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ABSTRACT OF THE DOCTORAL THESIS

Modeling the catalytic reduction of CO_2 on CuNi systems

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The increase in carbon dioxide concentration in the atmosphere which has been observed over the past 150 years, is largely correlated with the gradual increase in global temperature, thus contributing to climate change. The issue of utilizing this large-scale waste is particularly important, especially in the era of constant technological development. Currently, the vast majority of energy is obtained from fossil fuels, which leads to increased CO_2 emissions.

Both the technology for effectively reducing emissions through selective adsorption and the chemical reduction of CO_2 into valuable products are already known but not widely implemented. Challenges related to this issue include the high thermodynamic stability of CO_2 molecule, requiring significant energy input for conversion, as well as the need for highly active catalysts, often resulting in high costs of the process.

This doctoral thesis addresses research issues related to carbon dioxide reduction on selected copper-nickel materials, aiming to obtain high-value chemical compounds with the potential to be used as energy carriers. The work describes the electrocatalytic conversion of CO_2 on Cu/Ni surfaces, with pure Cu surfaces taken as a reference. Additionally, the possibility of electroreduction of CO_2 to HCOOH or CO on 13-atom CuNi nanoclusters was analyzed. Finally, a modification of the Cu/ZnO system, known for its hydrogenating properties in methanol synthesis, was proposed by adding Ni to the active phase.

The research conducted for this thesis is exploratory and employs computational chemistry techniques to determine reaction mechanisms and factors influencing process efficiency. The focus was mainly on modifying the properties of the copper phase by the presence of nickel, allowing for the determination of the synergistic effect of both metals, as well as their promotional or co-catalytic nature.