Materials Aspects of Hematite-Based Photoelectrochemical Water Splitting

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As a semiconductor oxide, hematite (alpha iron oxide) possesses many attractive properties for photoelectrochemical (PEC) water splitting, including the suitable bandgap (2-2.2 eV) for efficiencies as high as 16% and stability against corrosion over a wide range of pH. In addition, its abundance makes it possible to utilize the material in large scale. The utilization of hematite as a PEC electrode material also faces great challenges. For example, the short hole diffusion distance within hematite limits the effectiveness in charge separation; the relatively positive positions of the band edges renders complete water splitting unachieveable. To combat these problems, we proposed and tested a number of strategies, most of which are based on forming homo- or hetero-junctions. The idea is to keep the desirable properties of hematite and compensate its shortcomings using additional material components. Here we present our recent results toward this direction. To improve charge separation, we introduced a highly conductive nanostructure that we call nanonets, which help collect photogenerated electrons, thereby minimizing electron-hole recombinations. To reduce the need for externally applied potentials, we coated a p-type layer on top of n-type hematite, which produces a buried junction. The photovoltage created by the junction assists water splitting. To absorb photons with energies lower than the band gap of hematite, we combined Si nanowires with hematite and showed that the two absorbers can work in concert to greatly reduce the applied potential and still enable PEC water splitting. These proof-of-concept demonstrations show that with good synthesis controls, the goal of high-performance water splitting by hematite is within reach. The concepts demonstrated here should also be applicable to othe oxide-based semiconductors for water splitting purposes. They will likely contribute significantly to our efforts of building a renewable energy powered future.