II.F.5 Solar Water Splitting: Photocatalyst Materials Discovery and Systems Development

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California Institute of Technology, Pasadena, CA

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Objectives

- Develop and optimize novel photocatalyst(s) with bandgap(s) engineered for unbiased solar splitting of water.
- Develop bio-inspired metal complex catalysts to reduce the overpotential required for efficient solar splitting of water.
- Demonstrate a chemical conversion process efficiency of >8% for a photoelectrochemical system.
- Demonstrate a pilot-scale photoelectrochemical hydrogen system with >1,000 hours life.

Technical Barriers

This project addresses the following technical barriers from the Photoelectrochemical Hydrogen Production section (3.1.4.2.6) of the Hydrogen, Fuel Cells and Infrastructure Technologies Program Multi-Year Research, Development and Demonstration Plan:

(AP) Materials Efficiency
(AQ) Materials Durability
(AR) Bulk Materials Synthesis
(AS) Device Configuration Designs
(AT) Systems Design and Evaluation

Technical Targets

This project is conducting fundamental studies of oxide-based photocatalysts to understand the nature of bandgap engineering as it relates to photoelectrochemical splitting of water. In addition, bio-inspired electron and hole transfer catalysts are being studied in order to gain insight into the development of robust and low-cost non-precious metal catalysts for photoelectrochemical systems. Insights gained from these studies will be applied toward the design and synthesis of photoelectrochemical systems that meet the DOE 2010 production targets, especially bandgap, durability, and systems-level efficiency.

Approach

A two-pronged approach is envisaged, where studies of photoelectrochemical materials occur simultaneously with studies of electron and hole transfer catalysts.

Oxide-based photoelectrochemical systems, while chemically robust, generally exhibit bandgaps not suitable for efficient photoelectrochemical splitting of water. Common photoelectrochemical materials and their overlap with the water redox potentials are shown in Figure 1. Note that although the materials differ with respect to cation as well as crystal structure, the relative location of the valence band in these materials is common. This is because the valence band location is due to the oxygen 2p orbitals. Thus, promotion of an electron into the conduction band relates significantly to the electronegativity of oxygen. Consequently,

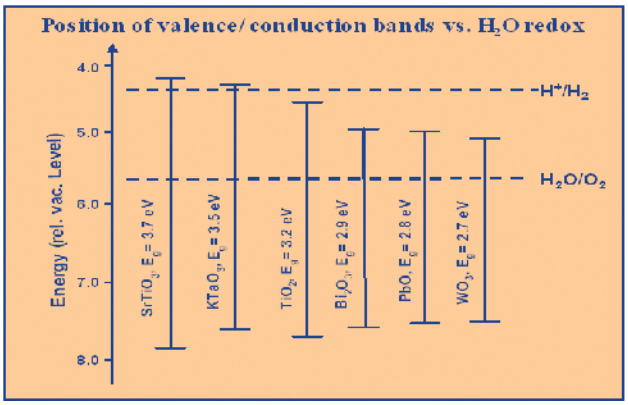

FIGURE 1. Location of Bandedges of Common Photocatalysts with Respect to Water Redox Potentials

anions with lower electronegativity, specifically carbides, nitrides, and phosphides, are better suited to efficiently split water. However, these materials are generally unstable in water, thus lifetime is greatly diminished. Therefore, the principal focus of this work is to develop photoelectrochemical materials with the durability of oxide materials and the bandgap of the non-oxides. Doping of oxide materials on the anion site with elements such as carbon and nitrogen has been performed for photocatalysts such as TiO_2. Evidence shows that this can indeed increase the photosensitivity of the system. Still, this has not been performed in a systematic fashion on materials not requiring an external bias (e.g., $SrTiO_3$, $KTaO_3$).

The lack of robust, low-cost electron and hole transfer catalysts greatly diminishes the solar-to-hydrogen efficiency of photoelectrochemical systems. Consequently, overpotentials on both the anodic and cathodic sides of the system are required to maintain a reasonable photocurrent. This increases the minimum bandgap requirement and thus the solar efficiency of the system. Precious metals such as platinum, though effective, are expensive and poison easily. Bio-inspired catalysts have become a hotbed for research in recent years. A greater understanding of how nature has solved this problem in plants has been achieved, but translation and development of this knowledge to solar water splitting is lacking.

FY 2006 Progress

This project did not receive funding in FY 2006. DOE plans to restart project funding in FY 2007.