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Cobalt, nickel/iron, and titanium oxide electrodes for water oxidation[1]

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Water splitting on metal oxide surfaces has attracted enormous interest for more than forty years. While a great deal of work has focused on titanium dioxide (TiO_2), recently cobalt and mixed Ni-Fe oxides have also emerged as promising electrocatalysts for water oxidation due to their low cost and high activity. In this talk I shall discuss various aspects of water oxidation on cobalt (hydro-)oxides, pure and mixed nickel and iron (hydro-)oxides, and TiO_2 surfaces. Using DFT+U calculations, I shall examine the composition and structure of cobalt and Ni-Fe oxides under electrochemical conditions, and present studies of the oxygen evolution reaction (OER) on the relevant stable compounds. I shall also present hybrid functional calculations of the first proton-coupled-electron transfer at the water/TiO_2 interface in the presence of a photoexcited hole. Our results provide evidence that the proton and electron transfers are not concerted but rather represent two sequential processes. They also suggest that the OER is faster at higher pH, as indeed observed experimentally.

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[2]Work in collaboration with Jia Chen and Ye-Fei Li.