# Computational Design of Electrocatalyst for High-Temperature Co-Electrolysis in Solid Oxide Electrolyser Cells

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High-temperature co-electrolysis of steam and CO2 mixture has been proposed as an alternative route for producing syngas and reducing the atmospheric CO2 concentration. The technology is highly promising because of its high selectivity and conversion efficiency toward the products. In addition, the produced syngas can also be further converted into very useful synthetic fuels. In this study, we investigated both electrochemical reaction and thermochemical reaction on a variety of transition metals to evaluate their ability to increase the activity of the conventional Ni catalysts used in the fuel electrode of solid oxide electrolyzer cells. We theoretically identified that the adsorption energies of O and H are the key descriptors of co-electrolysis of steam and carbon dioxide. We then performed microkinetic analysis to derive volcano plots to predict the activity of co-electrolysis on various transition metals. We could successfully suggest good candidates of Ni-based bimetallic alloy catalysts with excellent activities in the co-electrolysis. Our result will provide great insight to improve the high-temperature co-electrolysis system.