New trends on Oxygen Evolution Reaction (OER)

Divanis S., Kutlusoy T. ,Boye I., Isabela C. Man, Rossmeisl J.

Introduction:

Electrochemical splitting of water is a key process for Hydrogen production. One of the ways that this conversion can be achieved is by electrolysis using a potential difference obtained from a photovoltaic cell or from a wind turbine. In both cases effective catalysis for water oxidation to molecular oxygen , that is the oxygen evolution reaction (OER) is needed. The OER is the main drawback at the overall procedure , because of the high overpotential needed in order to evolve the oxygen at the anode electrode.

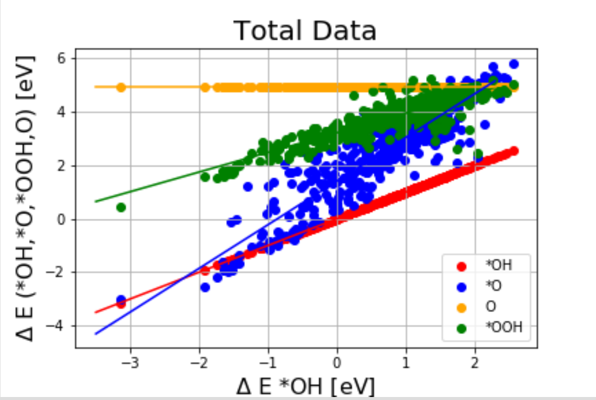


Fig.1: All the available DFT calculation data for the OER intermediates binding energies, obtained from various works, from 2011 until today.

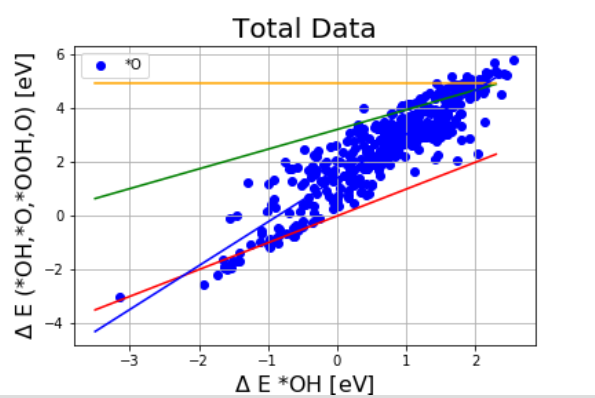


Fig.2:The binding of the atomic oxygen on the anode catalyst is the step that most of the times creates the overpotential for the evolution of the molecular oxygen.

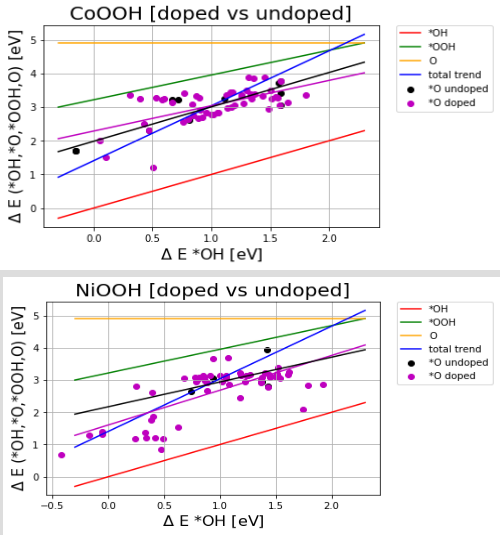
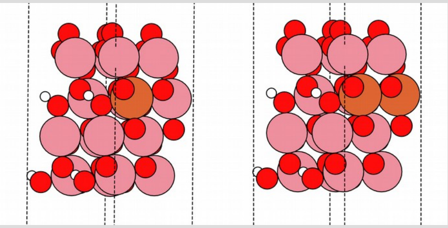


Fig.3:The different slope of the atomic oxygen adsorption trend from the total data trend, possibly indicates a different way of binding the oxygen on the surface.



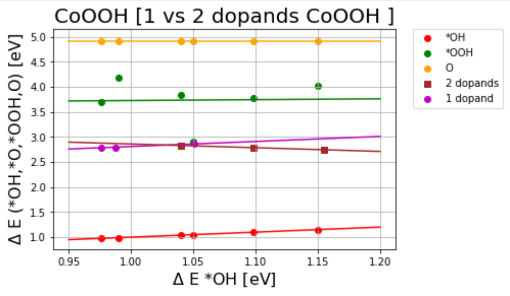


Fig.4:The effect of light and heavy doping does not affect the binding energy of the atomic oxygen when the metal oxide surface lacks a band gap.

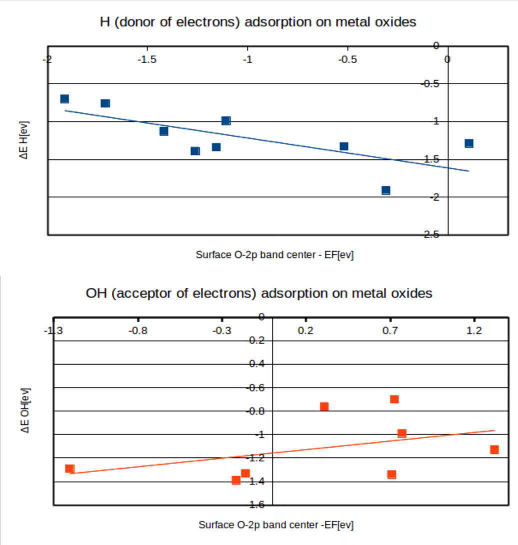


Fig.5:Adsorption of electron donors (H) and electron acceptors (OH) on different metal oxides respectively.

Conclusions

The gathering of all the available data from DFT calculations, for the OER revealed that the adsorption of the atomic oxygen is mainly the problem for the overall procedure since the data points have a big aberration from the trend, also it is obvious that there is a big overlap of data points, meaning that a lot of different works have actually produced the same results. Some metal oxides like NiOOH and CoOOH have a different adsorbing trend for the atomic oxygen. Adsorbing donors and acceptors of electrons on various metal oxides are creating trends with negative and positive slope respectively when they are drawn against a surface O-2p band center.

References:
Man, I. C. et al. ChemCatChem, 3: 1159-1165
Thomas Østergaard et al. J. Phys. Chem. **C 2018**, 122, 10442–10449,
Castelli et al. J. Phys. Chem. C , **2017**, 121, 18608-18614