

Light Induced H₂O Splitting: Device and materials science issues

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One of the most demanding areas for a holistic and sustainable energy economy is related to the integration of storage devices to renewable primary energy sources to overcome e. g. the discontinuous supply of solar power. The direct production and use of chemical fuels would provide a favourable solution. However, inherent problems in the direct production of H₂ from solar light has not been solved yet.

Direct H₂ formation by **photocatalytic or photoelectrochemical H₂O splitting** theoretically provides high light (photon) to fuel (H₂) efficiency. Advanced materials and design concepts based on the coupling of wide band gap semiconductors i.e. ZnTe, GaP, SiC or thin film Si tandem cells and nano sized metal catalysts provide very promising options. Alternatively band gap modified and defect engineered nanosized oxides are interesting alternatives to meet the requirements. Materials and devices of this type must be designed, grown, processed and characterized combining a solid knowledge of photovoltaic device physics and electrocatalysis.

The schematic arrangement of photo electrochemical devices for H₂O splitting is shown in Fig 1 for one and two (tandem) absorber materials.

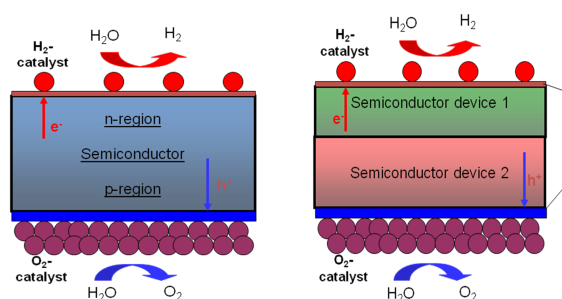


Fig. 1. Schematic arrangement of photoelectrochemical solar cells for H₂O splitting

From a consideration of the given thermodynamic and kinetic energetic condition to split H₂O only wide band gap absorbers or tandem structures with a sufficient splitting of the quasi-Fermi level comparable to the provided photovoltage of the solar device will be able to produce H₂O in reasonable amounts. As a consequence the first duty is to optimize the light converting devices structure in a similar way as it has to be done for electricity producing solar cells. This means that the transport lengths of charge carriers must exceed the thickness of the device, where the thickness of the absorber layer has to exceed the absorption length. Subsequently the separated charge carriers must be transferred to the reactants without loss in chemical potentials (photo voltage) and loss in photocurrent. In the case of multi electron transfer reactions catalysed by metal particles specific interactions of intermediates with the electro catalyst's surfaces must be taken into account. As is schematically shown in Fig. 2 the energetic conditions must be optimized to minimize any loss mechanism. The position of the band edges, metal Fermi level, and electrolyte density of states must be arranged in a proper way. Whereas surface science techniques may be one possible but also challenging way to measure the energetic conditions for equilibrium conditions, a detailed knowledge and optimisation of photo electrochemical devices would also need a better understanding of such devices under non-equilibrium conditions.

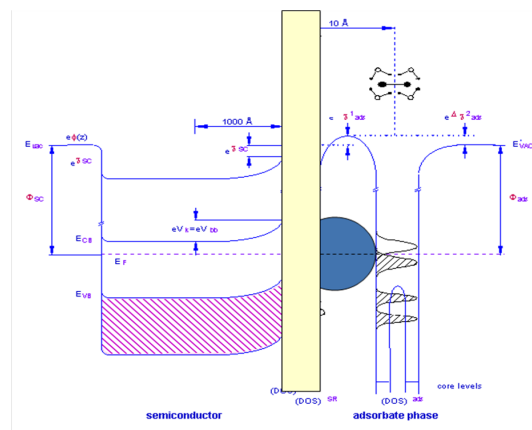


Fig. 2. Schematic sketch on a possible electron energy diagram of a photo electrochemical device in the dark composed of a semiconductor, passivation layer, metal particle and electrolyte.

We will present and discuss our recently revived research approach on photo electrochemical water splitting devices giving a survey on most interesting systems from our point of view. The materials science issues, which are needed to overcome given limitations of H₂O splitting devices will be discussed and first results of recent experimental investigations to verify our concepts will be presented.