Green Hydrogen Production via Steam Reforming of Light Alcohols on Ni-Cu Based Catalysts

M. Natália D.S. Cordeiro[1], J.L.C. Fajín[1]

[1]*LAQV@REQUIMTE, Department of Chemistry and Biochemistry, Faculty of Sciences, University of Porto, P-4169-007 Porto, Portugal*

Email: ncordeir@fc.up.pt

Fuel Cells (FCs) efficiently convert fuel into electricity, making them a promising alternative to thermal engines, particularly in the transportation sector. To be environmentally friendly, FCs must use renewable fuels obtained through green processes [1].

Hydrogen, with its high energy-density-to-mass ratio, is the primary fuel for FCs and can be produced renewably through water electrolysis or the reforming of light alcohols derived from biomass [1].

In this communication, we move a step forward and present results of periodic Density Functional Theory (DFT) calculations that elucidate the complete reaction mechanism for the methanol steam reforming (MSR) on a cost-effective Ni-Cu catalyst. The most plausible routes for products formation were identified, specifically highlighting desirable CO_2 and H_2 formation while considering undesired by-products such as CO, coke, or CH_4 [2].

Our findings demonstrate that MSR primarily occurs on the Ni-Cu catalyst through methanol decomposition on the catalytic surface, followed by the water gas shift (WGS) reaction. The WGS reaction converts the CO generated from methanol decomposition into CO_2 and H_2. Direct formation of CO_2 from methanol is a minor route, occurring predominantly on specific combed surfaces within the catalyst. Furthermore, the presence of a bimetallic Ni-Cu alloy effectively suppresses the production of undesirable methane, CO, and coke.

These DFT results pave the way for a more comprehensive theoretical understanding of key MSR mechanisms and can contribute to the rational development of Ni-Cu-based catalysts for hydrogen production.

Acknowledgments

This work received financial support from FCT - Fundação para a Ciência e Tecnologia through funding for the project PTDC/QUI-QIN/30649/2017 (REALM). The authors would like to thank also the FCT support to LAQV-REQUIMTE (UID/QUI/50006/2020). JLCF thanks FCT for funding into framework of Norma Transitória - DL 57/2016/CP1346/0019).

---

[1] Fuel cells. U.S. Department of Energy; Office of Energy Efficiency & Renewable Energy, 2021.

[2] **J.L.C. Fajín, M. Natália D. S. Cordeiro, ACS Catalysis, 12, 512-526 (2022).**