II.F.3 Photoelectrochemical Hydrogen Production Using New Combinatorial Chemistry Derived Materials

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Objectives

- Continue synthesis and screening of libraries designed in previous years and follow promising (lead) materials as they are identified.
- Explore the composition-function relationship of dopants in ZnO hosts.
- Investigate metal oxide libraries for electrocatalytic hydrogen production and expand high-throughput screening to include electrocatalytic overpotential as a routine screen.
- Develop a high-throughput optical screening system to measure the effective bandgap of metal oxides in libraries.
- Synthesize and screen model libraries optically for bandgap as a primary screen; create secondary libraries of compositions with solar spectrum adsorption and subsequently screen the derivate libraries for appropriate redox/flatband levels and finally for H_2 production.
- Continue to expand investigations of nanoporous materials with the emphasis on ZnO, WO_3 and TiO_2.
- Participate as a member of the USA Annex-14 Expert Group in the International Energy Agency's Hydrogen Implementing Agreement on photoelectrolytic hydrogen production.

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
(AS) Device Configuration Designs
(AT) Systems Design and Evaluation

Technical Targets

McFarland Group Progress Toward Meeting DOE Photoelectrochemical Hydrogen Production Targets

Characteristic	Units	2003 Target	2010 Target	2005 Status of Combinatorial Chemistry Derived Materials
Usable Semiconductor Bandgap	eV	2.8	2.3	2.75
Chemical Conversion Process Efficiency	%	4	10	1%
Plant Durability	hr	NA	1,000	(see following)

Although we have not directly measured the lifetime of our materials in photoelectrochemical systems, photocurrent stability under ultraviolet (UV) illumination (over 15 minutes or longer) is one of the key screening parameters used to identify promising material systems. Work on ZnO/Cu_2O systems and doped ZnO is partially aimed at improving the stability of these systems.

Introduction

The overall project objective is to discover and optimize an efficient, practical, and economically sustainable material for photoelectrochemical production of bulk hydrogen from water – a clean, renewable route to hydrogen energy. The properties of the semiconductors investigated for this application, which are similar to those in photovoltaic devices, must satisfy conditions in several areas if cost-effective hydrogen production is to be realized: (1) efficient solar absorption, (2) effective charge separation/transport, (3) appropriate conduction band/valence band energies relative to H_2 and O_2 redox potentials, (4) facile interfacial charge transfer, (5) long-term stability, and (6) low cost. A material which satisfies all the above conditions simultaneously could provide clean hydrogen in bulk and at low cost; unfortunately, no such material or system has been discovered or developed to date. The DOE has identified the following future targets for solar-to-hydrogen efficiency and durability: 2010, 8% and 1,000 hours; 2015, 10% and 5,000 hours.

Approach

This project involves the application of combinatorial chemistry methods to discover and optimize photoelectrochemical materials and systems for cost-effective hydrogen production. Our research paradigm features systematic and high-speed exploration of new metal-oxide based solid-state materials. By investigating large arrays of diverse materials, we are working to improve understanding of the fundamental mechanisms and composition-structure-property relationships within these systems while discovering new and useful energy-producing photocatalysts. It should also be noted that our approach focuses on the investigation of semiconductor materials that are inherently inexpensive, such as ZnO, WO_3, Fe_2O_3 and Cu_2O. Although more expensive systems (e.g., GaAs, InP, etc.) have generally demonstrated greater efficiency, cost and/or natural abundance, they could be problematic on a large scale. Thus, we are applying combinatorial techniques toward inexpensive host photocatalysts with the aim of significantly improving their properties while negligibly affecting cost.

FY 2006 Progress

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