A Multiscale Modelling Approach to Elucidate the Mechanism of the Oxygen Evolution Reaction at the Hematite-Water Interface

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Photoelectrochemical (PEC) cells that produce hydrogen from water are highly relevant in transition to a clean energy economy. Hematite is a promising semiconductor for PEC cells due to its suitable band gap (2.1 eV), availability, stability and non-toxicity. The oxygen evolution reaction (OER) largely determines the energy efficiency in PEC cells. Computational modelling of OER, a multiscale modelling problem, can improve the efficiency of PEC cells by mechanistic insight which is unavailable from experiments[1]. We present a multiscale computational model of OER which connects the thermodynamics and kinetics of elementary charge transfer reactions in OER to kinetics of OER at laboratory length and time scales (Figure 1). We couple density functional theory (DFT) and DFT based molecular dynamics (DFT-MD) simulations with solvent effects at an atomistic level with kinetic Monte Carlo (kMC) simulations at a coarse-grained level in our multiscale model. The time and applied bias potential dependent surface coverage, which are experimentally not known, and the O_2 evolution rate during OER at the hematite-water interface are calculated by the multiscale model. Furthermore, the multiscale model demonstrates the effect of explicitly modelling the interaction of water with the electrode surface via direct adsorption.

References

[1] V. Sinha, A. Bieberle-Hütter *et al.*, Reaction Mechanisms in Catalysis: Faraday discussion, April 2020. https://doi.org/10.1039/C9FD00140A

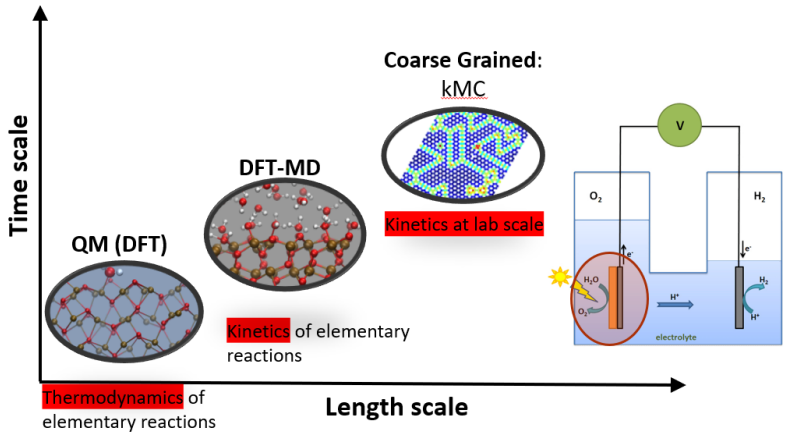

Figure 1. Multiscale model for Oxygen evolution Reaction at hematite (photo)anode.

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