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Catalysis Connected

Title
Theory-guided design and optimization of catalytic conversions of renewable feedstocks

Abstract
The transfer to sustainable energy and chemistry technologies is one of the key challenges for humanity in the 21st century. Catalysis plays a pivotal role in all chemical strategies towards novel more efficient and sustainable chemical conversion processes for the valorization of renewable feedstocks such as biomass and CO2. So far, most developments in catalysis have been largely based on trial-and-error approaches. The grand challenge in the field is to make a step towards the rational design of efficient catalysts for a given chemical reaction. To progress in this direction it is imperative to learn how catalysts promote chemical transformations and how their performance can be controlled. Over the last decade, computational chemistry has become one of the key components of catalysis research and has deserved a place in the catalysis toolbox next to common laboratory techniques such as FTIR, NMR or XRD [1]. State-of-the-art quantum chemical methodologies and, particularly, the density functional theory (DFT) methods have matured to the level that they can be nowadays routinely used not only to rationalize, but also to direct experimental catalysis studies. Accuracy is the corner stone of computational chemistry and it represents the key focus of this lecture. In this talk I will illustrate the problem of model definition in computational studies on industrially-relevant catalytic systems [2] and highlight the need for new operando modeling methods to adequately describe the catalytic processes. The discussion will be illustrated by representative examples from our recent research on heterogeneous catalysis for selective methane conversion [3] and reductive transformations of CO2 and biomass-derived substrates [4]. During this talk, I will touch upon possible implications of the selective agreements between reductionism-dominated theories and highly complex catalytic experiments. I will emphasize the necessity of establishing a balance between the reductionist and systems approaches and the development of new operando modeling approaches to studying complex multicomponent reactive systems and come closer to predictive models suitable for guiding the design of new and improved catalysts.

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MCEC Netherlands Center for Multiscale Catalytic Energy Conversion

Advanced Research Center Chemical Building Blocks Consortium

DCS Dutch Catalysis Society