

On The Activity and Selectivity of Syngas Conversion Processes

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Syngas, a mixture of CO, CO₂, and H₂, can be converted to bulk chemicals like methanol and transportation fuels like higher hydrocarbons or higher alcohols. Typically syngas is produced by steam reforming of natural gas, but other feedstocks like biomass can be used as well representing an interesting route to sustainable fuels. We investigate the catalytic conversion of syngas to methane and methanol on transition-metal surfaces using density functional theory (DFT) calculations.

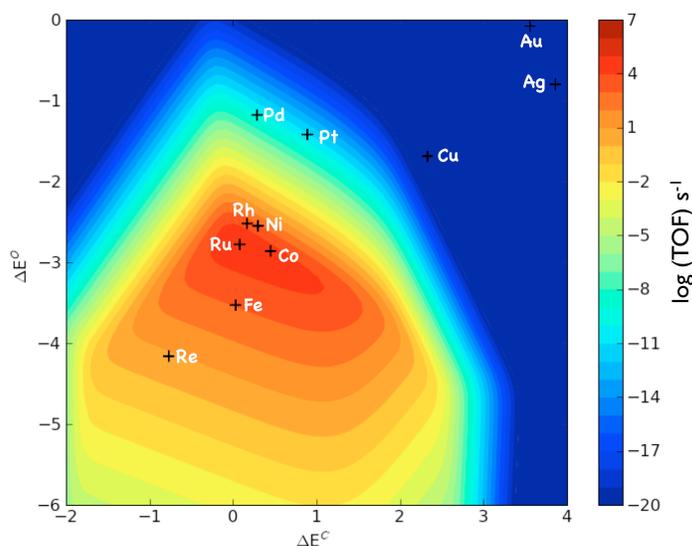


Figure 1. Theoretical volcano for the production of methane from syngas. The turnover frequency is plotted as a function of carbon and oxygen binding energies. Binding energies for the stepped 211 surfaces of selected transition metals are depicted. Reaction conditions are: 573 K, 40 bar H₂, 40 bar CO.

Based on scaling relations of adsorption energies [1] and transition-states [2] on transition-metal surfaces we were able to describe both, methane and methanol formation in terms of the carbon and oxygen binding energy of the transition-metal in question. The combination of these scaling relations with a microkinetic model leads to activity volcanoes for methane (see figure 1) and methanol formation as a function of carbon and oxygen binding energies [3, 4]. Having established volcanoes for the activity of these two competing reactions allows for the determination of the parent selectivity. Importantly, to map out the activity and selectivity as a function of only two parameters allows for fast computational screening for new leads of improved catalysts for syngas conversion processes.

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