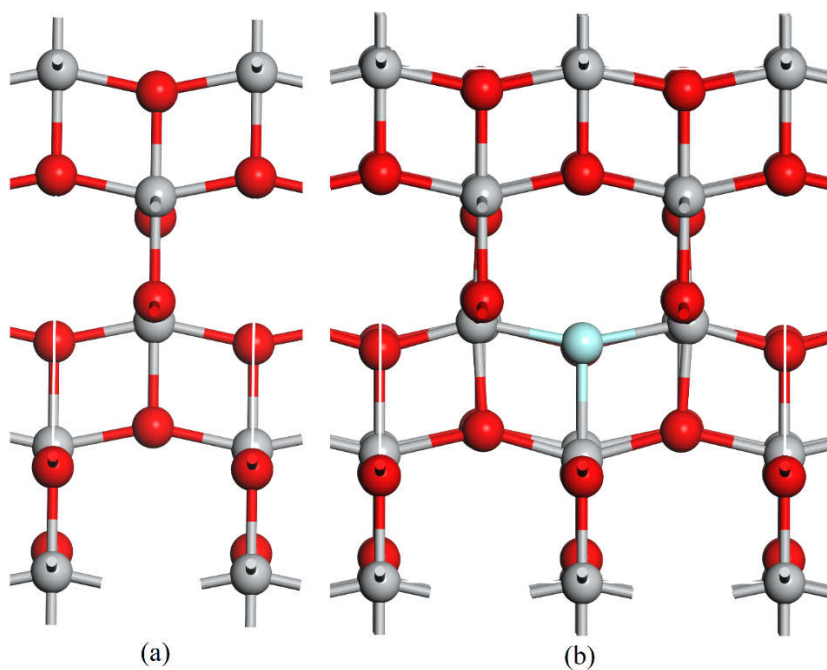


Figure S3. Geometry of pure and F doped TiO₂.

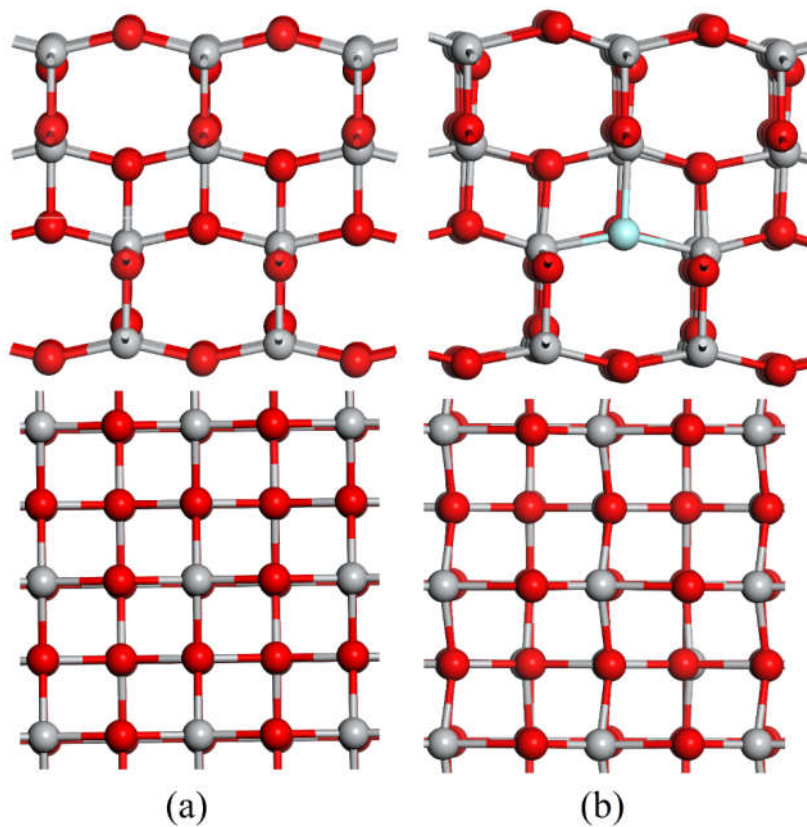


Figure S4. Side and top views of TiO₂ (001) and F doped TiO₂ (001).

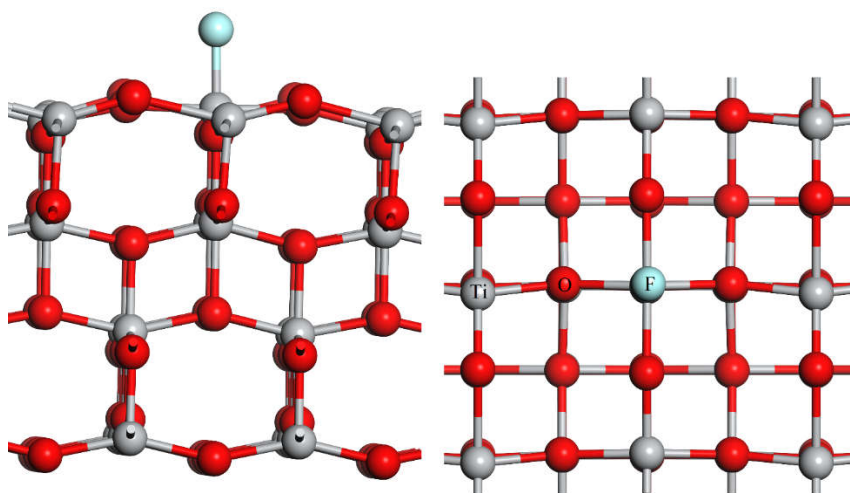


Figure S5. Side and top views of F adsorption on TiO₂ (001).

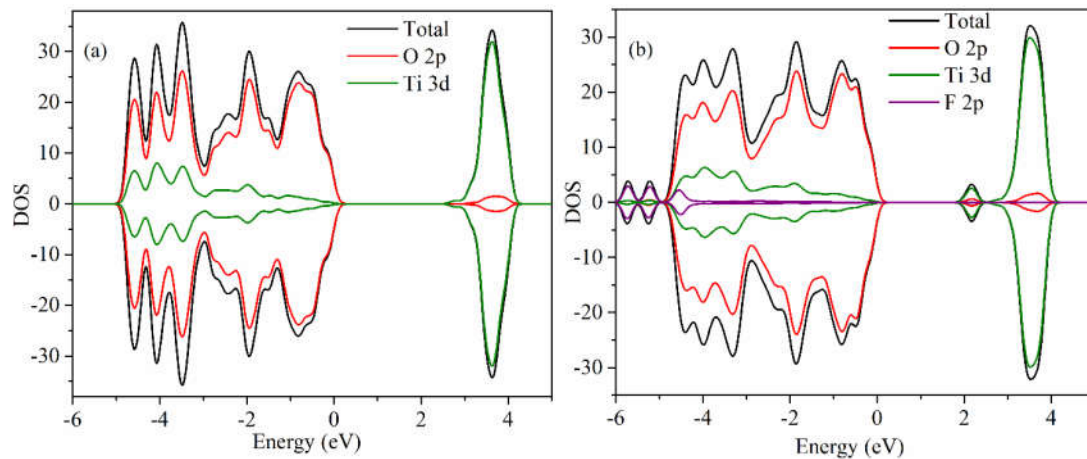


Figure S6. Total and partial density of states for pure bulk TiO_2 (a) and F doped TiO_2 (b).

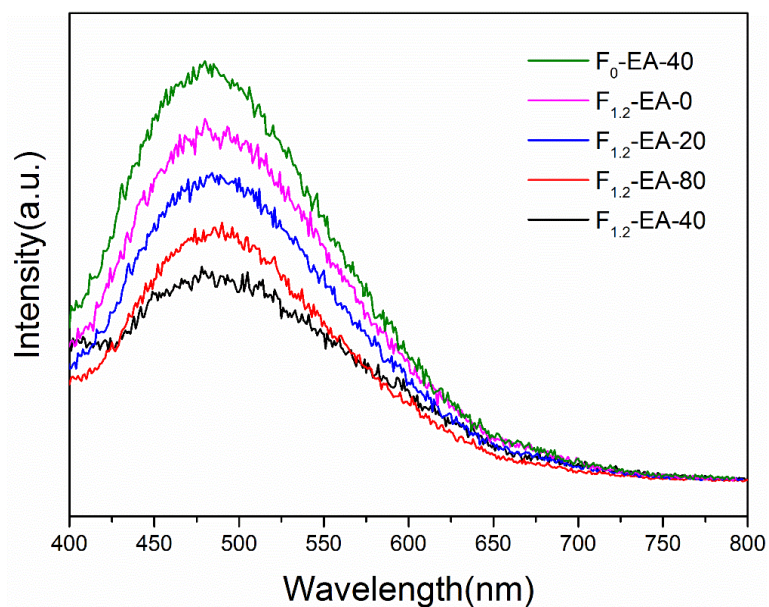


Figure S7. PL spectra of the as-synthesized samples under 325 nm excitation.

Table S1. Crystallite size of prepared samples calculated from the major (101) peak of XRD pattern

Samples	F ₀ -EA-40	F _{1,2} -EA-0	F _{1,2} -EA-20	F _{1,2} -EA-40	F _{1,2} -EA-80
Particle size (nm)	8	12	18	14	10

Table S2. The estimated energy gap (E_g), VBM and CBM of the samples

Samples	Energy gap (eV)	Valence Band Maxima (eV)	Conduction Band Minima (eV)
F ₀ -EA-40	3.12	2.94	-0.18
F _{1,2} -EA-0	3.09	2.94	-0.15
F _{1,2} -EA-40	2.97	2.94	-0.03