Surface Reconstruction and Molecular Adsorption on Anatase TiO$_2$(001)-(1×4) HUIJUAN SUN, YANG WANG, JIN ZHAO, BING WANG, JINLONG YANG, JIANGUO HOU, University of Science and Technology of China, UNIVERSITY OF SCIENCE AND TECHNOLOGY OF CHINA TEAM — TiO$_2$ is a large band gap semiconductor with a wide range of applications including in photocatalysis, decontamination, and solar-energy conversion. Comparing to the well studied rutile phase, the anatase phase appears more common in nanocrystals and shows higher activity in photocatalysis. However, only a few literatures investigated the surface structure of anatase(001), which is assumed to be the origin of anatase’s high reactivity, due to its thermodynamic instability and the difficulty in obtaining high quality samples. In the present work, reconstructed anatase TiO$_2$(001)(1×4)surface has been investigated by atomic resolved STM together with the first-principles calculations. Two types of defects were found on the surface, which appear as dark spots and bright spots. The adsorption behavior of H$_2$O, O$_2$ and CO$_2$ molecules were studied. Surprisingly, it was found that all the molecules only adsorbed on the defect sites, which is against to the current understanding of the high activity of anatase (001) surface. Based on first-principles calculations we provide a new structure model of O saturated TiO$_2$ (001) (1×4) surface, which behaves inactive in photocatalysis.