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Photo-excited carrier dynamics of single defects on TiO_2(110) probed by a laser-combined scanning tunneling microscope YING JIANG, CHAOYU GUO, XIANGZHI MENG, International Center For Quantum Materials, Peking University, Beijing, China, HUIXIA FU, SHENG MENG, Institute of Physics, Chinese Academy of Sciences, Beijing, China — Titanium dioxide (TiO_2) is well-known as one of the most widely used materials in photocatalysis and solar energy conversion. Although it is well accepted that the surface and near-surface defects play crucial roles as active sites in the photocatalytic and photoconcersion process of TiO_2, the atomic-scale information of photo-excited carrier dynamics of those defects is still lacking. Here, we addressed this important issue using a home-made laser-combined scanning tunneling microscope (STM). Surface and subsurface oxygen vacancies of rutile TiO_2(110) led to prominent in-gap states below the Fermi level (E_F). Upon the light illumination, those gap states exhibited significant energetic shift. Interestingly, the subsurface defects showed two distinct photo response: redshift and blueshift, while the surface defects only showed blueshift. Based on density functional theory calculations (DFT), the redshift/blueshift of the gap states were ascribed to the photo-excited charge transfer between the gap states and valance/conduction band, which changed the charge states of the oxygen vacancy. Time-resolved experiments suggested that the lifetime of the photo-excited hot electrons/holes can be in the order of nanoseconds. Our work highlights the importance of atomic environment in the photoactivity of the defects and may help to improve the photocatalytic efficiency by engineering the defect types properly.

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