Analysis of function induced on anatase TiO_2 surface which has photocatalytic activity: electronic states and surface structure

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The techniques to control the low-dimensional electronic states appearing at the surface and interface of oxide semiconductors have attracted huge attention for designing the future quantum electronic devices. Recently, the formation of two-dimensional electron liquid (2DEL) states has been reported at the surface of anatase titanium dioxide (a-TiO_2) [1]. The 2DEL is generated by irradiation of strong vacuum-ultraviolet light which induces oxygen vacancies near the surface. However, owing to the difficulty to control the distribution of the oxygen vacancies in depth, the dimensionality of the electronic states generated by photoirradiation remains a controversial issue [1,2]. Therefore, in this study, we have proposed an alternative route to address the 2DEL states: we adsorbed H atoms on the (001) surface of a-TiO_2 and investigated the formed 2DEL states by *in situ* angle-resolved photoelectron spectroscopy (ARPES).

Figure 1 shows the band structure near the Fermi level (E_F) for the bare and H-adsorbed surfaces of a-TiO_2 (001). At the bare a-TiO_2 (001) surface, the existence of a conduction band, which forms the Fermi surface, is clearly observed. By deposition of H atoms onto the a-TiO_2 surface, the value of Fermi momenta (k_F) increases. This result indicates that adsorbed H atoms act as electron donor and electrons transfer from H atoms to a-TiO_2. Moreover, subband structures are clearly visible at the H adsorbed surface, indicating the two-dimensional confinement of doped carriers near the a-TiO_2 (001) surface region. The simulation based on the wedge-shaped potential approximation suggests that the doped-electrons are confined within a few nm from the surface.

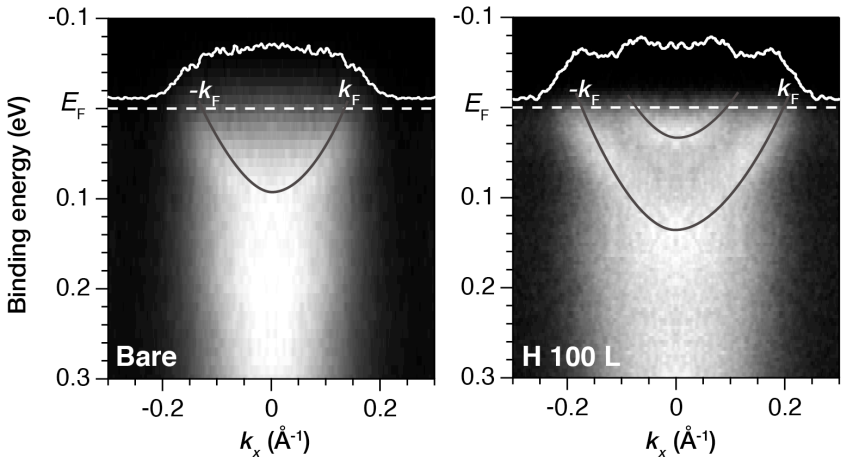

Fig. 1. ARPES images of the bare and H-adsorbed surfaces of a-TiO_2 (001). The momentum distribution curves at E_F are also shown in the respective images.

Bibliography

[1] T. C. Rödel *et al*., Phys. Rev. B **92**, 41106 (2015).

[2] S. Moser *et al*., Phys. Rev. Lett. **110**, 196403 (2013).