

# Interfacial Charge Transfer in PhotoElectroChemical Generation of Hydrogen from Water

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**Abstract**— One of the most crucial factors that govern the photoelectrochemical (PEC) conversion of solar radiation into hydrogen is the optimal control surface states and surface structures for an efficient photo-generation of charge carriers and improving the charge transport properties at the electrolyte-electrode interface. At the electrode-electrolyte interface, three most important steps take place for splitting water to generate hydrogen: (1) light absorption by the semiconducting electrode surface, (2) the charge carrier generation, and (3) the charge carrier separation with a sufficiently high energy for electrolyzing the redox couple. These three processes are common for all PEC systems used for hydrogen production. Our approach is to engineer the PEC interface to optimize the interfacial properties. The key issues of the current approach are to control the surface states and surface morphology and in achieving the effective band gap by doping at the surface.

A joint effort between University of Arkansas at Little Rock and the University of Nevada at Reno on electrode-electrolyte interface engineering studies for the improving photocurrent density of nanostructured TiO<sub>2</sub> photoanodes using plasma treatment is reported here. The objective is to develop methods for physical and chemical controls of surface band gaps by first removing contaminants from the surface and then doping the photoanode surface, leaving the crystalline uniformity of the bulk of the semiconductor nearly unaltered for increasing light absorption and minimizing the recombination rate of charge carriers. Since the previous studies with bulk-doping have been found to be ineffective in increasing light absorption and improving the photocurrent density of TiO<sub>2</sub> photoanodes due to Fermi level pinning and the associated adverse effect on the electron transport properties, the focus of our research is on the control of surface states and surface structures for generating hydrogen from water in an efficient manner. Plasma treatments of the TiO<sub>2</sub> electrode surface successively with He, O<sub>2</sub> and N<sub>2</sub> atmosphere for removing electron traps followed by n-type surface doping of the semiconductor showed an 80 percent increase in photocurrent density (to 1.68 mA/cm<sup>2</sup>) compared to that of the untreated photoanodes..