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?

Simulating thermodynamic and kinetic properties of surface states for OER catalysis

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Hematite is a widely material as an anode for water splitting, but the role of interactions between neighboring reaction sites is unknown. By combining DFT and Metropolis Monte Carlo simulations, we uncovered the relation between neighboring sites and their effect of overall surface coverage. We created large slabs with multiple intermediates to account for near-neighbor interactions. Incorporating the newly found reaction energies and a strong interaction of $*OH_2$ and *OOH intermediates revealed the rate determining step.

Adding activation energies and kinetic barriers to a Kinetic Monte Carlo simulation gave more evidence for *OOH formation as the rate determining step. We also developed a novel method for calculating the reorganization energy. By using halogens as hydrogen “traps” and using the relation of reorganization and activation energies from Marcus Theory, we calculated reorganization energies for all reactions involving charge transfer. Combining the new method with KMC enabled current calculation and J-V curve simulation.