Computational methods for modeling materials for H_2O splitting

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Functional materials are important for the application of water oxidation in the field of renewable energy. In order to push materials toward maximal efficiency, a better understanding of the intrinsic limitations is essential. We cover our latest results on identifying and finding ways to overcome bottlenecks by modelling electrochemical processes at three regimes: 1. at the bulk, the calculated hole effective mass is unfavorably high and conductivity can be improved through doping and alloying, 2. at the surface, catalysis is slow and involves long-lived surface states, but the catalytic overpotential can be reduced by adding a doping gradient or overlayers without strain, and 3. at the back contact the losses can be improved by selecting a proper metal contact. We provide unique analysis approaches that reveal fundamental understanding of electrochemistry with hematite. Special emphasis will be made on our development of charge transport calculations through materials. These models have made an impact on understanding experimental observations and have influenced subsequent theoretical investigations.