Engineering semiconductor materials and catalysts for photoelectrochemical solar fuel production

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The development of robust and inexpensive semiconducting materials that operate at high efficiency are needed to make the direct solar-to-fuel energy conversion by photoelectrochemical cells economically viable. In this presentation our laboratory's progress in the development new light absorbing materials and co-catalysts will be discussed along with the application toward overall solar water splitting tandem cells for H_2 production. Specifically, this talk will highlight recent results with the ternary oxide $CuFeO_2$, 2D transition metal dichalcogenides, and organic (π-conjugated) semiconductors as solution-processed photoelectrodes.

With respect to $CuFeO_2$, in our recent work [1] we demonstrate state-of-the-art sacrificial p-type photocurrent with optimized nanostructuring. Recent results addressing interfacial recombination by the electrochemical characterization of the surface states and attached co-catalysts will be presented along with approaches to overcome the limitations of this material.

In addition, two-dimensional (2-D) transition metal dichalcogenides (TMDs) generally have intriguing electronic properties making them promising candidates for high-efficiency solar energy conversion. However, it is notoriously difficult to fabricate thin films of 2-D TMDs over the large areas required to convert solar energy on a practical scale. We recently developed a simple method to fabricate high-quality thin films of 2-D layered TMDs at low cost and with good efficiency towards solar-to-fuel energy conversion [2]. The challenges with charge transport, separation [3] and water redox catalysis in these systems will also be discussed with respect to the 2D flake size.

Finally, with respect to π-conjugated organic semiconductors, in our recent work [4] we demonstrate a π-conjugated organic semiconductor for the sustained direct solar water oxidation reaction. Aspects of catalysis and charge-carrier separation/transport are discussed.

[1] Prevot, M. S.; Li, Y.; Guijarro, N.; Sivula, K. *J. Mater. Chem. A* **2016**, *4*, 3018-3026.
[2] Yu, X.; Prevot, M. S.; Guijarro, N.; Sivula, K., *Nat. Commun*. **2015**, *6*, 7596.
[3] Yu, X.; Rahmanudin, A.; Jeanbourquin, X. A.; Tsokkou, D.; Guijarro, N.; Banerji, N.; Sivula, K. *ACS Energy Lett*. **2017**, *2*, 524.
[4] Bornoz, P.; Prévot, M. S.; Yu, X.; Guijarro, N.; Sivula, K. *J. Am. Chem. Soc*. **2015**, *137*, 15338.