Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supporting Information

Understanding the effects of surface/bulk defects on the photocatalytic activity of TiO_2: Anatase versus Rutile

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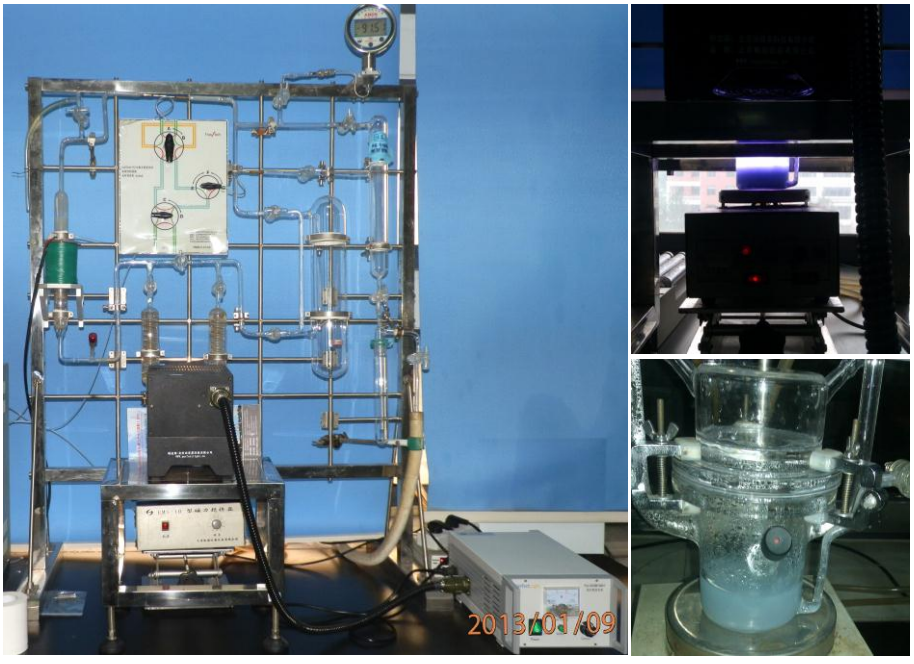

Figure S1 Experiment setup for the photocatalytic reforming of methanol

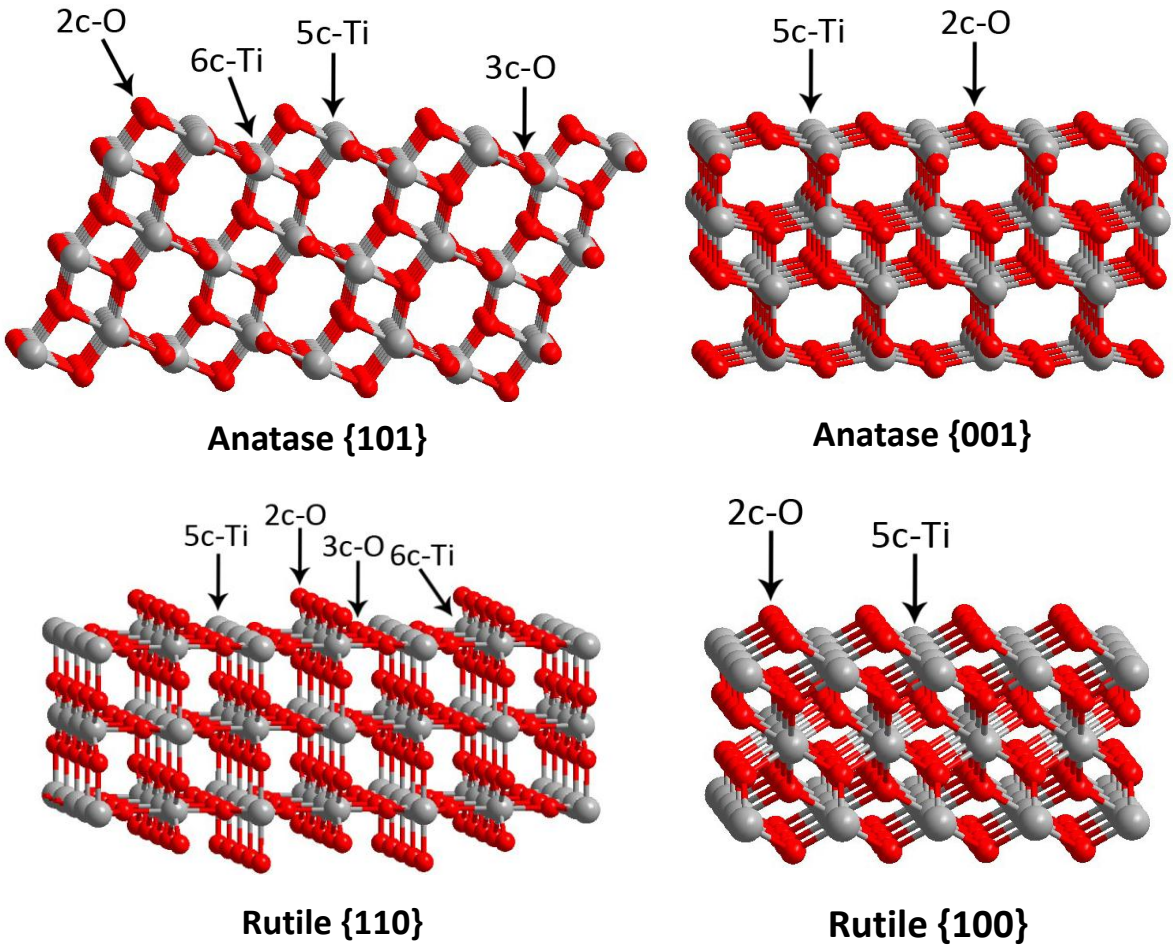

Figure S2 Structural modes of anatase TiO_2 {101} and {001} facets, and rutile {110} and {100} facets

For the anatase {101} facets, the bonding modes on the surface are mainly saturated 6c-Ti and 3c-O modes, and unsaturated 5c-Ti and 2c-O. For the anatase {001} facets, the bonding modes on the surface are mainly unsaturated 5c-Ti and 2c-O. For rutile {110} facets, the bonding modes on the surface are mainly saturated 6c-Ti and 3c-O modes, and unsaturated 5c-Ti and 2c-O. For rutile {100} facets, are mainly unsaturated 5c-Ti and 2c-O. The 6c-Ti and 3c-O are easy to exhibit the symmetric stretching vibration, and the 2c-O and 5c-Ti tend to exhibit the symmetric bending vibration and anti-symmetric bending vibration. In Raman spectra, the E_g mode is mainly caused by the symmetric stretching vibration of O-Ti-O in TiO_2, the B_{1g} mode is caused by symmetric bending vibration of O-Ti-O, and the A_{1g} mode is caused by anti-symmetric bending vibration of O-Ti-O.

Table S1 Intensity and the ratio between different Raman vibrational modes in anatase TiO_2

Sample	Raman intensity			Ratio		
	E_g / 140 cm^{-1}	B_{1g} / 395 cm^{-1}	A_{1g} / 515 cm^{-1}	A_{1g} / Eg	B_{1g} / Eg	A_{1g} / B_{1g}
anatase	2023	320	321	0.16	0.16	1.00
A-400	2116	283	287	0.14	0.13	1.01
A-500	5420	703	712	0.13	0.13	1.00
A-600	10870	1356	1370	0.13	0.12	1.01
A-700	12449	1560	1563	0.13	0.13	1.00

Table S2 Intensity and the ratio between different Raman vibrational modes in rutile TiO_2

Sample	Raman intensity			Ratio
	Multi-proton process / 230 cm^{-1}	E_g / 445 cm^{-1}	A_{1g} / 610 cm^{-1}	A_{1g} / Eg
rutile	1147	2688	2347	0.87
R-400	1276	2722	3125	1.15
R-500	2350	5034	5766	1.15
R-600	3116	6680	7744	1.16
R-700	3294	7358	8560	1.16

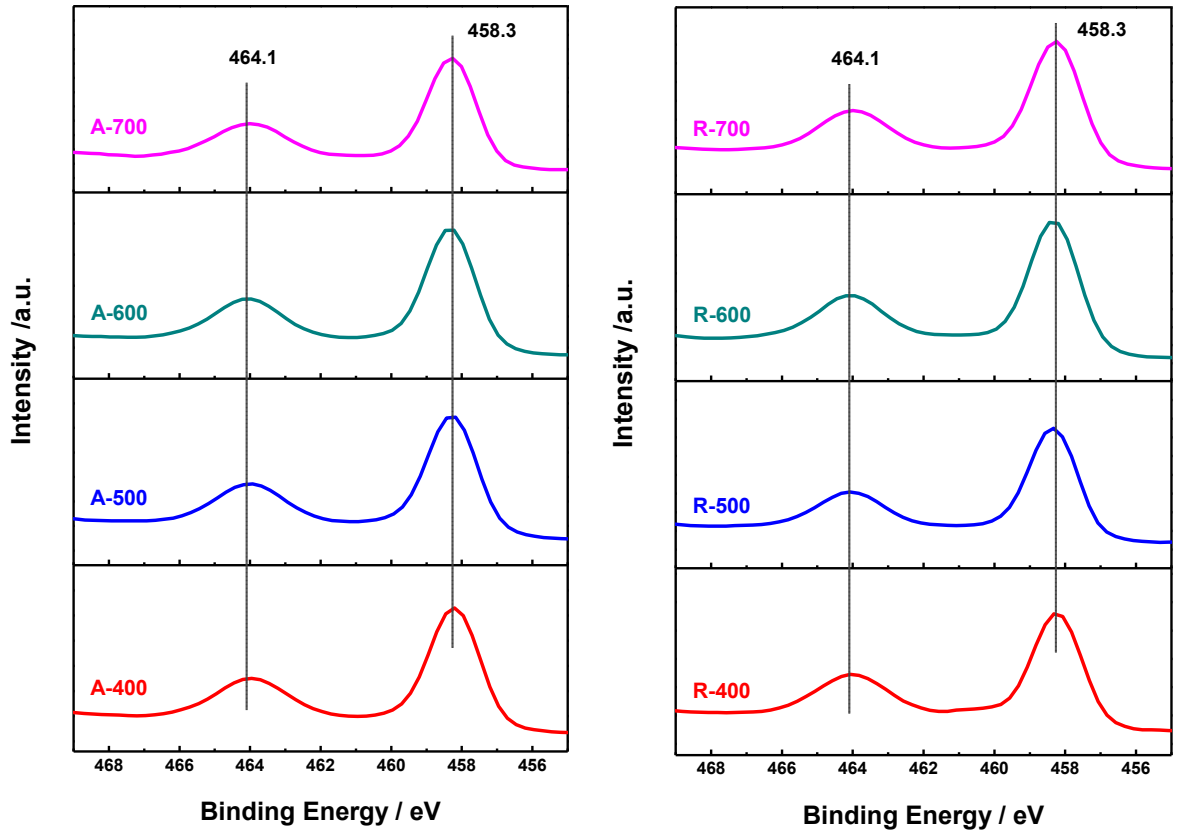

Figure S3 XPS of Ti 2p region of anatase and rutile TiO_2 calcined at different temperatures

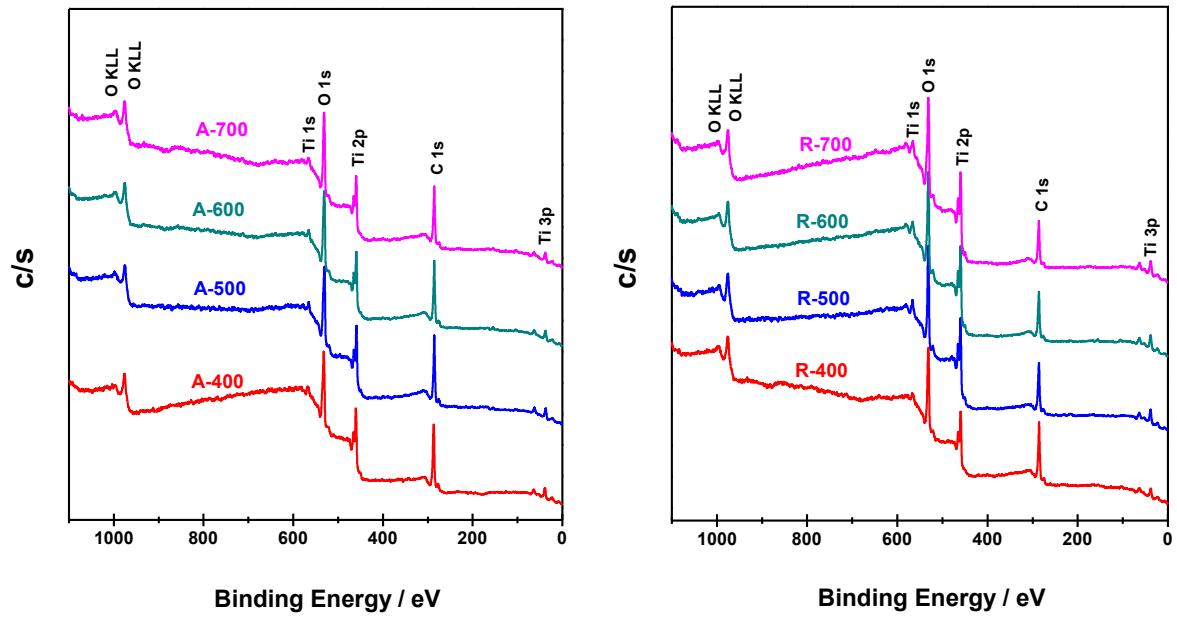

Figure S4 XPS survey spectra of anatase and rutile TiO_2 calcined at different temperatures