Tailoring the Activity for Oxygen Evolution Electrocatalysis on Rutile TiO2(110) by Transition-Metal Substitution - DTU Orbit (22/04/2019)

The oxygen evolution reaction (OER) on the rutile M-TiO2(110) (M = V, Nb, Ta, Cr, Mo, W, Mn, Fe, Ru, Ir, Ni) surfaces was investigated by using density functional theory calculations. The stability of different doped TiO2 systems was analyzed. The scaling relationship between the binding energies of OER intermediates (HOO* versus HO*) is found to follow essentially the same trend as for undoped oxides. Our theoretical analysis shows a lower overpotential associated with OER on the doped M-TiO2(110) than on the undoped TiO2(110). The theoretical activity of Cr-, Mo-, Mn-, and Ir-doped TiO2 is found to be close to that of RuO2(110) for some of the configurations in consideration.

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