

# Hydrogen Adsorption on Pd Surfaces and Its Effect on CO<sub>2</sub> Activation

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An accurate description of the surface of Pd-based catalysts under reaction conditions is a critical step toward a deeper understanding of catalyst reactivity. Herein, by modeling the phase diagram of the (111) and (100) surfaces of face-centered cubic Pd via ab initio atomistic thermodynamics, we predict the stable hydrogen coverages for a wide range of temperatures and H<sub>2</sub> pressures. The hydrogen coverage at the experimental conditions used for CO<sub>2</sub> hydrogenation plays a major role in the reactivity, as it hinders the chemisorption of activated CO<sub>2</sub>. The calculated data will serve as basis for subsequent subgroup-discovery analysis on CO<sub>2</sub> activation.

## Poster title

Poster

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