Annual meeting of the COST Action: Computational materials sciences for efficient water splitting with nanocrystals from abundant elements (CA18234)

"Computational water splitting, where we are now and where to go?

"Efficient Generation of Black Titania – Insights from Atomistic Simulations"

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Abstract

Black TiO_2 is one of the most actively studied materials in the field of renewable energy applications including photocatalytic, photoelectrochemical and electrochemical energy conversion techniques. Black TiO_2 is commonly generated via hydrogenation, i.e. exposure of TiO_2 to an atmosphere of molecular, atomic or ionic hydrogen species. Although a plethora of different hydrogenation approaches has been devised, a deeper mechanistic understanding and an efficient method suitable for industrial upscaling has been missing.

Here, we report ab initio thermodynamics and molecular dynamics simulations which elucidate the different underlying mechanisms and efficiencies of molecular, atomic and plasma-based hydrogenation techniques. The theoretical findings can also explain the hitherto unprecedented efficiency of a novel experimental hydrogenation approach based on a modified plasma-based hydrogenation approach. The latter method is not only efficient and suitable for industrial upscaling but as a low-temperature process has no detrimental side-effects on the substrate and hence allows photocurrents that are among the highest which have been measured for black TiO_2.