Hydrogen Evolution Reaction on Ni-based catalysts: From extended to nanoscale surfaces

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Hydrogen production via alkaline water electrolysis stands as a promising avenue in the pursuit of scalable solutions for renewable energy storage and conversion. To achieve this, the development of non-precious metal-based electrocatalysts with low overpotential is imperative, aiming to reduce the overall cost of electrolysis devices. Despite the longstanding exploration of nickel-based electrocatalysts spanning nearly a century, the understanding of their performance in both the cathodic hydrogen evolution reaction (HER) and anodic oxygen evolution reaction (OER) is still proving challenging in the present day. This is reflected in the diverse range of reported overpotential values and Tafel slopes, indicative of catalytic activity and reaction mechanisms, respectively, across the literature. This diversity underscores the complexity inherent in nickel-based catalytic surfaces, alongside discernible gaps in comprehending the plethora of processes occurring on Ni electrodes contingent upon applied potential.

In this presentation, we delve into elucidating the influence of chemisorbed species, both non-covalently and covalently bound, alongside thicker passive films and their morphological attributes at the electrochemical interface on the rate of HER across well-defined Ni-based extended surfaces, employing a combination of experimental and computational methodologies. Subsequently, we embark on a comparative analysis of these surfaces vis-à-vis Ni, NiO, $Ni(OH)_2$, among others, synthesized in-house, alongside commercially available benchmark Ni nanomaterials, delineating their shared traits and distinguishing characteristics.

Finally, we introduce a novel modified Ni nanocatalyst tailored for HER, evaluating its performance under real-world electrolysis conditions. Through this multifaceted investigation, we aim to not only enhance the fundamental understanding of nickel-based electrocatalysts but also open potential avenues for the design and implementation of more efficient and economically viable alkaline water electrolysis systems for sustainable hydrogen production.