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Investigation of the influence of calcination temperature on the production of iron and cobalt electrocatalysts derived from ZIF-67 and impacts on performance in OER

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The global demand for energy necessitates investment in the production of alternative energy sources to replace fossil fuels. Green hydrogen, produced from the water splitting via electrolysis, is one of the most promising candidates for this purpose. Two half-reactions are involved: the Hydrogen Evolution Reaction (HER) and the Oxygen Evolution Reaction (OER), with the latter being the main obstacle to the large-scale feasibility of water electrolysis (only about 4% of all H_2 produced worldwide is done via this synthesis route). Therefore, the use of electrocatalysts is necessary to make this reaction viable. Oxides derived form Zeolitic Imidazolate Frameworks-67 (ZIF-67) have shown good performance as electrocatalysts in the OER. In this context, this work proposes the synthesis of iron-modified ZIF-67 and its use as a template for the production of electrocatalysts, subsequently applied in the OER. To analyze the influence of calcination temperature on electrocatalytic activity, the oxides were obtained at temperature of 260, 350, and 500°C from the Fe-impregnated samples. According to the X-ray powder patterns, the formation of composites was observed for the three produced electrocatalysts: the ZIF-67/Fe(260) exhibits peaks corresponding to the ZIF-67 phase in addiction to iron cobaltite due to the occurrence of the process at a temperature lower than the degradation of ZIF-67; for ZIF-67/Fe(350), the formation of a cobalt-rich phase and an iron-rich phase (Co_3O_4 and $Fe_2Co_2O_4$, respectively) is noted; whereas for ZIF-67/Fe(500), the presence of three crystalline phases was observed: $Fe_2Co_2O_4$, Fe_3O_4, and Fe_2O_3. Characteristic bands of the formed materials can be observed in the infrared spectra. The working electrodes were prepared by drop-casting of the catalytic ink containing 5 mg of the electrocatalysts, 20 µL of Nafion (binder agent) and 500 µL of isopropyl alcohol onto a nickel foam (99% porosity) with an area of 1 cm^2. The electrocatalytic activity was measured via Linear Sweep Voltammetry (LSV), in which the overpotentials were: η_{10} = 298, 318, and 342 mV vs. RHE for ZIF-67/Fe(260), ZIF-67/Fe(350), and ZIF-67/Fe(500), respectively. This demonstrates that with increasing temperature, there is a loss in the efficiency of the electrocatalyst in the OER, with ZIF-67/Fe(260) being classified as ideal, but all samples produced in this work exhibit electrocatalytic activity superior to various materials highlighted in the literature.

Table 1. Values related to the OER performance to the electrocatalysts made in this work.

Electrocatalyst	η_{10} (mV vs. RHE)	η_{100} (mV vs. RHE)	Tafel Slope (mV dec^{-1})
ZIF-67/Fe(260)	298	364	61.43
ZIF-67/Fe(350)	318	419	72.26
ZIF-67/Fe(500)	342	464	95.65

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References

[1] A. S. César *et al*, Journal of Cleaner Production, **207**, 751-763 (2019).
[2] Q. Zhao *et al.*, Journal of Nanoparticle Research, **22**, 299 (2020).