

Abstract Submitted
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Interplay between hydrogen bonding and electron solvation on hydrated TiO₂ surface JIN ZHAO, Dept. of Physics and Astronomy, Univ. of Pittsburgh, KENNETH JORDAN, Dept. of Chemistry, Univ. of Pittsburgh, JINLONG YANG, Hefei Natl. Lab. for Physical Sciences at Microscale, Univ. of Science and Technology of China, HRVOJE PETEK, Dept. of Physics & Astronomy, Univ. of Pittsburgh — At metal-oxide/protic-solvent interfaces, partially hydrated or “wet electron” states represent the lowest energy pathway for electron transfer.¹ Through a joint two-photo photoemission (2PP) experiment and density function theory (DFT) study, we identified the electronic states corresponding to the partially solvated or wet electron state in H₂O overlayers on rutile TiO₂(110) surface. We find that a network of dangling H atoms can stabilize photoexcited electrons, in so-called wet-electron states. The energies of the “wet electron” states correlate closely with the number and configuration of the dangling H atoms involved in stabilizing them. We also performed DFT calculations of H₂O and H covered anatase (101) surface. Comparing with rutile (110), anatase (101) surface accommodates weaker H₂O molecule-surface hydrogen bonding. Our calculated wet electron state on anatase (101) surface has a lower energy than on rutile. Moreover, the longer distance between the adjacent adsorbate sites and the lower binding energy of H₂O allow for greater freedom for the adsorbed molecules to undergo structural relaxation in solvation of injected electrons. These differences might contribute to the higher photocatalytic activity of anatase compared with rutile. [1] K. Onda B. Li, J. Zhao, K.D. Jordan, J. Yang and H. Petek, *Science* **308**, 1154 (2005).

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