

Supplementary Information

Nature of visible-light responsive fluorinated titanium dioxides

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The atomic Coordinates and energies of F2c and F3c doped anatase TiO₂ (001) surfaces.

Unit cell box vectors:

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3.819109300 0.000000000 0.000000000
0.000000000 3.819109300 0.000000000
0.000000000 0.000000000 26.733765103
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Atomic coordinates of F2c doped surface ($E_{tot} = -164.38\text{eV}$):

Ti	0.000000	2.882871	1.207509
Ti	1.909555	2.884527	3.634658
Ti	1.909555	0.974843	6.052195
Ti	0.000000	0.970408	8.507256
Ti	1.909555	0.968822	23.068289
Ti	0.000000	0.973148	25.523313
F	0.000000	2.879780	8.490475
F	1.909555	2.878284	23.081741
F	0.000000	0.969088	10.295931
F	1.909555	0.968130	21.279815
O	0.000000	0.972558	0.788804
O	1.909555	2.882185	1.629935
O	0.000000	2.884314	3.212425
O	1.909555	0.974133	4.053065
O	1.909555	2.883373	5.639903
O	0.000000	0.973198	6.460541
O	1.909555	0.970991	8.097754
O	0.000000	0.969365	23.477869
O	1.909555	0.971835	25.114916
O	0.000000	2.881820	25.935706

Atomic coordinates of F3c doped surface ($E_{tot} = -162.69\text{ eV}$):

Ti	0.000000	2.885778	1.200371
Ti	1.909555	2.874517	3.641174
Ti	1.909555	0.954359	6.026532
Ti	0.000000	1.172771	8.777351
Ti	1.909555	0.775006	22.798274
Ti	0.000000	0.986786	25.548768

F	1.909555	0.973341	8.213912
F	0.000000	0.969385	23.362070
F	0.000000	1.016280	10.556214
F	1.909555	0.936256	21.020124
O	0.000000	0.975752	0.773513
O	1.909555	2.884397	1.632819
O	0.000000	2.875100	3.208803
O	1.909555	0.964864	4.068013
O	1.909555	2.875049	5.625009
O	0.000000	0.980115	6.492691
O	0.000000	2.915962	8.600571
O	1.909555	2.850557	22.973514
O	1.909555	0.962476	25.082253
O	0.000000	2.884921	25.950128