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BIFUNCTIONAL IrO_X-DOPED NICKEL SELENIDE ELECTROCATALYSTS FOR THE HYDROGEN AND OXYGEN EVOLUTION REACTIONS

Resumo: The water electrolysis has been regarded as an excellent option for the production of green hydrogen. This process involves two half-reactions, the hydrogen and oxygen evolution reactions (HER and OER), that should be promoted by a catalyst for improving the energy conversion efficiency of the system. Different kinds of cost-effective and earth-abundant metal-based materials have been actively studied for applications on the electrocatalysis of the water electrolysis reactions, and among these, nickel selenide stands out advantageously as it features dual electrocatalytic activity for OER and HER, but its activity is found to be limited by the number of surface-active sites [1]. However, the doping of this electrocatalyst has been considered a potential approach to increase its number of active sites as well as to regulate its electronic structure to enhance its activity for the aforementioned reactions [2,3]. In this study, the electrocatalysis of the HER and OER were investigated in IrO_X-doped nickel selenide nanoparticles supported on carbon black, synthesized using a hydrothermal methodology with different contents of IrO_X (Ni:Ir atomic ratios of 2:0.1, 2:0.2, 2:0.4, and 2:0.8). The presence of IrO_X in the samples was clearly evidenced by EDS, while XRD showed the cubic $NiSe_2$ structure (PDF #89-7161) of the materials, but with the doped composites having the $NiSe_2$ diffraction peaks broadened and slightly shifted towards higher Bragg angles. This confirms the incorporation of IrO_X into the $NiSe_2$ lattice and the consequent reduction of nanoparticles crystallinity. Electrochemical active surface areas (ECSA) estimated by cyclic voltammetry indicated an increased number of actives sites in the IrO_X-doped $NiSe_2$, while linear sweep voltammograms (LSV) obtained in N_2-saturated 1 M KOH electrolyte demonstrated that the presence of dopant enhances the catalytic performance of $NiSe_2$ for both, OER and HER. This effect is particularly pronounced for the OER and for the catalysts with 2:0.1 and 2:0.2 Ni:Ir atomic ratios. Tafel diagrams obtained from the LSV data allowed a quite clear understanding of either reaction mechanisms. From the results, it is concluded that IrO_X-doped $NiSe_2$ obtained by the hydrothermal method is a potential material to be used in alkaline electrolyzers, as catalysts of both, the hydrogen and oxygen evolution reactions.

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