Complementation of thermodynamic volcano analysis on oxygen evolution catalysts with a unifying approach: considering the symmetry of reaction steps and kinetics

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The oxygen evolution reaction (OER) is considered as an important bottleneck in the overall water-splitting reaction because of its sluggish kinetics. Computational studies using high-throughput screening on the OER catalysts have focused on the conventional volcano plots that solely rely on the thermodynamic overpotential and binding energies of reaction intermediates. In this study, the OER activities for candidates were evaluated by combining the overpotential-dependent volcano plots with electrochemical-symmetry index (ESSI) and a single experimental parameter that accounts for the kinetics, resulting in an ESSI-descriptor activity map. On the example of OER over transition metal oxides (TMOs) and their heterostructures on rutile TiO_2 (110) substrate, two different frameworks were intuitively compared to evaluate the catalytic activities. This unifying approach provides insights into the intrinsic properties of the heterostructure as well as materials that can be used to lower the overpotential of the OER.