Electrochemical chlorine evolution at rutile oxide (110) surfaces

Based on density functional theory (DFT) calculations we study the electrochemical chlorine evolution reaction on rutile (110) oxide surfaces. First we construct the Pourbaix surface diagram for IrO$_2$ and RuO$_2$, and from this we find the chlorine evolution reaction intermediates and identify the lowest overpotential at which all elementary reaction steps in the chlorine evolution reaction are downhill in free energy. This condition is then used as a measure for catalytic activity. Linear scaling relations between the binding energies of the intermediates and the oxygen binding energies at cus-sites are established for MO$_2$ (M being Ir, Ru, Pt, Ti). The linear relations form the basis for constructing a generalized surface phase diagram where two parameters, the potential and the binding energy of oxygen, are needed to determine the surface composition. We calculate the catalytic activity as function of the oxygen binding energy, giving rise to a Sabatier volcano. By combining the surface phase diagram and the volcano describing the catalytic activity, we find that the reaction mechanism differs depending on catalyst material. The flexibility in reaction path means that the chlorine evolution activity is high for a wide range of oxygen binding energies. We find that the required overpotential for chlorine evolution is lower than the overpotential necessary for oxygen evolution.

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