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FAKULTÄT FÜR CHEMIE

Einladung zum Vortrag von

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Structural Transformations Leading to the Oxygen Evolution Active Phase for Fe Containing Layered Double Hydroxides

NiFe based (oxy)hydroxides are among the most active electrocatalysts for the oxygen evolution reaction (OER) in alkaline electrolytes. Their crystal structure, known as layered double hydroxide (LDH), is composed of layers of edge sharing metal oxygen octahedra that are intercalated with water molecules and charge balancing anions. While Fe-free $Ni(OH)_2$ catalysts show low OER activity, the incorporation of Fe^{3+} ions in $Ni(OH)_2$ layers is responsible for a dramatic activity enhancement. Similarly, incorporation of Fe^{3+} into $Co(OH)_2$ leads to CoFe LDH, which has also superior OER activity respect to Fe-free $Co(OH)_2$. Oxidative deprotonation and possibly the electrocatalytic OER reaction lead to reversible structural changes that are only observable with *in operando* or *in situ* methods. Despite several structural and electronic features were reported to change from the catalytically silent to the active state, key aspects of the catalytically active site remain elusive and more investigations are necessary. Theoretical predictions based on density functional theory (DFT) can guide this process, however so far different atomic models have been used in DFT calculations due the lack of clear structural information concerning the crystalline phase of Fe containing LDHs under OER active conditions.
In this contribution our results obtained using *in operando* wide angle X-ray scattering (WAXS) and X-ray absorption spectroscopy on crystalline NiFe and CoFe LDH nanostructured catalysts will be presented. We identified the structure of the active catalyst state and observed that the lattice spacing contracts under operating conditions to a similar value for both catalysts. The results extracted from *operando* WAXS measurements are in agreement with our DFT calculations, which could further unravel how the OER mechanism proceeds on these catalysts.

Dienstag, 26. März 2019, 15:00 Uhr
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