Vortragsankündigung

Mittwoch, 28. November 2018, 11.15 Uhr

Seminarraum I (JAK2AOG1.33), Jakob-Haringer-Straße 2a

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"Modelling of particle-based photoelectrochemical and photocatalytic water splitting"

Fabrication of photocatalytic semiconductor particle-based photoelectrodes (PE) using simple dipping procedures – scaled in commercial battery production – can be a route to overcome the efficiency-cost trade-off of solar hydrogen. Additionally, the particles can be directly dispersed in the electrolyte for photocatalytic water-splitting. The ability to vary the morphology of the particles allows for designing high-performing particle-based PE or photocatalytic devices. In addition, particle arrangement, inter-particle necking procedure, surface passivation and co-catalyst deposition can further improve the PE's or photocatalytic device performance. The impact of morphology, arrangement, and material combinations on multi-physical transport and, consequently, solar to hydrogen efficiency must be understood to provide design guidelines for high-performing particle-based PE or photocatalytic devices.

In the first part of my talk, I will report on a combined experimental-numerical approach which we used to model particle-based PEs made of $LaTiO_2N$. Morphological characteristics, calculated based on exact, 3D structural information of the PE obtained by nano-tomography, are incorporated in the model. The model is validated using photocurrent measurements of the PE using front and back illumination, and then used to explore the impact of co-catalyst deposition, surface passivation, necking procedure, and modification of bulk material properties on the performance of particle-based PE. In the second part of my talk, I will discuss a transient model of a photocatalytic device utilizing these particles. This model allows to assess the feasibility and limits of photocatalytic water splitting and provides guidance on the design choices.