**OBJECTIVE AND SIGNIFICANCE:** The objective of this research is to improve the durability and efficiency of chalcopyrite and perovskite thin-film photo-absorbers for photoelectrochemical (PEC) production of solar fuels, aiming for a $1/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 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.

Under two consecutive DOE awards received in 2014 and 2017, HNEI partnered with the University of Nevada, Las Vegas (UNLV), Stanford, the National Renewable Energy Laboratory (NREL), and Lawrence Livermore National Laboratory (LLNL) to establish a unique tool chest of theoretical modeling, state-of-the-art synthesis, and advanced material and interface characterization to provide deeper understanding of PEC materials and engineer high-performance devices. Focusing on the chalcopyrite material class, our group was able to synthesize solar absorbers capable of generating photocurrent densities relevant to high solar-to-hydrogen (STH) efficiencies (>12%). We also demonstrated that tungsten oxide (WO₃) films only few atoms thick could increase the stability of chalcopyrites in acid by a factor of 2 when compared to un-coated samples.

A key challenge remains: materials integration into “multi-junction” (MJ) PEC water splitting devices, an integration scheme in which thin film materials are monolithically stacked on top of each other to maximize STH efficiency. With such architecture, the deposition process of each layer must not damage the previously deposited layers and interfaces in any way. Our results showed that chalcopyrites are not compatible with monolithic MJ integration.

**PROJECT STATUS/RESULTS:** In 2023, HNEI and partners at Stanford, UNLV, LLNL and NREL received DOE funding to specifically develop a novel integration scheme in which material classes can be combined regardless of their nature while preserving their intrinsic performance. Such a scheme, pioneered by HNEI and known as semi-monolithic integration, relies on 2D materials-assisted exfoliation and room temperature bonding techniques to transfer fully integrated cells from their original substrates onto new handles. With this integration scheme, sub-cells can be successively transferred onto a new host to create a fully functional MJ structure. By design, semi-monolithic integration allows to circumvent all material incompatibilities, enabling new MJ architectures otherwise not possible with conventional monolithic integration. With this integration scheme, HNEI was able to fabricate the world’s first chalcopyrite triple junction PEC device with 3% STH efficiency (proof-of-concept). HNEI will leverage this new technology to combine chalcopyrites and perovskites photo-absorbers, aiming for MJ devices with STH efficiencies of at least 15%.

To date, this project has produced five peer reviewed papers, which are listed on the following page.

**Funding Source:** Department of Energy

**Contact:** Nicolas Gaillard, ngaillard@hawaii.edu

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ADDITIONAL PROJECT RELATED LINKS

PAPERS AND PROCEEDINGS:


