

Materials Issues for Photoelectrochemical Water Splitting: Chalcopyrite Thin-Films and III-V Nitrides.

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The direct photoelectrochemical (PEC) splitting of water is a one-step process for the production of H₂ using solar irradiation; water is split directly upon illumination. This direct conversion system utilizes the process where an illuminated semiconductor material immersed in aqueous solution, is used to decompose water directly. Light is absorbed in the semiconductor and water is split at the semiconductor surface. The key is to match the light-harvesting properties of the semiconductor with a catalyst that can efficiently collect the energy and direct it towards the water splitting reaction. The simplest PEC based direct water splitting system would consist of an illuminated single gap semiconductor having a bandgap greater than 1.6 electron volts coupled to a surface catalyst immersed in an aqueous solution.

To date, no semiconducting material has been discovered that simultaneously meets all the criteria required for economical hydrogen production via light-driven direct water splitting. Whilst considerable work has been directed at metal oxides due to their expected stability, little thought has been given to the requirement that these PEC devices must have the same fundamental internal quantum efficiency as the commercial high efficiency PV devices. Chalcopyrite materials in the family of Cu(In,Ga)(SSe) are known to have high PV conversion efficiencies and can be made with low-cost thin film approaches, making them appealing candidates for PEC water splitting. CuGaSe₂, with an energy gap close to 1.7eV, is at the lower end of the desired band gap range for water splitting materials but nonetheless of interest. The III-V nitride materials have shown excellent stability as evidenced by corrosion analysis; however, they show a significant decrease in overall conversion efficiency as compared to other non-nitride III-Vs.

This report will summarize our efforts on these materials and their application to tandem cells for photoelectrochemical water splitting. Issues relating to metal oxides will also be discussed.