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Hydrogen Adsorption on Pd Surfaces and Its Effect on CO2 Activation

Monday, 11 April 2022 19:00 (1h 30m)

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 H2 pressures. The hydrogen coverage at the experimental conditions used for CO2 hydrogenation plays a major role in the reactivity, as it hinders the chemisorption of activated CO2. The calculated data will serve as basis for subsequent subgroup-discovery analysis on CO2 activation.

Poster title

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