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Reactivity and Structural Dynamics of Catalysts

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Message from the Guest Editors

Dear Colleagues,

Transition-metal nanostructured catalysts typically operate under high pressure and high-temperature conditions, and these reactive environments may substantially influence their morphology and surface composition and change their reactivity. However, the current understanding of catalytic properties of these catalysts is generally based on simplified models with a static surface, where the structural dynamics of interfaces with liquid or gas is neglected and no account is taken for possible modification during the reaction. This serious drawback may prevent a reliable description of catalysts' reactivity that mainly depends on the configuration of the surface. Today, investigating the equilibrium structure of catalysts in a reactive environment is still barely studied and remains an extremely challenging task. In this Special Issue, we want to focus on the recent experimental and theoretical works dedicated to the description and the prediction of the reactivity and the structural dynamics of transition metal nanocatalysts under reactive environments.