FOXSI
Functional Oxide Surfaces and Interfaces

EINLADUNG

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von

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From benchmarks to biomass:
Transformations of hydrocarbons over metals from first principles calculations

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Abstract:

We present results for reactions of hydrocarbon molecules on transition metal surfaces. For the transformation of ethylene to ethylidyne, kinetic Monte-Carlo simulations, based on DFT results alone, allowed to identify the rate-limiting steps on Pd(111) and Pt(111). With that expertise at hand, we turned to the ring opening of methylcyclopentane, a model for understanding Diesel fuel upgrading, aiming at size effects of supported metal nano particles. Finally we illustrate the conversion of biomass derived oxygenates in aqueous medium, on the example of the model system propanol over Pt. We addressed the reforming pathway, yielding H_2 and CO_2, as well as the formation of homologue alkanes (propane).

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