



Kyushu University
Institute for Materials Chemistry and Engineering

九州大学
先導物質化学研究所

24.09.2013

先導物質化学研究所講演会

Understanding the behavior of catalytic reactors: In situ probe techniques and multi-scale modeling

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Optimization of design and operation of catalytic reactors do not only require the understanding of the reaction paths on the catalysts surface and the mass and heat transport in the reactor but also the interactions of them. In addition, homogeneous and electrochemical reactions may occur as well. Therefore, a variety of methods have been developed recently to study these interactions in detail using in-situ probe techniques and multi-scale modeling. The presentation will discuss the potentials, challenges, and limitations of some of the recently developed methods. On the experimental side, the focus is on capillary and laser spectroscopy techniques to spatially resolve concentration profiles. On the modeling side, the focus is on the use of molecular computations for the simulation of technical reactors. Exemplarily, the catalytic conversion of light hydrocarbons from natural/bio gas and alcohols towards hydrogen, syngas, and olefins will be discussed.

References

- [1] Modeling and Simulation of Heterogeneous Catalytic Reactions: From the Molecular Process to the Technical System. O. Deutschmann (Ed.), Wiley-VCH, Weinheim, 2012.
- [2] M. Hettel, C. Diehm, B. Torkashvand, O. Deutschmann. Critical Evaluation of In-situ Probe Techniques for Catalytic Honeycomb Monoliths. Catalysis Today
<http://dx.doi.org/10.1016/j.cattod.2013.05.005>

日時： 2013年10月2日(水) 15:00～
場所： 九州大学筑紫キャンパス総理工第三講義室

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