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Probing photoactivity of single defects on TiO2(110) at atomic scale CHAOYU GUO, XIANGZHI MENG, International Center For Quantum Materials, Peking University, HUIXIA FU, SHENG MENG, Beijing National Lab for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, YING JIANG, International Center For Quantum Materials, Peking University — Titanium dioxide (TiO2) is one of the most widely used materials in photocatalysis. Although it is well accepted that the surface/near-surface defects play crucial roles in the photocatalyticthe atomic-scale information of photo-excited carrier dynamics is still lacking. Here, we addressed this issue using a laser-combined scanning tunneling microscope. Surface and subsurface oxygen vacancies of rutile TiO2(110) were created through sputtering and annealing, leading to the appearance of in-gap states. Upon the light illumination, those gap states exhibited energetic shift. Interestingly, the subsurface defects showed two distinct photo response: redshift and blueshift, while the surface defects only showed blueshift. Based on ab initio density functional theory calculations, the energy shift of the gap-states were ascribed to the photo-excited charge transfer between the gap states and valance or conduction band, which changed the oxygen vacancy's charge states. Further time-resolved experiments suggested that the lifetime of hot electrons/holes can be in the order of tens of nanoseconds. Our work highlights the importance of atomic environment in the photoactivity and may help to improve the photocatalytic efficiency by engineering the defect types properly.

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