In operando characterization of catalytically active faceted nano-particle-electrolyte interfaces by Atomic Force Microscopy

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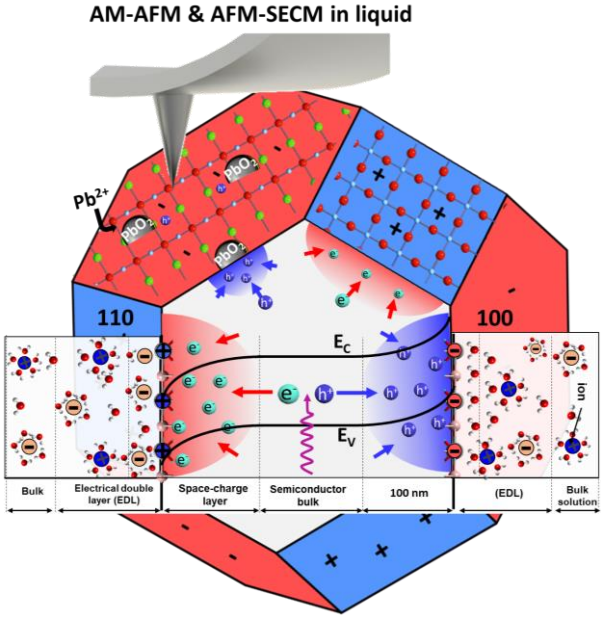
The electro- and photo-catalytic conversion of renewable electricity and solar energy into stable chemical fuels and other products is a core element of the transition towards a sustainable economy. According to the current paradigm, optimum performance is achieved by using faceted nanoparticles of metal or semiconducting materials functionalized in a facet-selective manner with suitable cocatalysts for the desired redox reactions, such as water splitting or CO2 reduction. Yet, neither the strength of the internal electric fields that drive efficiently separate photo-generated electron-hole pairs nor their dominant source are well understood. The primary reason for this lack of knowledge is the absence of suitable experimental techniques that allow quantification of local surface properties such as potentials, charge densities, defect distributions, and hydration effects with the required sub-particle resolution. Applying theoretical modelling and the state of the AFM-based methods (force spectroscopy for surface charge mapping and atomic resolution imaging) with their unique resolution to well-known high-performance photocatalytic materials, we gain unprecedented insights into facet-dependent properties and microscopic mechanisms of charge separation and transfer in photo/electro-catalyst systems and thereby lay the ground for a systematic development of more efficient materials.



[1] Su, S., Siretanu, I., van den Ende, D., Mei, B., Mul, G., & Mugele, F. Facet-Dependent Surface Charge and Hydration of Semiconducting Nanoparticles at Variable pH. *Advanced Materials*, *33*(52), 2106229 (2021).