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Ultrafast proton coupled charge transfer dynamics in photocatalysis

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In this talk I will present our experimental and theoretical studies on the nature of electron and hole acceptor states and their dynamics for protic solvent molecule (H_2O , CH_3OH) covered TiO_2 surfaces. Electron-hole pair generation by band gap excitation can introduce charges into protic solvent/ TiO_2 interface, which can drive photocatalytic processes. By time resolved two-photon photoemission and DFT electronic structure calculations we identify the partially solvated or “wet” electron acceptor states, and their proton-coupled electron transfer (PCET) dynamics. Because holes are through to be the primary reagents for photocatalysis on TiO_2 , we also explore possible hole driven PCET dynamic pathways.