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Using oxide nanostructures to control carrier transport properties ANDERS HELLMAN, Chalmers Univ of Tech — Selecting suitable material(s) for water splitting is an intricate dilemma, as materials with high solar-to-hydrogen (STH) conversion are typically not stable in aqueous environment and/or are scarce, whereas stable and abundant materials often exhibit unacceptable performance for commercialization [1]. For example, Fe_2O_3 is an abundant n-type semiconductor that has excellent stability in neutral and alkaline electrolytes, but so far the reported STH conversion efficiency has not exceeded 3% [2]. A major factor hampering the performance Fe_2O_3, is the high charge recombination rate inside the semiconductor. Thus, there is a need to develop methods and designs to reduce charge recombination. Recently we showed that by joining different oxides we were able to control the charge recombination rate [3]. The control mechanism relies on the formation of dipole-like electric fields at the interface which, depending on the field direction, attract or repel minority carriers from the interface. Here we investigate the built-in electric field generated at the interfaces of Fe_2O_3/TiO_2 and Fe_2O_3/Cu_2O using first-principles methods. The results show how electronic band alignment and defects doping at the interface determine the direction and strength of the built-in field. Our understanding of the oxide nanostructures can be employed for designing and improving the performance of water-splitting photoelectrodes. [1]: A. Fujishima, et al., *Surf. Sci. Rep.*, **2008**, 6, 515-582. [2]: D. K. Bora, et al., *Energy Environ. Sci.*, **2013**, 6, 407-425. [3]: B. Iandolo, et al., *Nano Lett.*, **2016**, *16*, 2381–2386.

Anders Hellman
Chalmers Univ of Tech

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