**OBJECTIVE AND SIGNIFICANCE:** 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.

**BACKGROUND:** Sometime referred 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 (typically a strong acid) 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 2017, 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 power 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).

**PROJECT STATUS/RESULTS:** 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. For example, the HNEI team collaborated with Stanford and UNLV to develop coatings for prolonged PEC operations. We demonstrated that molybdenum disulfide (MoS$_2$) films only few atoms thick could effectively protect cadmium sulfide (CdS) in acid for 7 hours, whereas unprotected CdS samples dissolved instantly (Hellstern, 2019). Likewise, we reported that tungsten oxide (WO$_3$) could increase the stability of copper gallium selenide (CuGaSe$_2$) in acid by a factor of 2 when compared to un-coated samples (Palm, 2020).

The HNEI team also partnered with LLNL and UNLV to discover novel PEC materials. Theoreticians at LLNL used an algorithm to determine the chemical composition a material should possess to meet specific optoelectronic properties. At HNEI, the team synthesized specimens following LLNL’s theoretical calculations. Then, the fundamental properties of the newly formed materials were measured at UNLV. Experimental data were finally fed back into LLNL’s model to refine its prediction. Using this theory-synthesis-characterization feedback loop, a novel class of absorbers known as *ordered vacancy compounds* was successfully fabricated (Gaillard, 2021).

The listed publications are linked on the following page.

**Funding Source:** Department of Energy

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ADDITIONAL PROJECT RELATED LINKS

PAPERS AND PROCEEDINGS:


