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How organic switches grafting on TiO_2 modifies the surface potentials: Theoretical insights

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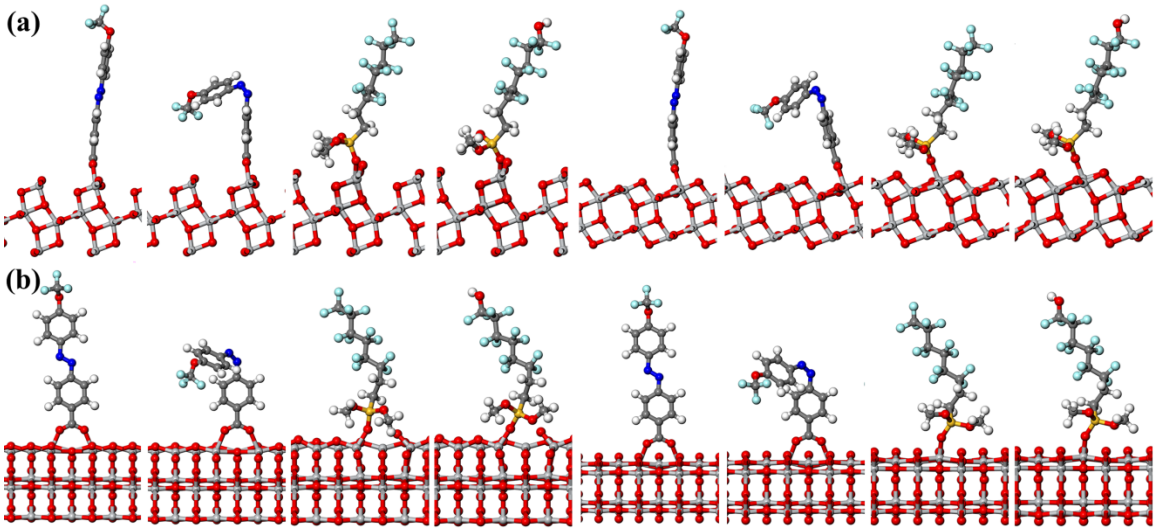

Figure S1 Adsorbed structures of trans-FAZB, cis-FAZB, PFOS-F and PFOS-OH on anatase (101)-I (four leftmost) and anatase (101)-II (four rightmost) surface viewed along (a) y-axis and (b) x-axis. The white, gray, blue, red, gold, light gray and light blue spheres represent hydrogen, carbon, nitrogen, oxygen, silicon, titanium and fluorine atoms, respectively.

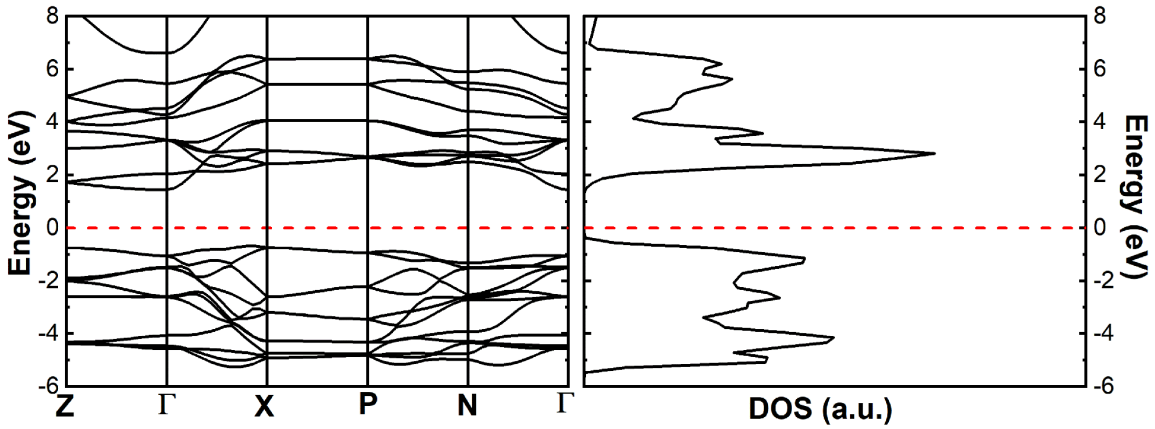

Figure S2 The electronic band structure (left panel) and the corresponding density of states (right panel) of bulk anatase. The Fermi level is set to zero.

Table S1 Parameterization schemes in adsorption energy calculation for trans-FAZB on TiO_2 (101)-II surface.

Scheme Number	Cutoff (eV)	Force Convergence Criteria (eV/Å)	Adsorption Energy (eV)
1	300	0.01	-2.94
2	350	0.01	-2.42
3	400	0.01	-2.15
4	500	0.01	-2.12
5	600	0.01	-2.16
6	400	0.001	-2.15

Table S2 Height difference between the outermost atom of the organic unit and the interface for 12 species of considered hybrid systems.

Structure (label as in Fig.1 and S1)	Distance (Å)
trans-FAZB/(100)	16.27
cis-FAZB/(100)	6.20
trans-FAZB/(101)-I	15.95
cis-FAZB/(101)-I	5.62
trans-FAZB/(101)-II	15.79
cis-FAZB/(101)-II	6.42
PFOS-F/(100)	13.28
PFOS-OH/(100)	13.63
PFOS-F/(101)-I	12.19
PFOS-OH/(101)-I	11.72
PFOS-F/(101)-II	12.53
PFOS-OH/(101)-II	12.99