Hawaiʻi 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*, 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 (WO_3) 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, ngaillar@hawaii.edu

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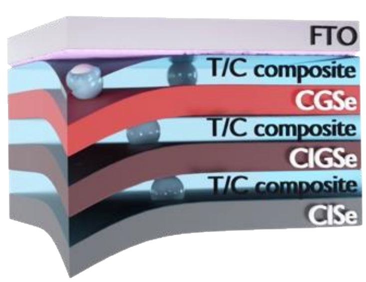

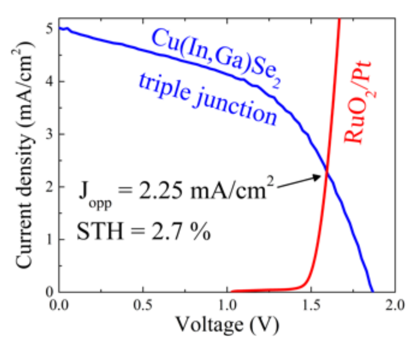

ADDITIONAL PROJECT RELATED LINKS

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 $CuGa_3Se_5$ 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.