Site Specific Molecular Chemisorption of $O_2$ on TiO$_2$(110): A Scanning Tunneling Microscopy Study

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The investigation of $O_2$ adsorption on TiO$_2$ is critical since it can help us to better understand the photooxidation mechanism of TiO$_2$. In our work, molecularly chemisorbed $O_2$ were directly imaged on reduced TiO$_2$(110) at 50 K with scanning tunneling microscopy (STM). Two $O_2$ adsorption channels, one at bridging oxygen vacancies ($V_O$) and another at five-fold coordinated Ti atoms (Ti$_5$c), have been identified. While $O_2$ at Ti$_5$c appears as a single protrusion, the $O_2$ at $V_O$ manifests itself by a disappearance of the $V_O$ feature. It is found that STM tip can easily dissociate $O_2$ and the dissociation details strongly depend on the tunneling conditions and the type of the $O_2$ adsorption site. The chemisorbed $O_2$ at these two distinctive sites are the most likely precursors for the two previously established $O_2$ dissociation channels, observed at temperatures above 150 and 230 K at the $V_O$ and Ti$_5$c sites, respectively.

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