FLAIR Colloquium

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Room R77, Building L2|01

Role of Oxophilicity in the Performance of Transition Metal Based Electrocatalysts for the Alkaline Hydrogen Evolution Reaction

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Abstract

Oxophilicity plays a significant role in the performance of catalysts for the hydrogen evolution reaction (HER) by influencing the adsorption and activation processes of water molecules on the catalyst's surface. This property refers to the affinity of a catalyst's surface for oxygen-containing species, which can significantly impact the catalytic activity and stability, particularly in the alkaline HER since the water adsorption/dissociation often limits the reaction rate. For instance it has been observed that the HER kinetics over Pt(111) under alkaline conditions is drastically enhanced by the presence of oxophilic groups, such as Pt-islands (defects) and $Ni(OH)_2$ on the catalyst surface[1], and it was associated with an easier H_2O dissociation.

In this sense, we have been recently studying the performance of oxophilic transition metal (TM)-based electrocatalysts for the alkaline HER, such as chalcogenides and nanostructured metal. By changing synthesis and operation conditions, the oxophilicity of these compounds can be modulated, which has a strong effect in their catalytic performance. In my talk, I will discuss the direct correlation between oxophilicity and catalytic activity for TM sulphides and the elucidation of reaction mechanisms that we have been elucidating based on operando spectroscopy supported by DFT calculations.[2] We find that the increase of oxophilicity does not only increase the degree of surface oxidation but also the stability of oxide species under strongly reducing condition of the HER, which we argue is the key for the observed high performance of oxophilic TM-based electrocatalysts.

References

[1] R. Subbaraman et al., Science, 2011, 334(6060), 1256–1260.

[2] Xingyu Ding et al., Nature Communications 15, 5336 (2024).