Maximizing Solar-to-Fuel Conversion Efficiency in Photo-Electrochemical Cells with Heat and Concentrated Sunlight

**Investigators**
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**Objective**
The objective is to develop a photo-electrochemical cell (PEC) for efficient and stable solar fuel production using Earth-abundant materials that combine the beneficial traits of room-temperature PECs and high-temperature thermochemical decomposition. Ambient-temperature PECs are among the most intensely studied technologies for storing intermittent solar energy in hydrogen, hydrocarbons, and other fuels. Despite the high theoretical efficiency of PECs, actual values are typically low, and most devices become unstable after a few hours. To substantially increase the stability and solar-to-fuel conversion efficiency of PECs, the research team will harness the thermal energy and intense light from concentrated solar radiation, which is normally discarded as waste heat.

**Background**
PECs that operate at room temperature suffer from instability due to photo-corrosion, and low efficiency caused by electrocatalytic and electron-transfer losses. The proposed project offers a novel PEC design that combines the conventional semiconductor photo-excitations and thermal energy from concentrated sunlight. Both thermal and electrical energy will be used to help chemical reactions overcome energetic barriers.

**Approach**
This basic design of this new class of PEC consists of a heterojunction between an oxide light absorber and a catalytically active, wide band-gap mixed oxygen ion and electron conducting (MIEC) oxide. The device operates at elevated temperatures (500°C to 700°C) with concentrated solar flux (Figure 1). Replacing a liquid or polymeric solid electrolyte in a conventional PEC with an oxygen-ion-conducting MIEC will extend the operating temperature to a much higher range. At the same time, thermal energy will greatly enhance carrier transport and electrocatalysis in the oxide heterojunction. Combined with the fast removal of products in the gas phase, the heterojunction will substantially decrease the probability of carrier recombination and result in higher efficiencies.
Identify and develop oxide light absorber and MIEC materials for the elevated-temperature hetero-junction photo-anode

Research efforts will be focused on understanding the critical material parameters that control solar-to-fuel efficiency and stability, and optimizing the semiconductor/MIEC heterojunction by tuning the material composition. Three critical material parameters that directly control the solar-to-fuel conversion efficiency will be emphasized: (1) light absorber band gap and doping level; (2) interfacial recombination velocity; and (3) band alignment between the light absorber and the MIEC. The team has identified several promising oxides with hematite and perovskite structures, and will begin by optimizing a hematite Fe$_2$O$_3$/Fe-SrTiO$_3$ system. Other PEC components, such as the solid-electrolyte membrane and the cathode, are readily available.

Fabrication and rapid characterization

To rapidly assess the light absorber/MIEC heterojunctions, researchers will fabricate planar, thin-film structures and characterize their optoelectronic properties at elevated temperature. Two single-chip platforms have been designed to measure a wide range of properties in a single experiment. A heterojunction platform will provide measurements – such as photocurrent, current-voltage curves and electrical conductivity of the light absorber – as a function of temperature and gas composition. An electrochemistry platform will be used to assess oxygen-evolution activity and hydrogen production of the MIEC, allowing its electrical and ionic conductivity to be characterized as a function of temperature and pressure.

Demonstration of a working PEC device

A completed device will be tested using a solar simulator at 1 to 50 suns concentration. A gas chromatograph will quantify the hydrogen and oxygen production rate in the cathode and anode chambers. The objective is to demonstrate a working PEC device with efficiencies exceeding 10% that achieves stable performance after 100 hours of operation, with a long-term goal of 1,000 hours.