



Hawai'i Natural Energy Institute Research Highlights

Alternative Fuels

Solar Fuels Generation

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*, to reduce the 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 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.

PROJECT STATUS/RESULTS: Under two consecutive U.S. DOE awards received in 2014 and 2017, HNEI partnered with the University of Nevada, Las Vegas, Stanford University, the National Renewable Energy Laboratory, and Lawrence Livermore National Laboratory 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 uncoated 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.

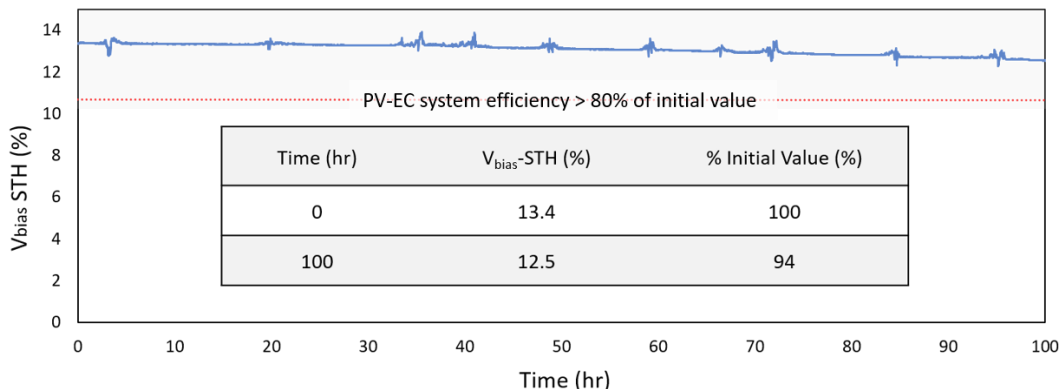
In 2023, HNEI and its partners received additional DOE funding to develop a novel integration scheme in which material classes can be combined regardless of their nature while preserving their intrinsic performance. Such a scheme, pioneered by HNEI and known as *semi-monolithic* integration, relies on 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 combine two promising—yet thermally incompatible—material classes, *chalcopyrites* and *perovskites*, into tandem cells producing hydrogen with an initial efficiency of 13.4% and capable of maintaining over 90% of its efficiency for over 100 hours of operation.

To date, this research has produced the publications and presentations listed on the following page.

Funding Source: U.S. Department of Energy

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ADDITIONAL PROJECT LINKS

PAPERS AND PROCEEDINGS:

1. 2022, K. Outlaw-Spruell, J. Crunk, W. Septina, C.P. Muzzillo, K. Zhu, N. Gaillard, [Semi-monolithic Integration of All-Chalcopyrite Multijunction Solar Conversion Devices via Thin-Film Bonding and Exfoliation](#), ACS Applied Materials and Interfaces, Vol. 14, Issue 49, pp. 54607-54615.
2. 2021, N. Gaillard, [A perspective on ordered vacancy compound and parent chalcopyrite thin film absorbers for photoelectrochemical water splitting](#), Applied Physics Letters, Volume 119, Issue 9, Paper 090501.
3. 2021, I. Khan, C.P. Muzzillo, C.L. Perkins, A. Norman, J. Young, N. Gaillard, A. Zakutayev, [Mg_xZn_{1-x}O contact to CuGa₃Se₅ absorber for photovoltaic and photoelectrochemical devices](#), JPhys Energy, Vol. 3, Issue 2, Paper 024001. (Open Access: [PDF](#))
4. 2021, D.W. Palm, C.P. Muzzillo, M. Ben-Naim, I. Khan, N. Gaillard, T.F. Jaramillo, [Tungsten oxide-coated copper gallium selenide sustains long-term solar hydrogen evolution](#), Sustainable & Energy Fuels, Vol. 5, Issue 2, pp. 384-390.
5. 2020, A. Sharan, F.P. Sabino, A. Janotti, N. Gaillard, T. Ogitsu, J.B. Varley, [Assessing the roles of Cu- and Ag-deficient layers in chalcopyrite-based solar cells through first principles calculations](#), Journal of Applied Physics, Vol. 127, Paper 065303.

PRESENTATIONS:

1. 2024, N. Gaillard, [Semi-Monolithic Integration of Dissimilar Material Classes into Efficient Water Splitting Devices](#), Presented at the Electrochemical Society PRiME Meeting, October 6-11, Honolulu, Hawai'i, Symposium L04, Abstract 3947.
2. 2024, K. Outlaw-Spruell, C. Muzzillo, K. Zhu, N. Gaillard, [Semi-Monolithic Multijunction Devices for Unassisted Photoelectrochemical Water Splitting](#), Presented at the Electrochemical Society PRiME Meeting, October 6-11, Honolulu, Hawai'i, Symposium L04, Abstract 3932.
3. 2024, N. Gaillard, [Semi-Monolithically Integrated Photoelectrochemical Devices for Unassisted Water Splitting](#), Presented at the 245th Electrochemical Society Meeting, May 26-30, San Francisco, California, Symposium I02, Abstract 1990.
4. 2024, K. Outlaw-Spruell, C. Muzzillo, K. Zhu, N. Gaillard, [Anisotropic Conductive Adhesive for Semi-Monolithic Integration of Multi-Junction PV and PEC Devices](#), Presented at the Materials Research Society Spring Meeting, April 22-26, Seattle, Washington, Symposium EN05.07.04.