Computational Screening of Rutile Oxide Heterostructures for Oxygen Evolution Reaction (OER)

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The oxygen evolution reaction (OER) plays a key role for the efficiency of the water splitting process while high overpotential is required. Many studies have been dedicated to lower the energy barrier of OER on transition metal oxides (TMOs), which are considered as promising candidates for OER electrocatalysts. The OER activity and electronic structure of conventional TMOs can be tuned by the strategic formation of heterostructure with another TMO. Accordingly, computational screening was conducted on a wide range of rutile-type transition metal dioxide films (MO_2) supported on another rutile-type MO_2 (1 1 0) substrate to investigate their OER efficiency by using density functional theory (DFT) calculations. In this work, the electrochemical-step symmetry index (ESSI) was employed for the exhaustive screening of the heterostructures for electrode materials in addition to the conventional volcano approach based on simple binding energies of reaction intermediates. The scaling results provide a valuable insight into the active candidate materials to lower the overpotential.