

III REUNIÃO DO GRUPO DO CARBONO

LIVRO DE RESUMOS

26-27 MARÇO 2024 PORTO, PORTUGAL







FICHA TÉCNICA

TÍTULO

III Reunião do Grupo de Carbono

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EDIÇÃO

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DATA Março de 2024

ISBN (VERSÃO DIGITAL) 978 989 8124 43 2

CATALOGAÇÃO RECOMENDADA

III Reunião do Grupo de Carbono Faculdade de Engenharia da Universidade do Porto, Porto, Portugal (2024)

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Transition metal-doped CNT as bifunctional oxygen electrocatalysts

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The negative impacts of fossil fuels on our ecosystems and the growing global energy demand have accelerated the need to employ renewable sources-based technologies to generate electricity. Nowadays, the use of hydrogen as an energy vector is one of the hottest research topics towards achieving a sustainable future and one of the main strategies of the European Commission to achieve climate neutrality [1]. Therefore, hydrogen-based devices play a crucial part in this matter and are required to be optimized to ensure their industrial viability. Accordingly, the unitized regenerative fuel cell (URFC) presents itself as one of the most attractive alternatives to employ hydrogen as an energy vector. This device is comprised of a fuel cell and an electrolyzer, which allows the electrolysis of water to be carried out when the electrical energy production is higher than its demand and, inversely, reconverting the resulting reactants into water and electricity when the renewable energy production is unable to suppress the energy requirements. Nonetheless, the compartmentalization of the URFC into two different pairs of reactions leads to the need for bifunctional catalysts for each pair. The oxygen pair of reactions, oxygen reduction and evolution (ORR and OER, respectively), presents the most sluggish kinetics in comparison to the hydrogen pair and, consequently, requires more investigation. This drawback is usually surpassed by using noble metal electrocatalysts that are scarce and expensive. Therefore, the proper design of widely available and low-cost carbon electrocatalysts can be an interesting and important alternative to reduce the operational costs of the URFC. Moreover, the modification of the material's chemical properties by incorporating transition metals is crucial to enhance the electroactivity of the catalyst. Considering our previous investigations, the use of iron phthalocyanine (FePc) towards ORR and Ni or Co species towards OER has led to individually high electroactivities towards each reaction, whereas the simultaneous presence of FePc and Ni or Co on the same carbon support has led to remarkable bifunctional oxygen electrocatalytic performances [2, 3]. Therefore, the preparation of bimetallic- and trimetallic-doped carbon nanotubes (CNT) derived from FePc, cobalt nitrate, and/or nickel nitrate was studied towards the oxygen reactions. The bifunctionality features of the optimized electrocatalyst are among the best ever reported for carbon-based electrocatalysts and largely surpassed those of conventional noble metal-containing electrocatalysts, making it a good candidate for upscale testing in more industrially relevant applications.

Funding

This work was supported by BiCat4Energy, PTDC/EQU-EQU/1707/2020. This research was also funded by FCT/MCTES (PIDDAC): LSRE-LCM, UIDB/50020/2020 (DOI: 10.54499/UIDB/50020/2020) and UIDP/50020/2020 (DOI: 10.54499/UIDP/50020/2020); and ALICE, LA/P/0045/2020 (DOI: 10.54499/LA/P/0045/2020).

Acknowledgements

RSR acknowledges the FCT funding under Stimulus of Scientific Employment, Individual Support Call – 5th Edition, 2022.04079.CEECIND (DOI: 10.54499/2022.04079.CEECIND/CP1733/CT0006). RGM acknowledges the research grant from FCT (2020.06422.BD).

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