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Screening Using Artificial Neural Network of Additives for Cu-Zn Oxide Catalyst for Methanol Synthesis from Syngas

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The activity of Cu-Zn oxide catalysts for methanol synthesis from syngas varies depending on the additives to the oxide, and optimum composition is sensitive to the reaction conditions. An artificial neural network (ANN) was applied to identify the most effective additives based on the experimental results already reported. The physicochemical characters of element X, such as ionic radii and ionization energy, and the activity of Cu-Zn-X oxide catalyst were correlated using the ANN. Twenty-two types of X were supplied for the training of the ANN, and 29 activities of Cu-Zn-X, the X of which was not included in the training data, were predicted. Beryllium was predicted as the most effective additive, which was verified experimentally.

Keywords: [Methanol synthesis](#), [Neural network](#), [Physicochemical property](#), [Copper zinc catalyst](#)

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