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Site-Specific Photosimulated Reactions of O_2 on TiO_2(110)[1] ZHITAO WANG, Pacific Northwest National Laboratory, N. AARON DESKINS, Worcester Polytechnic Institute, IGOR LYUBINETSKY, Pacific Northwest National Laboratory — We report the direct observation at an atomic level with high-resolution scanning tunneling microscopy of photostimulated reactions of single O_2 molecules on reduced TiO_2(110) surfaces at 50 K. Two distinct reactions of O_2 desorption and dissociation occur at different active sites of terminal Ti atoms and bridging O vacancies, respectively demonstrating the critical relation between photoreactivity and adsorption sites on TiO_2. These two reaction channels follow very different kinetics. Hole-mediated O_2 desorption is promptly and fully completed, while electron-mediated O_2 dissociation is much slower and is quenched above some critical O_2 coverage. Density functional theory calculations indicate that both coordination and charge state of an O_2 molecule chemisorbed at specific site largely determine a particular reaction pathway.

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