Activity Descriptors for CO2 Electroreduction to Methane on Transition-Metal Catalysts - DTU Orbit (16/05/2019)

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The electrochemical reduction of CO2 into hydrocarbons and alcohols would allow renewable energy sources to be converted into fuels and chemicals. However, no electrode catalysts have been developed that can perform this transformation with a low overpotential at reasonable current densities. In this work, we compare trends in binding energies for the intermediates in CO2 electrochemical reduction and present an activity "volcano" based on this analysis. This analysis describes the experimentally observed variations in transition-metal catalysts, including why copper is the best-known metal electrocatalyst. The protonation of adsorbed CO is singled out as the most important step dictating the overpotential. New strategies are presented for the discovery of catalysts that can operate with a reduced overpotential.

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