Supplementary Information

Structure of a Superhydrophilic Surface: Wet Chemically Prepared Rutile-TiO_2(110)(1×1)

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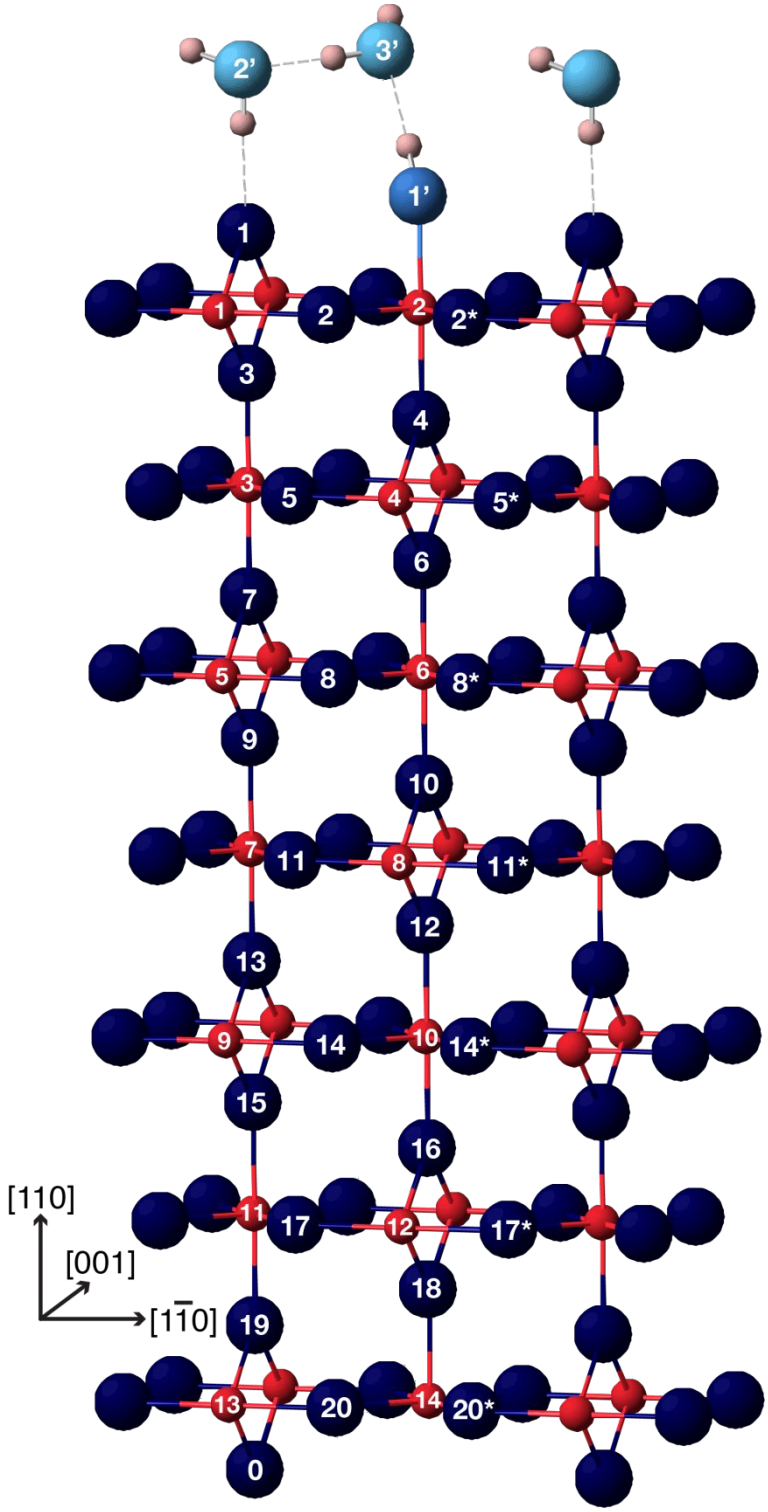

Figure S1. Ball and stick model of optimised superhydrophilic TiO_2(110) surface, showing all atoms displaced during fitting of SXRD data. The numerical labelling of the atoms is employed in Table S1 for identification purposes. Symmetry paired atoms are denoted by *.

Table S1. Optimised coordinates of atoms obtained from fitting of SXRD data acquired from superhydrophilic rutile-TiO_2(110). Fractional occupancies of adsorbate atoms are indicated by a subscript in the atom column. DW factors are also listed. The origin, (0,0,0), is located on O(0) (see Figure S1). Values in italics have not been displaced during fitting. Bulk terminated coordinates are also given.

Atom	Coordinates (Å)						DW-factor
	x	x-bulk	y	y-bulk	z	z-bulk	($Å^2$)
$O(3')_{0.60}$	2.38	-	1.30	-	24.87	-	4.67
$O(2')_{0.89}$	-0.01	-	0.09	-	24.57	-	1.39
$O(1')_{1.00}$	3.18	-	0.12	-	22.63	-	1.24
O(1)	*0.00*	0.00	*0.00*	0.00	21.89	22.25	4.19
Ti(1)	*0.00*	0.00	*1.48*	1.48	20.81	20.76	2.05
Ti(2)	*3.25*	3.25	*0.00*	0.00	20.75	20.76	0.97
O(2)	1.98	1.98	*1.48*	1.48	20.84	20.76	2.42
O(2*)	4.51	4.51	*1.48*	1.48	20.84	20.76	2.42
O(3)	*0.00*	0.00	*0.00*	0.00	19.55	19.49	1.35
O(4)	*3.25*	3.25	*0.00*	0.00	18.81	18.77	0.25
O(5)	*1.25*	1.26	*1.48*	1.48	17.52	17.51	1.36
O(5*)	*5.24*	5.23	*1.48*	1.48	17.52	17.51	1.36
Ti(3)	*3.25*	3.25	*1.48*	1.48	17.54	17.51	0.25
Ti(4)	*0.00*	0.00	*0.00*	0.00	17.54	17.51	0.25
O(6)	*3.25*	3.25	*0.00*	0.00	16.23	16.24	0.54
O(7)	*0.00*	0.00	*0.00*	0.00	15.51	15.52	0.54
Ti(5)	*0.00*	0.00	*1.48*	1.48	14.29	14.26	0.25
Ti(6)	*3.25*	3.25	*0.00*	0.00	14.29	14.26	0.25
O(8)	1.97	1.98	*1.48*	1.48	14.26	14.26	0.54
O(8*)	4.52	4.51	*1.48*	1.48	14.26	14.26	0.54

O(9)	*0.00*	0.00	*0.00*	0.00	13.01	12.99	0.49
O(10)	*3.25*	3.25	*0.00*	0.00	12.28	12.28	0.49
O(11)	*1.26*	1.26	*1.48*	1.48	11.00	11.01	0.49
O(11*)	*5.23*	5.23	*1.48*	1.48	11.00	11.01	0.49
Ti(7)	*3.25*	3.25	*1.48*	1.48	11.03	11.01	0.25
Ti(8)	*0.00*	0.00	*0.00*	0.00	11.04	11.01	0.25
O(12)	*3.25*	3.25	*0.00*	0.00	9.73	9.75	0.25
O(13)	*0.00*	0.00	*0.00*	0.00	9.02	9.03	0.25
Ti(9)	*0.00*	0.00	*1.48*	1.48	7.78	7.76	0.25
Ti(10)	*3.25*	3.25	*0.00*	0.00	7.78	7.76	0.25
O(14)	1.98	1.98	*1.48*	1.48	7.76	7.76	0.25
O(14*)	4.52	4.51	*1.48*	1.48	7.76	7.76	0.25
O(15)	*0.00*	0.00	*0.00*	0.00	6.49	6.50	0.33
O(16)	*3.25*	3.25	*0.00*	0.00	5.77	5.78	0.33
O(17)	1.26	1.26	*1.48*	1.48	4.51	4.51	0.33
O(17*)	5.24	5.23	*1.48*	1.48	4.51	4.51	0.33
Ti(11)	*3.25*	3.25	*1.48*	1.48	4.52	4.51	0.25
Ti(12)	*0.00*	0.00	*0.00*	0.00	4.52	4.51	0.25
O(18)	*3.25*	3.25	*0.00*	0.00	3.24	3.25	0.25
O(19)	*0.00*	0.00	*0.00*	0.00	2.52	2.53	0.25
Ti(13)	*0.00*	0.00	*1.48*	1.48	1.27	1.26	0.25
Ti(14)	*3.25*	3.25	*0.00*	0.00	1.27	1.26	0.25
O(20)	1.99	1.98	*1.48*	1.48	1.26	1.26	0.25
O(20*)	4.50	4.51	*1.48*	1.48	1.26	1.26	0.25
O(0)	*0.00*	0.00	*0.00*	0.00	*0.00*	0.00	0.25