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The electrocatalytic properties of doped TiO₂ RASMUS KARLSSON, SUNCAT Center for Interface Science and Catalysis, SLAC and Dept. of Chemical Engineering, Stanford University, HEINE HANSEN, DTU Energy, DTU Technical University of Denmark, THOMAS BLIGAARD, SUNCAT Center for Interface Science and Catalysis, SLAC and Dept. of Chemical Engineering, Stanford University, ANN CORNELL, Applied Electrochemistry, School of Chemical Science and Engineering, KTH Royal Institute of Technology, LARS PETTERSSON, Dept. of Physics, AlbaNova University Center, Stockholm University — "Dimensionally stable anodes" (DSA), rutile oxide electrode coatings of 30% RuO₂ and 70% TiO₂, deposited on Ti substrates, have been used industrially for electrosynthesis of chlorine gas since the 1970s. Nevertheless, a fundamental understanding of the origin of their high activity and chlorine selectivity has been lacking. In this presentation, I will indicate how calculations using density functional theory and the computational hydrogen electrode have been used to model the electrocatalysis of both the oxygen evolution reaction (OER) and the chlorine evolution reaction (CIER) on surfaces with the typical DSA composition. Our calculations suggest a fundamental reason for the high CIER selectivity of Ru-doped TiO₂: Ru dopants activate nearby Ti surface sites, and create active sites with the optimal descriptor value for high CIER activity and selectivity. I will also present results from a broad screening study, where we examine the effects from doping TiO₂ with each of the fourth, fifth and sixth-row transition metals. We suggest several dopants that can activate TiO₂ for either the OER or the CIER, including dopants not previously tested experimentally.

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