Supplementary Material (ESI) for PCCP

A shortcut for evaluating activities of TiO_2 facets: Water dissociative chemi-sorption on TiO_2-B (100)

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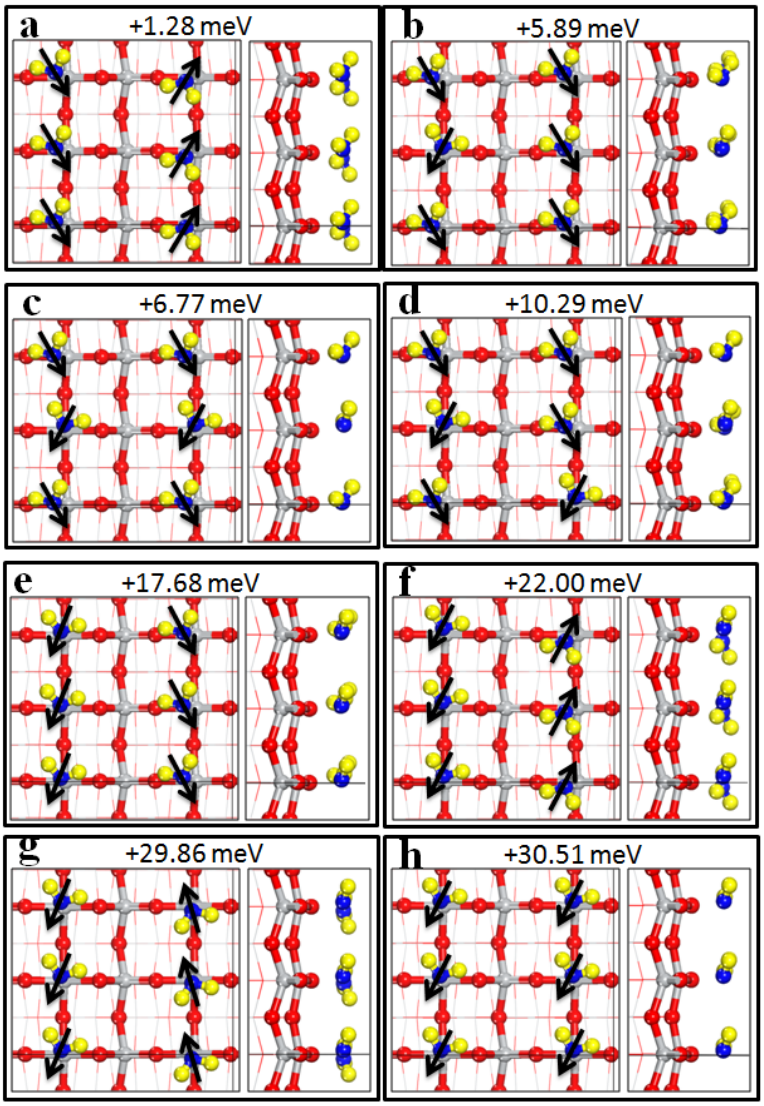

Fig. S1 Top (left) and side (right) views of water adsorbed molecularly on TiO_2-B (100) surface at 1ML coverage. Different relative orientations of water are considered and only the stable structures are shown here. The relative adsorption energy in millielectronvolts (meV) per water molecule compared with the structure displayed in Fig. 6a is marked on the top of each structure. Positive values indicate the configuration is less stable than the one shown in **Fig. 6a**. (The more negative the adsorption energy is, the more stable the configuration will be.) The direction of the viewer is same as **Fig. 6a**. Ti atoms and O atoms of TiO_2 are in gray and red respectively. H atoms and O atoms of water are in yellow and blue respectively.

Table S1 Atomic positions and charges in the TiO_2-B lattice

	Coordination number	Thomas P. Feist[c]		Mouna Ben Yahia[c]		This work		
		Atomic positions / fractional unit						charge/ e
		x	z	x	z	x	z	
Ti (1)	**6**	**0.197**	**0.292**	**0.193**	**0.287**	**0.195**	**0.283**	**1.58**
Ti (2)	**6**	**0.099**	**0.705**	**0.100**	**0.709**	**0.100**	**0.711**	**1.59**
O (1)	**2**	**0.132**	**0.004**	**0.131**	**0.004**	**0.133**	**0.004**	**-0.66**
O (2)	**4**	**0.264**	**0.653**	**0.262**	**0.654**	**0.264**	**0.653**	**-0.82**
O (3)	**3**	**0.060**	**0.371**	**0.059**	**0.373**	**0.058**	**0.369**	**-0.76**
O (4)	**3**	**0.362**	**0.293**	**0.360**	**0.290**	**0.362**	**0.294**	**-0.77**

[a] Atoms in first column are labeled as right part of **Fig. 1**

[b] The data of Mouna Ben Yahia in the table was transformed according to the crystallographic symmetry (C2/m)

[c] The origin data from T. P. Feist and M. B. Yahia is published on J. Solid State Chem., 1992, 101, 275 and J. Chem. Phys., 2009, 130, 204501 respectively.

Table S2 Calculated displacement and Lowdin charge of surface atoms for TiO_2-B (001) and (100)

Surface	Atoms	Coordination Number	Displacement / Å			Charge / e
			[100]	[010]	[001]	
(001)	Ti(1)	5	0.006	0	0.002	1.61
	Ti(2)	5	-0.054	0	0.020	1.60
	O(1)	3	0.062	0	0.139	-0.82
	O(2)	2	-0.008	0	0.018	-0.73
	O(3)	3	0.031	0	0.001	-0.83
(100)	Ti(1)	5	0	0.143	-0.149	1.58
	Ti(2)	6	0	0.156	0.164	1.57
	O(1)	2	0	-0.251	-0.019	-0.70
	O(2)	2	0	0.107	0.245	-0.72
	O(3)	3	0	-0.130	-0.099	-0.76
	O(4)	4	0	0.119	0.082	-0.84

[a] Atoms in first column are labeled as right panel of **Fig. 2**