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Beyond the Top of the Volcano? – A unified approach to electrocatalytic oxygen reduction and oxygen evolution.

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Abstract

We study the oxygen reduction (ORR) and the oxygen evolution reaction (OER) and based on previous obtained mechanistic insight we provide a unified general analysis of the two reactions simultaneously. The analysis shows that control over at least two independent binding energies is required to obtain a reversible perfect catalyst for both ORR and OER. Often only the reactivity of the surface is changed by changing from one material to another and all binding energies scale with the reactivity. We investigate the limitation in efficiency imposed by these linear scaling relations. This analysis gives rise to a double volcano for ORR and OER, with a region in between, forbidden by the scaling relations. The reversible perfect catalyst for both ORR and OER would fall into this "forbidden region". Previously, we have found that hydrogen acceptor functionality on oxide surfaces can improve the catalytic performance for OER beyond the limitations originating from the

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