Solar Fuels: Importance of Material Compatibility in Their Production

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Abstract
Research and implementation of clean energy alternatives are paramount, not only for the earth but to more efficiently harness energy from renewable alternatives, such as the sun, which provides 10,000 times the daily global energy demand. Artificial photosynthesis, or so-called solar fuel technology, presents an alluring prospect in harnessing solar energy and offers a pathway into the investigation of energy-rich technologies while enabling a potential option of large and continued enhancement of renewable energy options. Fuels are sought after because of the incomparable energy density that they offer, as well as current establishments that rely upon fuel consumption. Hydrogen, a common solar fuel, is produced by water splitting. Alcohols and other fuels can also be produced by the sequestering of CO_2, which is invaluable on its own. This makes solar fuels a great alternative to fossil fuels, which are exhaustible and destructive options. Nonetheless, all the components in the photoabsorbing system must be intelligently selected to work in tandem. Like any new technology, the solar fuel field faces challenges, e.g. low current density, expensive catalysts, and high costs. The main aim of this talk is to bring insight into the importance of material selection and design to produce an efficient photoabsorbing system for solar fuel production and to highlight the significance of building knowledge upon the successful methods that have been previously accomplished.

Introduction
The increase in greenhouse gasses has brought momentous changes to the climate of the earth, generating an urgent need for fossil fuel alternatives. Solar fuels are a type of renewable energy that offers a great alternative to store solar energy through chemical bonds. A prominent approach in creating solar fuels is through photoelectrochemical devices, often referred to as artificial photosynthesis (AP)[1]. AP mimics naturally occurring photosynthesis processes, where sunlight is used to generate reactions such as HER (hydrogen evolution reaction) or OER (oxygen evolution reaction), in the case of water splitting for hydrogen[2]. The basic components of an AP cell are: photoabsorbers, catalysts and electrolyte. Finding suitable photoabsorbing materials, enhancing catalyst efficiency, and understanding the full integration of these materials, is paramount in improving design and performance[1].

Photoabsorbing materials

In principle, the photoabsorbing material captures photons and initializes an electron transport chain. A large variety of photoabsorbing materials have been previously studied, including oxides, oxynitrides, chalcogenides, carbon and carbon nitride-based materials, as well as traditional semiconductors (III–V and III–V nitrides)[1]. Despite different system arrangements, there are shared expectations for photoabsorbers that are believed to create a highly efficient AP system. These include: i) good charge transport, ii) long-term stability and iii) supplying enough photovoltage. Most importantly, an appropriate bandgap to utilize a broad solar spectrum. The bandgaps should allow enough energy necessary for water splitting (>1.23 eV) but not too high where sunlight can't be effectively used (<3.0 eV)[1,3]. However, even when using highly efficient catalysts, overpotentials are at least 0.3 V. There is currently no photoabsorber that meets all the requirements.

Catalyst design

Catalysts in the AP cell expedite the reactions that take place for solar fuel production by assisting in both the bond making and breaking reactions for solar fuel generation[1]. Improving the catalytic efficiency, will directly aid the efficiency of solar fuel generation. There have been great strides in catalyst designs, notably those of metal-organic frameworks and noble metals[4], but overpotentials remain high, and obtaining a decreased overpotential with earth abundant materials for either HER and OER reactions proves to be even more difficult[1]. However, moving forward, there must be a focus in realizing efficient earth abundant catalysts to make them economically viable[3].

Material compatibility

Developing one material to serve both as the photoabsorber and the catalysts, a *photoelectrode*, entails a single material to have both an adequate band structure and suitable surface properties is extremely challenging. Instead, integrated systems with different materials are a popular research avenue which can also improve the efficiency of an AP device. For example, a catalyst overlayer serving as a corrosion layer on a photoabsorber[1]. However, this consolidation introduces complexities, such as certain current densities bringing dangerous mixing of the product gases, however this can be addressed through introducing a membrane. A membrane can bring mechanical support, material hosting flexibility and more efficient charge transport[5]. To improve the performance of integrated systems, engineering interfaces between photoabsorber materials and catalysts (e.g. heterojunctions and surface modification) are potential methods for overcoming intrinsic limitations[6].

Conclusion

The biggest challenge in solar fuel generation via AP is material discovery. Experimental and computational screening of new materials exist, but there are still many to be simulated and tested. Improving the individual components of the AP device does not assure enhanced performance, in fact comprehension of the whole system in terms of not only the performance of individual components but their interplay, is essential to increase their performance. It is essential to understand trends of previously studied devices and where the most efficiencies lie, both in experimental work and in theoretical calculations, for more comprehensive designs. We are far from having an ideal AP device for solar fuel generation, but we cannot rely solely on trial-and-error strategies to solve the challenges ahead, but instead build knowledge upon the successful methods that have been previously accomplished.

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