Hawaiʻi Natural Energy Institute Research Highlights

Alternative Fuels

Solar Fuels Generation

<u>Objective and Significance</u>: The objective of this research is to improve the durability and conversion efficiency of novel *chalcopyrite* thin-film photo-absorbers for photoelectrochemical (PEC) production of *solar fuels*, aiming for a $2/kg production cost of renewable hydrogen.

<u>Background</u>: Sometimes referred to as *Artificial Photosynthesis*, PEC technology combines advanced photovoltaic (PV) materials and catalysts into a single device that uses sunlight as the sole source of energy to split water into molecular hydrogen and oxygen. In a typical PEC setup, the solar absorber is fully immersed into an electrolyte solution and solar fuels are generated directly at its surface. Fuels produced with this method can be stored, distributed and finally recombined in a fuel cell to generate electricity, with water as the only byproduct.

In 2014, the team at HNEI's Thin Films Laboratory teamed up with several National Laboratories (LLNL, LBNL, and NREL) and mainland academic teams (Stanford, UNLV) to develop new semiconducting materials for PEC water splitting, with primary focus on *chalcopyrites*. This material class, typically identified by its most popular PV-grade alloy $CuInGaSe_2$, provides exceptionally good candidates for PEC water splitting. A key asset of this thin-film semiconductor material class is its outstanding photo-conversion efficiency, as demonstrated with $CuInGaSe_2$-based PV cells (>23%). In a PEC configuration, our group has demonstrated that chalcopyrite-based systems are also efficient at storing solar energy into hydrogen bonds without the need of expensive precious catalysts (Gaillard, 2013).

<u>Project Status/Results</u>: HNEI's Thin Films Laboratory is now combining theoretical modeling with state-of-the-art materials synthesis and advanced characterization capabilities to provide deeper understanding of *chalcopyrite*-based PEC materials and engineer high-performance devices. Our recent study demonstrates that alloying *chalcopyrites* with sulfur can improve light collection and increase their photo-conversion from 30% to 65% of the theoretical limit (Gaillard, 2019). Also, we recently demonstrated that a 3-5 nanometer thick metal oxide or sulfide layer can be used to effectively passivate *chalcopyrites* surface against photocorrosion, improving their durability from only few days to up to 6 weeks (Hellstern, 2019). Finally, we are investigating new device integration schemes involving thin-films *exfoliation* and *bonding* techniques to transfer multiple fully integrated chalcopyrite devices onto each other to create multi-junction devices (Gaillard, 2019 presentation). We demonstrated that over 90% of the devices electrical properties are preserved after exfoliation and bonding, leading to multijunction structures capable of producing the large voltages required for water splitting.

This project has produced the following publications:

- 2019, T.R. Hellstern, et al., **<u>Molybdenum Disulfide Catalytic Coatings via Atomic Layer Deposition for Solar Hydrogen Production from Copper Gallium Diselenide Photocathodes</u>**, ACS Appl. Ener. Mats.
- 2019, N. Gaillard, et al., **<u>Wide-Bandgap $Cu(In,Ga)S_2$ Photocathodes Integrated on Transparent Conductive $F:SnO_2$ Substrates for Chalcopyrite-Based Water Splitting Tandem Devices</u>**, ACS Appl. Ener. Mats.
- 2019, N. Gaillard, **<u>Novel Chalcopyrites for Advanced Photoelectrochemical Water-Splitting</u>**, Presented at the U.S. DOE AMR.
- 2013, N. Gaillard, et al., **<u>Development of Chalcogenide Thin Film Materials for Photoelectrochemical Hydrogen Production</u>**, Proceeding of MRS Meeting.

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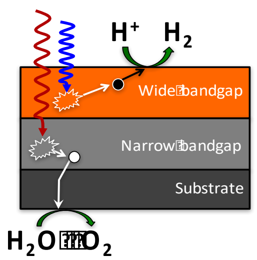
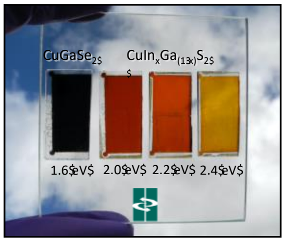
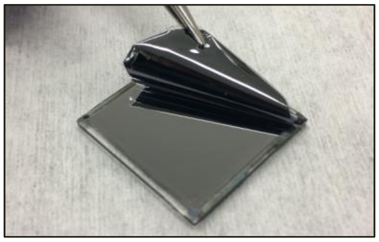
Tandem PEC device concept



Bandgap tunable photoelectrodes



Transferable PEC layers for efficient devices



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