# Theoretical investigation on the water adsorption conformations at the aqueous anatase TiO$_2$/water interfaces

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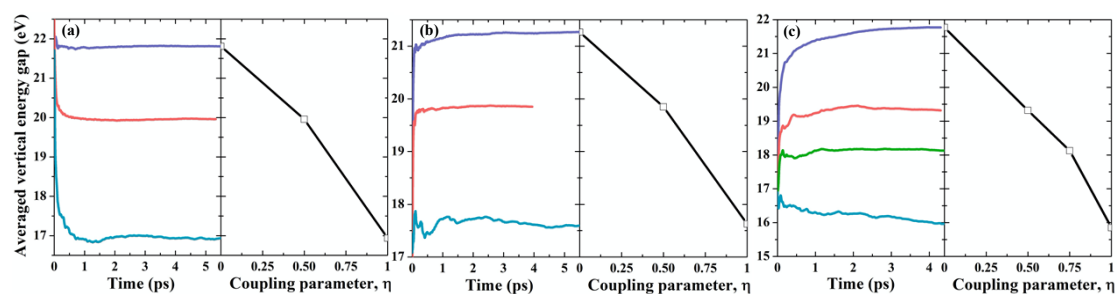
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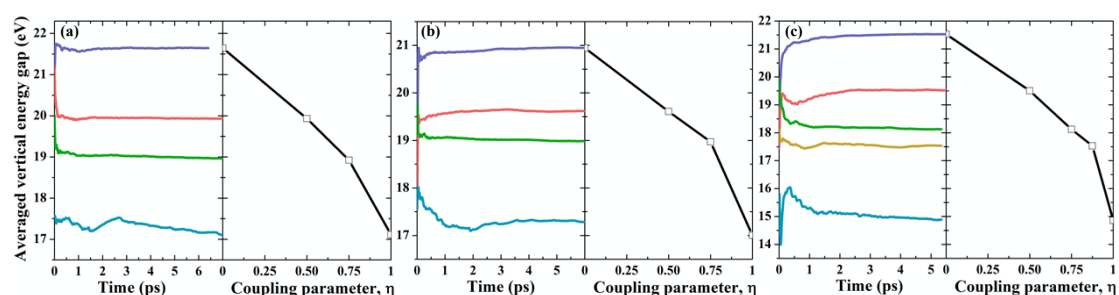
Fig. S1 Time accumulative averages of vertical energy gaps against the coupling parameters for the deprotonation reactions of the aqueous anatase (101) surface: (a) the deprotonation of TiOH$_2$; (b) the deprotonation of Ti$_2$OH$^+$; (c) the deprotonation of H$_3$O$^+$ at (101)/water interface.
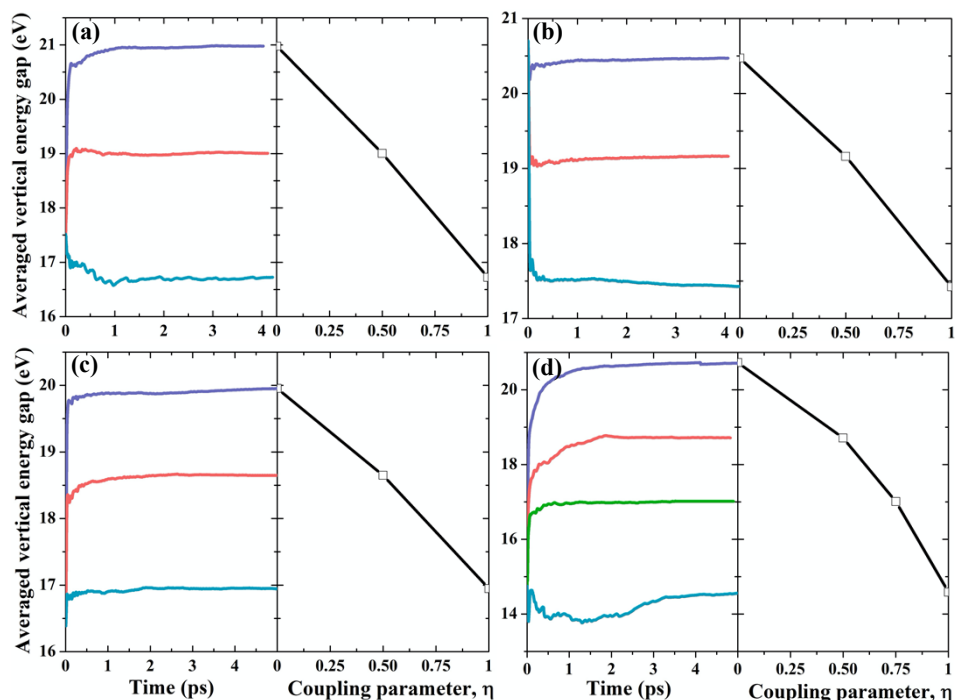
Fig. S2 Time accumulative averages of vertical energy gaps against the coupling parameters for the deprotonation reactions of the aqueous anatase (001) surface: (a) the deprotonation of $TiOH_2$; (b) the deprotonation of Ti_2OH^+ for O_A site; (c) the deprotonation of Ti_2OH^+ for O_B site; (d) the deprotonation of H_3O^+ at (001)/water interface.

Fig. S3 Time accumulative averages of vertical energy gaps against the coupling parameters for the deprotonation reactions of the aqueous anatase (100) surface: (a) the deprotonation of $TiOH_2$; (b) the deprotonation of Ti_2OH^+; (c) the deprotonation of H_3O^+ at (100)/water interface.

Table S1 The average electrostatic potentials of solid phase (V_{solid}, eV), vacuum phase (V_{vac}, eV) and the electrostatic potential difference (ΔV, eV) for anatase (101) surface.

Layer	V_{solid}	V_{vac}	ΔV
3L	-7.16	5.62	12.78
4L	-6.38	6.56	12.94
5L	-5.68	7.24	12.92
6L	-5.10	7.83	12.93

Table S2 The average electrostatic potentials of solid phase (V_{solid}, eV), vacuum phase (V_{vac}, eV) and the electrostatic potential difference (ΔV, eV) for anatase (001) surface.

Layer	V_{solid}	V_{vac}	ΔV
3L	-8.51	3.77	12.28
4L	-8.84	3.51	12.35
5L	-7.93	4.55	12.48
6L	-7.09	5.40	12.49
7L	-6.60	5.87	12.47

Table S3 The average electrostatic potentials of solid phase (V_{solid}, eV), vacuum phase (V_{vac}, eV) and the electrostatic potential difference (ΔV, eV) for anatase (100) surface.

Layer	V_{solid}	V_{vac}	ΔV
3L	-7.49	5.09	12.63
4L	-7.50	4.79	12.29
5L	-7.01	5.42	12.43
6L	-6.65	5.84	12.49
7L	-6.20	6.32	12.52
8L	-5.84	6.67	12.51
9L	-5.51	7.01	12.52