

Transition states of NH, CH and OH bond activation

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Transition states of NH, CH and OH bond activation

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Based on computational studies of stepped and non-stepped transition metal surfaces the reaction paths and energetics of ammonia, methane and water activation have been studied. Clean surfaces as well as surfaces with coadsorbed oxygen have been studied. A coherent framework for the interpretation of activation-free energy relationships will be presented. Transition state energetics is mainly determined by variations in the interaction of reacting fragments in the transition state with the metal surface. For example ammonia dissociation on Pt is a specific case where transition state and final state conformation is very different. This has as a consequence that activation of ammonia on Pt is similar on different surfaces and independent of surface topology. For methane activation this appears to be quite different. Such differences in behaviour will be analysed on the basis of the underlying electronic factors that control the surface chemical bonds. Bronsted-Eyring-Polanyi proportionality constants in the corresponding activation-free energy relationship relate to the relative energy of (sometimes transient) reaction fragments. Knowledge of the transition state structures in combination with an understanding of the chemical bonding features that determine site preference of reaction fragments provide a rational basis to analyse trends in activation energy as a function of metal composition as well as surface topology.

COLL 41

Modeling reactivity of metal catalysts

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Atomistic, density-functional based, simulations of surface processes can play an important role in the understanding of the factors determining surface chemical reactivity.

Insight gained in the study of simple model catalysts can extend to more complex and realistic situations.

Of particular potential importance is the possibility of using predictive atomistic simulations in order to identify reactivity indicators that encode in a simple approximate way this insight.