

On the effect of coverage-dependent adsorbate-adsorbate interactions for CO methanation on transition metal surfaces - DTU Orbit (09/11/2017)

On the effect of coverage-dependent adsorbate-adsorbate interactions for CO methanation on transition metal surfaces

Heterogeneously catalyzed reactions involving the dissociation of strongly bonded molecules typically need quite reactive catalysts with high coverages of intermediate molecules. Methanation of carbon monoxide is one example, where CO dissociation has been reported to take place on step sites with a high coverage of CO. At these high coverages, reaction intermediates experience interaction effects that typically reduce their adsorption energies. Herein, the effect of these interactions on the activities of transition metals for CO methanation is investigated. For transition metals that have low coverages of reactants, the effect is minimal. But for materials with high coverages under reaction conditions, rates can change by several orders of magnitude. Nevertheless, the position of the maximum of the activity volcano does not shift significantly, and the rates at the maximum are only slightly perturbed by adsorbate-adsorbate interactions. In order to accurately describe selectivities, however, adsorbate-adsorbate interactions will likely need to be included.

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