

On the Computational Optimization of Electrocatalysts

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While various approaches exist for the modelling of electrocatalytic reactions, not so many univocal and effective guidelines for catalyst optimization are at hand. For example, it is widely accepted that the adsorption-energy scaling relation of $^*\text{OOH}$ vs $^*\text{OH}$ is responsible for the considerable overpotentials observed experimentally during the oxygen evolution reaction (OER) [1,2]. Hence, breaking such a scaling relation is supposedly crucial for the enhancement of OER electrocatalysts.

In this talk, I will test this hypothesis using literature data [3]. I will show that the breaking of that scaling relation is necessary but insufficient to optimize OER electrocatalysts. Simple and quantitative alternatives are the “delta-epsilon” optimization and the concept of “electrocatalytic symmetry”, which provide guidelines for the improvement of electrocatalysts for oxygen evolution and reduction [3,4,5].

Furthermore, I will show that the use of density functional theory introduces sizable errors in computational electrocatalysis models [6]. As the errors modify calculated equilibrium potentials, reaction energies, adsorption energies and volcano plots, it is generally advisable to incorporate corrections into materials screening routines for electrocatalysts [7,8].

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