

## Supporting Materials

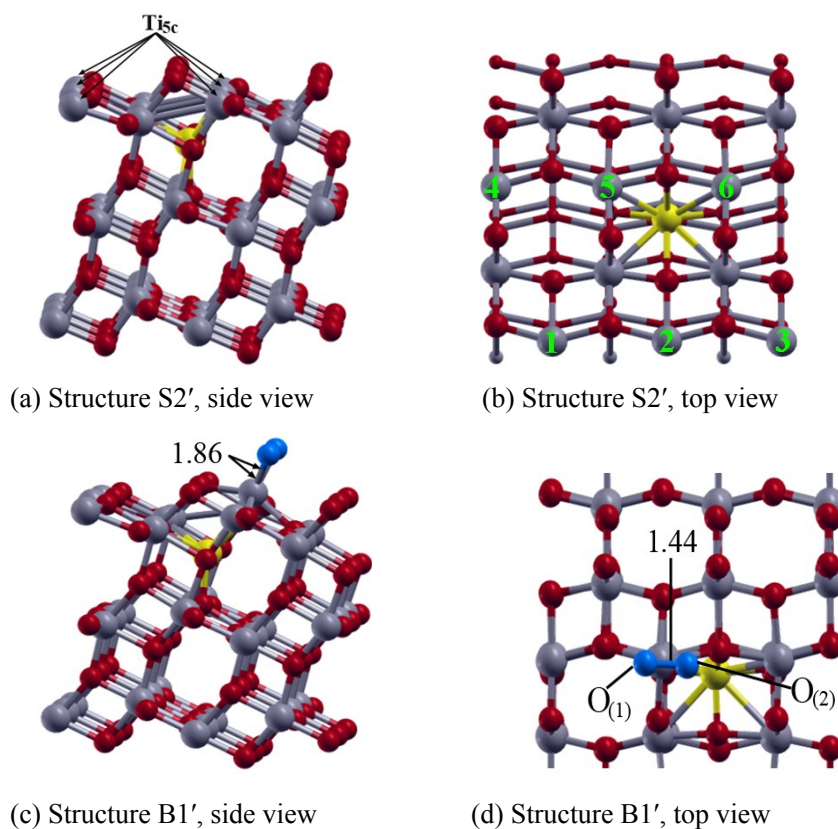


Fig. S1: (a) and (b) configuration of an anatase slab with a subsurface Ti interstitial under a (101) surface (S2'). (c) and (d) the energy favorable adsorption configuration of an oxygen molecule on the surface of S2', (B1').

Adsorption energy of an oxygen molecule on the (101) surface of configuration S2'

S2'	1, 3	2	4	5, 6
adsorption energy (eV)	-1.31	-1.45	-0.87	-2.01