Molecular and physical aspects of dye sensitization of photoelectrodes with copper-based sensitizer molecules

J. Top[1,3], B. S. Mun[2], A. Stephens[3], C. E. Housecroft[3]*, A. Braun[1]*

[1]Empa, [2]GIST, [3]University of Basel

Early work on dye sensitization dates back almost a hundred years and became a field of energy conversion in the late 1960s[1] and early 1970s[2]. Dye sensitized solar cells (DSSC) are basically a technology of artificial photosynthesis. Ruthenium is a favourite component in high performance dye molecules.[3,4]

Because of the low abundance and high cost of Ruthenium, our research focusses on Copper based dye molecules.

For DSSCs, the charge transfer between dye molecules and metal oxide semiconductor photoelectrode is very important. We show how we determine the electronic structure of the metal oxide – dye interface[4] operando with ambient pressure photoelectron spectroscopy for electronic structure determination, and electroanalytical methods for determination of the charge carrier dynamics.[5,6]

Furthermore, ab initio calculations are employed to aid in the interpretation of these results.

[1] Gerischer, H., Michel-Beyerle, M., Rebentrost E., Tributsch, H., *Electrochimica Acta*, **1968**, 13, 1509–1515
[2] Tributsch, H., Calvin, M., *Photochem. Photobiol.*, **1971**, 14, 95–112
[3] O'Regan B., Gratzel M., *Nature,* **1991**, 353, 737–740.
[4] Hagfeldt A, Gratzel M., *Accounts of Chemical Research,* **2000**, 33, 269–277.
[5] Braun A., Boudoire F., Bora D., Faccio G., Hu Y., Kroll A., Mun B., Wilson S, *Chemistry–a European Journal,* **2011**, 21, 4188–4199.
[6] Faccio G., Gajda-Schrantz K., Ihssen J., Boudoire F., Hu Y., Mun B., Bora D., Thöny-Meyer L., Braun A., *Nano Convergence,* **2015**, 2, 1–11.