Supporting materials

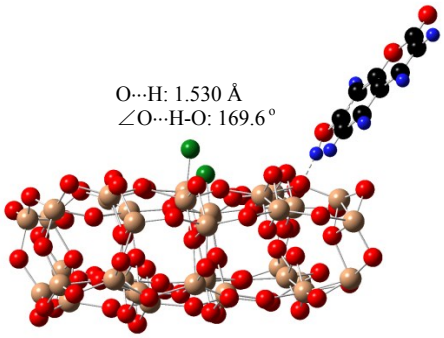

Figure S1. The optimized structure of **7-CN$^{\bullet+}$&F-**TiO_2 with **7-CN$^{\bullet+}$** interacting with the bridging oxygen atom. The calculated H-bonding property is shown in the figure. H, blue; O, red; **C**, black; Ti, gold; F, green.

Table S1. Isotropic proton coupling constants for **7-CN$^{\bullet+}$&F-**TiO_2 with **7-CN$^{\bullet+}$** interacting with the bridging oxygen atom.

Atom	Gauss
H at C3	-8.012
H at C4	2.511
H at C5	1.191
H at C6	-4.313
H at C8	-1.259
H at C7-OH	-3.279

Table S2. Anisotropic proton coupling constants for **7-CN**$^{\bullet+}$**&F-**TiO_2 with **7-CN**$^{\bullet+}$ interacting with the bridging oxygen atom.

Atom		Gauss
H at C3	Baa	-4.808
	Bbb	-0.361
	Bcc	5.180
H at C4	Baa	-1.052
	Bbb	-0.473
	Bcc	1.522
H at C5	Baa	-0.841
	Bbb	-0.183
	Bcc	1.020
H at C6	Baa	-2.648
	Bbb	-0.548
	Bcc	3.212
H at C8	Baa	-0.719
	Bbb	-0.702
	Bcc	1.423
H at C7-OH	Baa	-3.218
	Bbb	-1.751
	Bcc	4.972