Promotion of electrocatalytic activity of oxygen evolution reaction via induced crystal lattice defects and porosity in Borophene/Ni2+

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Ir/Ru-based electrocatalysts have been extensively studied for the oxygen evolution reaction (OER). However, an anodic process requires a substantial overpotential to achieve a significant current becoming a bottleneck in the electrocatalytic water splitting. This inefficiency results in low oxygen production rates limiting the hydrogen generation by means of electrolyzers in industrial scale in respect to other routs. Therefore, the rational design and comprehensive characterization of promising electrocatalysts are crucial for the advancing of energy conversion technologies. Deep characterization under reaction conditions is necessary to uncover the chemical nature and activity descriptors of the OER mechanism, which, despite being ideally-studies, remains complex and enigmatic.

In this context, a novel approach to understanding the OER mechanism using a borophene-based catalyst supported by Ni(NO3)2 (U-Borophene+Ni(NO3)2) with induced lattice defects and porosity will be explored. The catalyst was synthesized via chemical intercalation, effectively exfoliating bulk boron into few-layered borophene. This material was then combined with Ni(NO3)2·6H2O and subjected to rapid dehydration, inducing crystal lattice defects and porosity.

A series of ex-situ techniques, including nitrogen adsorption/desorption, XPS, EPR and XRD were employed to characterize the catalyst. Electrochemical experiments confirmed that the U-Borophene+Ni(NO3)2 electrocatalyst possesses a tailored structure with active sites that facilitate both conventional OER and lattice oxygen ER. As a result, this catalyst demonstrates an overpotential of 169.56 mV at 10 mA/cm² and a low Tafel slope of 31 mV per decade in a 1M potassium hydroxide electrolyte, outperforming ruthenium oxide and other leading electrocatalysts. Thus, this study not only advances the development of effective borophene based OER catalysts by highlighting the crucial physicochemical features of efficient electrocatalysts but also contributes to a deeper understanding of the reaction mechanism.