On the way to sustainable hydrogen

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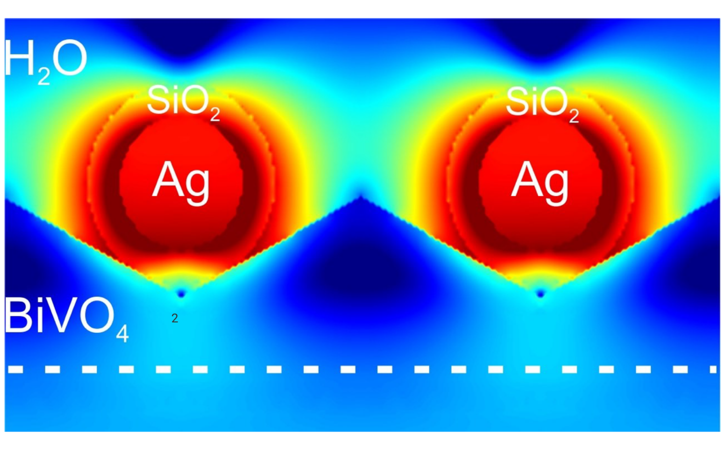
Researchers in the SNI network have developed a theoretical method to analyze and optimize water splitting by exploiting optical effects.

The work, published in the *Journal of Physical Chemistry C*, will help to advance sustainable hydrogen production without emitting CO .



Theoretical calculations were used to calculate the light intensity distribution during the splitting of water. A photoelectrode made of bismuth vanadate (BiVO4) structured with silver nanoparticles on its surface was used. The silver nanoparticles help to concentrate more light in the photoelectrode (light blue areas). They are surrounded with a silica shell to protect the silver from corrosion in water (Image: L. Driencourt, CSEM Muttenz and Swiss Nanoscience Institute, University of Basel)

Material nanostructuring and optical phenomena on a nanoscale such as plasmonic effects and light scattering have been widely studied for improving the solar-to-hydrogen efficiency of photoelectrochemical (PEC) water-splitting electrodes. In this work, we report a method for analyzing the contributions of optical effects from nanostructures for enhancing the PEC performances.

Electromagnetic simulations are performed for the precise calculation of generated power density in a semiconductor material. In addition, the transport and transfer of photogenerated charges to the electrolyte are modeled by using the conservation of minority carriers.

The surface loss parameter, diffusion length, and doping density of the semiconductor material are determined by fitting the model to an incident photon to current efficiency (IPCE) curve experimentally measured on the bare reference photoelectrode. These parameters are then used to compute the IPCE spectra of the photoelectrode for which an optical enhancement strategy is used, such as nanostructuring or plasmonics. The method is validated using published experimental data.

The calculated IPCE enhancement ratio originating from optical effects is in quantitative agreement with experimental observations for both periodic and random optical structures. The model can be used to study in detail the key enhancement mechanisms for the IPCE from optical nanostructures and, in particular, discriminate between optical and nonoptical (e.g., catalytic) enhancement.

Source: University of Basel