Solar hydrogen: Photoanodes promise high efficiencies

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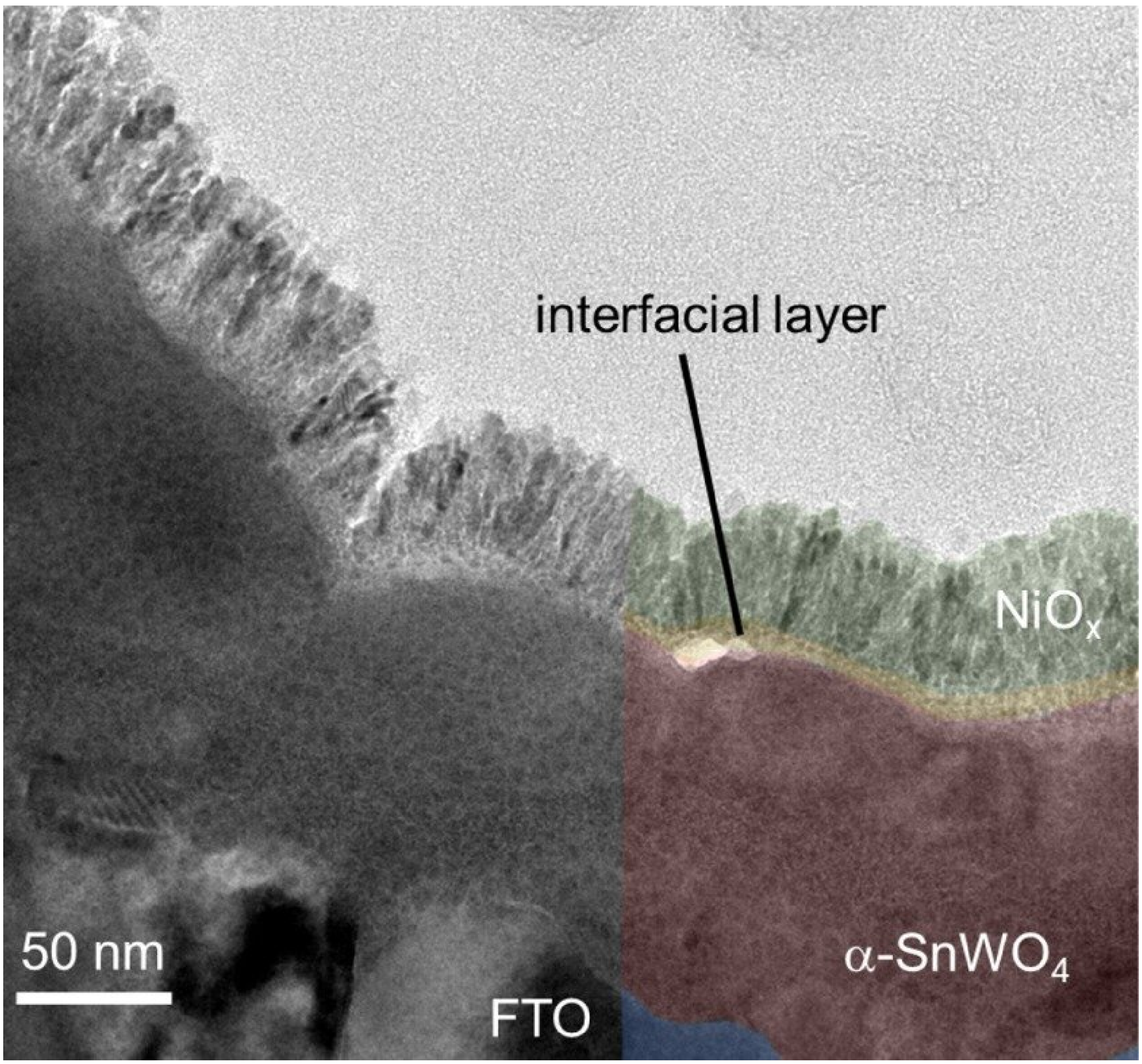

TEM-Image of a α-SnWO4 film (green) coated with 20 nm NiOx (pink). At the interface of α-SnWO4 and NiOx an additional interfacial layer can be observed. Credit: HZB

Photoanodes made of metal oxides are considered to be a viable solution for the production of hydrogen with sunlight. α-$SnWO_4$ has optimal electronic properties for photoelectrochemical water splitting with sunlight, but corrodes easily. Protective layers of nickel oxide prevent corrosion, but reduce the photovoltage and limit the efficiency. Now a team at HZB has investigated at BESSY II what happens at the interface between the photoanode and the protective layer. Combined with theoretical methods, the measurement data reveal the presence of an oxide layer that impairs the efficiency of the photoanode.

Hydrogen is an important factor in a sustainable energy system. The gas stores energy in chemical form and can be used in many ways: as a fuel, a feedstock for other fuels and chemicals or even to generate electricity in fuel cells. One solution to produce hydrogen in a climate-neutral way is the electrochemical splitting of water with the help of sunlight. This requires photoelectrodes that provide a photovoltage and photocurrent when exposed to light and at the same time do not corrode in water. Metal oxide compounds have promising prerequisites for this. For example, solar water splitting devices using bismuth vanadate ($BiVO_4$) photoelectrodes achieve already today ~8% solar-to-hydrogen efficiency, which is close to the material's theoretical maximum of 9%.

Theoretical limit is 20% in α-$SnWO_4$

To achieve efficiencies beyond 9%, new materials with a smaller band gap are needed. The metal oxide α-$SnWO_4$ has a band gap of 1.9 eV, which is perfectly suited for photoelectrochemical water splitting. Theoretically, a photoanode made of this material could convert ~20%

of the irradiated sunlight into chemical energy (stored in the form of hydrogen). Unfortunately, the compound degrades very quickly in an aqueous environment.

Protection against corrosion comes with a price

Thin layers of nickel oxide (NiOx) can protect the α-$SnWO_4$ photoanode from corrosion, but were found to also significantly reduce the photovoltage. To understand why this is the case, a team led by Dr. Fatwa Abdi at the HZB Institute for Solar Fuels has analyzed the α-$SnWO_4$/NiOx interface in detail at BESSY II.

Interface explored at BESSY II

"We studied samples with different thicknesses of NiOx with hard X-ray photoelectron spectroscopy (HAXPES) at BESSY II and interpreted the measured data with results from calculations and simulations," says Patrick Schnell, the first author of the study and a Ph.D. student in the HI-SCORE International Research School at HZB. "These results indicate that a thin oxide layer forms at the interface, which reduces the photovoltage," explains Abdi.

Outlook: Better protection layers

Overall, the study provides new, fundamental insights into the complex nature of interfaces in metal oxide-based photoelectrodes. "These insights are very helpful for the development of low-cost, scalable metal oxide photoelectrodes," says Abdi. α-$SnWO_4$ is particularly promising in this regard. "We are currently working on an alternative deposition process for NiOx on α-$SnWO_4$ that does not lead to the formation of an interfacial oxide layer, which is likely to be SnO_2. If this is successful, we expect that the photoelectrochemical performance of α-$SnWO_4$ will increase significantly."

More information: Patrick Schnell et al, Interfacial Oxide Formation Limits the Photovoltage of α-SnWO 4 /NiO x Photoanodes Prepared by Pulsed Laser Deposition, *Advanced Energy Materials* (2021). [DOI: 10.1002/aenm.202003183](https://doi.org/10.1002/aenm.202003183)

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