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"Computational water splitting, where are we now and where to go?"
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# Electrochemical water splitting: state of the art

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The most widely used approach for the modelling of water splitting [1, 2] is based on the fact that the adsorption energies of the archetypal intermediates (*O, *OH, *OHH) on countless heterogeneous and homogeneous catalysts follow linear scaling relations [3]. In multistep electrocatalytic reactions such relations appreciably simplify the elaboration of computational electrocatalysis models but lower their degrees of freedom, which may impose limits to the optimization of electrocatalysts.

Of interest for water splitting is the common belief that the scaling relation of *OOH vs *OH causes a sizable intrinsic overpotential for water splitting [2, 4]. Thus, breaking such scaling relation is considered crucial for the enhancement of water splitting electrocatalysts.

In my talk, I will put this widespread notion to the test using data from the literature [5]. The results show that breaking the scaling relation of *OOH vs *OH is a necessary yet insufficient condition to optimize water splitting electrocatalysts. Alternatively, one can use delta-epsilon optimization, a swift and affordable approach that provides quantitative guidelines for the improvement of water splitting catalysts [6-8] and bifunctional catalysts [9].

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