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SEMINAR SERIES

HIGHLIGHTS IN ENERGY RESEARCH

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Recent Progress on Ternary Metal Oxide Photoelectrodes for Water Splitting

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The direct photo-electrochemical conversion of water and CO2 into chemical fuels represents an exciting new pathway for the combined conversion and storage of solar energy. One of the main challenges in this field is to find semiconducting light absorbers that are efficient, chemically stable, and easy to synthesize. I will show some recent progress on BiVO4 , a promising photoanode material with a bandgap of 2.4 eV. We have investigated the carrier dynamics of undoped and doped BiVO4 with ultrafast timeresolved spectroscopy, and found that carrier trapping at defects and the formation of polarons play an important role. Hydrogen was found to be a particularly effective dopant, since it simultaneously passivates bulk defect states and increases the dark conductivity [1]. A second 'trick' to improve the performance of BiVO4 is by functionalizing its surface with cobalt phosphate (CoPi). We recently showed that the main role of this 'catalyst' is not to enhance the charge transfer kinetics, but to passivate surface defects on BiVO4 [2]. Using ambient pressure photoemission techniques, we now have some first clues about the chemical nature of these surface states and a better insight in how the solid/liquid interface behaves under illumination. These initial results are the first steps towards a molecular-level understanding of the BiVO4 /electrolyte interface that may eventually help to design efficient solar fuel generators. Scale-up is the next step, and I will show recent results on 50 cm2 complete water splitting devices based on BiVO4 photoelectrodes that we developed within the EU project PECDEMO. Finally, if time permits, I will show some of our efforts on CuBi2 O4 , a promising new photocathode material with a bandgap of about 1.7 eV [3].

References

[1] J.W. Jang et al., *Adv. Energy Mater.* 1701536 (2017)
[2] C. Zachäus et al., *Chem. Sci.* 8, 3712 (2017)
[3] F. Wang et al., *J. Am. Chem. Soc.* 139, 15094 (2017)

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Roel van de Krol (1971) is director of the Insitute for Solar Fuels at the Helmholtz-Zentrum Berlin für Materialien und Energie (HZB) and professor at the Chemistry Department of TU Berlin. After earning his PhD from TU Delft in 2000 and a postdoctoral stay at MIT (USA), he returned to TU Delft where he was an assistant professor until he moved to HZB in 2012. His research focuses on the development of materials and devices for the photoelectrochemical conversion of sunlight to chemical fuels. One of the specialties of his group is the work on multinary metal oxides for application as semiconducting photoelectrodes. Understanding how surface and bulk defects affect light absorption, charge transport, recombination, and catalytic activity in these materials is at the heart of these efforts.