



Energy Transition
RESEARCH & INNOVATION

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ETRI 2023

BOOK OF ABSTRACTS



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high hydrogenation capacity, producing the two active species $^*\text{CO}$ and $^*\text{CH}_x$, confirmed by DRIFTS analysis, in abundance and in an optimal proportion, favoring chain growth reactions.

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Abstract Title: Surface modification of copper electrodes for electrochemical CO_2 reduction

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Abstract: The aim of this project is to produce metallic copper (Cu) electrodes coated with the polymer polybenzimidazole (PBI) for use in Electrochemical reduction of CO_2 (ECO2RR). Following the chemical coordination of PBI on the Cu surface, we observed enhanced selectivity toward methane and ethylene as well as a decrease in the competitive hydrogen (H_2) evolution.

Keywords: CO_2 reduction, copper, surface modification, polybenzimidazole.

Introduction and Objectives: Copper (Cu) catalysts have shown the highest ability to produce hydrocarbons and alcohols such as ethylene and ethanol via Electrochemical Reduction of CO_2 (ECO2RR). However, the development of systems capable of converting CO_2 on an industrial scale into multicarbon compounds (C_2^+) employing electrocatalysts with high selectivity, stability, and Faradaic efficiency is still a long way off. One strategy in this approach is the covering of Cu electrodes with organic molecules. In general, the coating improves Faradaic efficiencies for C_2^+ products, reduces H_2 generation, and improves catalyst stability when compared to the respective electrodes without the coating. Therefore, the aim of this project is to produce metallic copper (Cu) electrodes coated with the polymer polybenzimidazole (PBI) for use in Electrochemical reduction of CO_2 (ECO2RR).

Methodology: The copper electrode is immersed in HNO_3 (5 M) solution for 5 minutes, washed with water, dried in air, and then, reacted in a DFM solution of polybenzimidazole (0,03 %) at 50 °C for 15 minutes. Then, the copper electrodes are placed in a closed vial for drying. The electrochemical experiments were performed in a homemade H-type cell equipped with three electrodes. The cathode and anode were separated by a Nafion membrane. A platinum mesh was used as counter electrode, and a Ag/AgCl as a reference electrode. All reported potentials were converted to the reversible hydrogen electrode (RHE) scale. All working potentials were controlled with a Autolab Potentiostat (PGSTAT30) under room temperature.

The working electrolyte was an aqueous 0.1 M KHCO_3 solution. Before every CO_2 reduction experiment, CO_2 was bubbled through the electrolyte for at least 45 min to obtain a CO_2 saturated solution. The Ohmic resistance was evaluated by electrochemical impedance spectroscopy (EIS) at Open circuit potential (OCP), and 85% Ohmic drop compensation was applied to all subsequent experiments. Electrolysis was performed at fixed potentials for 60 min, constantly purging the electrolyte with CO_2 at 10 mL/min for a stable pH and continuous CO_2 supply. A gas sample was taken during 10 min in a gas sampling bag (Tedlar). Four samples for each potential taken (average and standard deviation). The gas products from CO_2 reduction were analyzed using a Agilent 8860 GC system. The GC system was equipped with a FID, used to detect hydrocarbons, and a TCD for H_2 . The Faradic efficiencies (FE) were calculated by combining the electrochemical and GC data in using $\text{FE} = (F \times n_{e^-} \times \text{mol product} / \text{electrolysis charge})$, where F = Faraday constant and n_{e^-} = number of electrons necessary to generate each product.

Preliminary results: Copper-modified with PBI were characterized by Raman and nano-FTIR (s-SNOM) and the spectra have shown the characteristic bands of the PBI polymer. Scanning Electron Microscopy (SEM) revealed significant differences on the surface of the Cu electrode modified with PBI (CuPBI) in comparison with the pristine Cu. A homogeneous granular pattern was observed in the surface of CuPBI. S-SNOM experiments also revealed a homogeneous distribution of PBI over the surface of Cu. The Preliminary FE experiments revealed that H_2 production was lower in CuPBI vs. Cu, and the production of CH_4 and C_2H_4 was higher in CuPBI.

Preliminary conclusions: In summary, a methodology for producing copper electrodes coated with PBI was devised, and characterization results utilizing spectroscopic and microscopy techniques revealed that the copper surface was uniformly covered with PBI. According to the electrocatalysis results, Cu coated with PBI inhibited the H_2 evolution while favoring the generation of methane and ethylene. Our findings contribute to a deeper understanding of ECO_2RR activity and selectivity in PBI-modified Cu electrodes, and they demonstrate that coordination with functional molecules is a potential technique for developing selective, stable, scale-up catalysts.

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Abstract Title: Micractinium sp., mangroves, and biorefineries: A sustainable trio for third-generation ethanol

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