Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Electronic Structures of Bare and Terephthalic Acid Adsorbed TiO_2(110)-(1×2) Reconstructed Surface: Origin and Reactivity of the Band Gap States

Wenhua Zhang,[1] Liming Liu,[2] Li Wan,[1] Lingyun Liu,[1] Liang Cao,[3] Faqiang Xu,[1] Jin Zhao,[*, 2,4]

Ziyu Wu[*,1,5]

[1]*National Synchrotron Radiation Laboratory, University of Science and Technology of China, Hefei 230029, People's Republic of China.*

[2]*Department of Physics and Hefei National Laboratory for Physical Sciences at the Microscale, University of Science and Technology of China, Hefei 230026, People's Republic of China.*

[3]*High Magnetic Field Laboratory, Chinese Academy of Sciences, 350 Shushanhu Road, Hefei 230031, Anhui, P. R. China.*

[4]*Synergetic Innovation Center of Quantum Information & Quantum Physics, University of Science and Technology of China, Hefei 230026, People's Republic of China.*

[5]*Beijing Synchrotron Radiation Laboratory, Institute of High Energy Physics, Chinese Academy of Sciences, Beijing 100039, People's Republic of China.*

[*]J. Zhao: tel, 86-551-63602832; email: zhaojin@ustc.edu.cn.

[*] Z. Wu: tel, 86-551-63602077, email: wuzy@ustc.edu.cn.

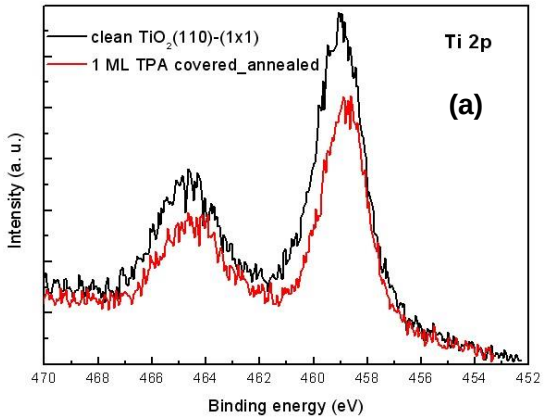
1. Calculation of TPA Coverage

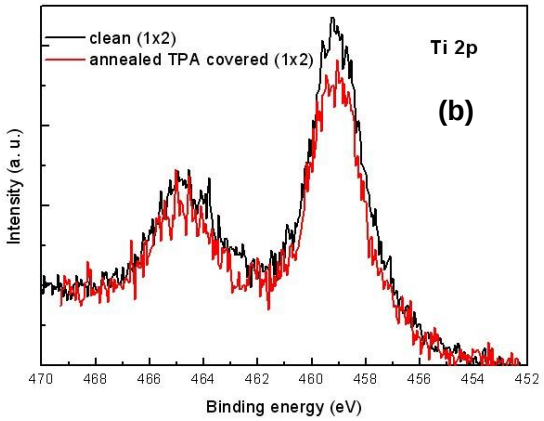
One monolayer (ML) is defined as the saturated chemisorbed single layer of TPA on the TiO_2(110)-(1×1) surface, which is prepared by the annealing of multilayer thick TPA film at 400 K for several minutes on the substrate. For depositions of TPA on TiO_2(110)-(1×2) reconstructed surface, the coverage at each step is calculated through the attenuation of Ti 2p signal assuming a simple layer-by-layer growth mode of TPA on the surface. According to this growth mode, the attenuation of Ti 2p intensity upon the deposition of TPA molecules can be written as

$$\ln I_0/I = t/\lambda,$$

where I_0 and I is the intensity of Ti 2p signal of the clean and the molecules deposited substrate, respectively, *t* is the film thickness measured with quartz thickness monitor and λ is the inelastic mean scattering distance. It can be seen the thickness of TPA is proportional to the value of $ln(I_0/I)$. Therefore the coverages of TPA can be obtained from the Ti 2p XPS data.

Fig. S1 shows (a) the Ti 2p XPS spectra for the clean TiO_2(110)-(1×1) and 400 K annealed TPA/TiO_2(110)-(1×1) samples, (b) the Ti 2p spectra for the clean TiO_2(110)-(1×2) and 400 K annealed TPA/TiO_2(110)-(1×2) samples, and (c) the Ti 2p spectra of TPA/TiO_2(110)-(1×2) samples at different deposition thickness. The peak intensities and calculation results are summarized in **Table S1**. It can be seen that the coverage value of the annealed sample is somewhat close to half the saturated chemisorbed TPA layer on the (1×1) surface, in conformance to the Ti_2O_3-added model for the (1×2) surface.





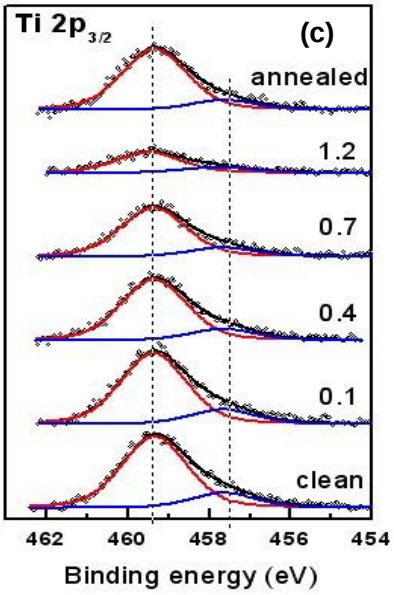


Fig. S1 (a) Ti 2p XPS spectrum of clean TiO_2(110)-(1x1) substrate and 1 ML TPA covered surface that obtained by annealing TPA multilayer at 400 K on the (1×1) surface. (b) Ti 2p XPS spectrum of clean TiO_2(110)-(1×2) substrate and the 400 K annealed TPA layer on the (1×2) surface. (c) Ti 2p evolution with TPA deposited on the (1×2) surface.

Table S1 The coverage estimations from the attenuation of Ti $2p_{3/2}$ features for TPA adsorption on TiO_2(110)-(1×2) reconstructed surface. I_0(Ti2p) and I(Ti2p) represent the Ti 2p XPS intensity of the clean substrate and the TPA covered sample, respectively.

	TPA on (1×2)						**TPA on (1×1)[a]**
Deposition Time /s	10	30	60	120	240	annealed	annealed
I_0(Ti2p)/I(Ti2p)	1.08	1.19	1.49	3.46	8.77	1.18	1.4
ln [I_0(Ti2p)/I(Ti2p)]	0.077	0.174	0.399	1.241	2.171	0.163	0.3365
Coverage /ML	0.23	0.52	1.2	3.7	6.5	0.49	**1**

Notes:

a) This column represents the calculation results of the as defined 1 ML TPA on the (1×1) surface.