FOXSI
Functional Oxide Surfaces and Interfaces

EINLADUNG

zum Vortrag
von

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What can computational catalysis do for you?
Catalyst structure, activity, stability and more

am

Mittwoch, 09. November 2016 um 16:00 Uhr

Technische Universität Wien, Hoftrakt
BD - Hoftrakt, Seminarraum BD 02, 2.OG
1060 Wien, Getreidemarkt 9

Abstract:

Catalyst design and kinetic modeling often start from molecular-scale hypotheses about the reaction mechanism, the structure of the active sites and the nature of the rate and selectivity determining steps. Computational catalysis has become a crucial tool to analyze such molecular-scale concepts and elucidate their electronic origin. In combination with characterization and experimental kinetic validation, insights gained from computational catalysis can be translated all the way to the industrial scale. This pas-de-deux between experiment and theory is becoming the new paradigm in catalyst design and kinetic modeling, both in academia and in industry.

In this presentation, I will illustrate how this approach can contribute to the different aspect of catalysis research, such as, the determination of the structure of the catalyst under reaction conditions, [1] discrimination of potential reaction mechanisms [2], and design of improved catalysts [3].

References

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[3] Tan, Chang, Borgna, Saeys, J. Catal., 280, 50 (2011)

FWF SFB F45 „Functional Oxide Surfaces and Interfaces (FOXSI)“
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