CALIFORNIA STATE SCIENCE FAIR
2015 PROJECT SUMMARY

Name(s)

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Project Number

S0613

Project Title

Correlating the Bandgaps of Earth-Abundant Metal Oxides to Photocurrent Generation for Water Splitting Applications

Abstract

Objectives/Goals

Solar-driven water splitting with earth-abundant, efficient and robust photoelectrode and catalyst materials can meet the challenges of providing sustainable energy globally. In my experiment, I sought to determine the correlation between the bandgaps of mixed metal oxide photoanodes for a photoelectrochemical cell and their photocurrent generation under visible light illumination.

Methods/Materials

Chemicals used were iron (iii) nitrate, zinc nitrate, sodium molybdate, copper (ii) nitrate, cerium nitrate, bismuth (iii) nitrate, vanadyl acetylacetonate, 2,4-pentanedione, sodium tetraborate decahydrate, and boric acid. Materials used to prepare metal oxide electrodes were FTO (fluorine-doped tin oxide) conductive glass plates, black spray paint, silver paint, glass tubing, wire, epoxy, and a kiln. Equipment used for photocurrent generation included an Ag/AgCl reference electrode, a Ni mesh, a potentiostat, and a light bulb. A UV-visible spectrophotometer equipped with an integrating sphere was used for bandgap measurements.

Six earth-abundant mixed-metal oxide materials were prepared on FTO glass plates and made into electrodes. The materials# bandgaps were obtained from Tauc analysis of diffuse reflectance spectra that were measured in a spectrophotometer with integrating sphere. Photoelectrochemical performance was experimentally determined using cyclic voltammetry in aqueous electrolyte and under simulated sunlight illumination. Generated photocurrents were correlated with the materials# bandgaps and compared to a prediction of how efficiency depends on bandgap.

Results

Bismuth-containing metal oxides followed the predicted trend that materials with mid-range bandgaps (in this case, a bandgap of around 1.95 eV) produced the highest photocurrents, while materials with larger and smaller bandgaps produced smaller photocurrents. The iron-containing metal oxides all produced small photocurrents that did not follow the predicted trend, which could be due to other limiting factors such as carrier lifetime.

Conclusions/Discussion

Experimental data indicated that photoanode materials not based on iron oxide, such as doped bismuth vanadates, followed the theoretically predicted photocurrent densities that peak at an optimal bandgap of ~2.0 eV. Materials with bandgaps both larger and smaller than this value showed, as expected, lower maximum solar photocurrent densities.

Summary Statement

The purpose of my project is to characterize metal oxides that can serve as anodes for the oxidation of water under visible light illumination to produce hydrogen as a clean fuel source.

Help Received

Used lab equipment at Caltech under the supervision of Dr. Astrid Mueller.