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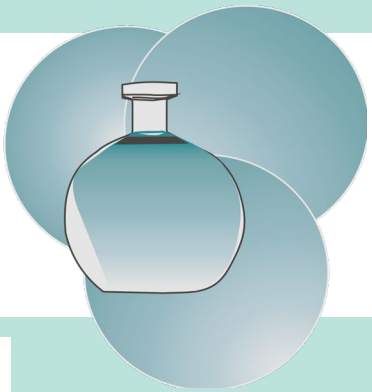

lädt ein

gemeinsam mit der Gesellschaft Deutscher Chemiker zum

GDCh
GESELLSCHAFT DEUTSCHER CHEMIKER

Vortrag

von Herrn

Prof. Raimund Horn

Hamburg University of Technology
Reacnostics GmbH

"Looking Into Catalytic Reactors at Work: Profile Measurements, Modeling & Operando Spectroscopy"

am: 11. April 2024

um: 16:00 Uhr

wo: im Raum 1/232

Die kleine Kaffeerunde vor dem Vortrag beginnt um 15:30 Uhr im Raum 1/232.
Das Mitbringen von eigenen Trinkgefäßen ist erwünscht.

Gäste sind herzlich willkommen!

TECHNISCHE UNIVERSITÄT
IN DER KULTURHAUPTSTADT EUROPAS
CHEMNITZ

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Fakultät für Naturwissenschaften

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Prof. Raimund Horn

Hamburg University of Technology
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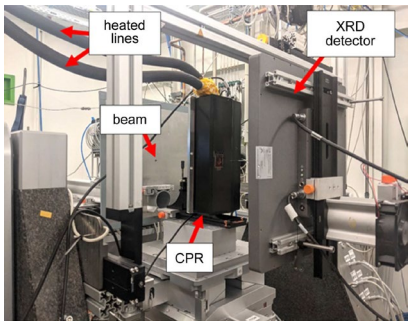
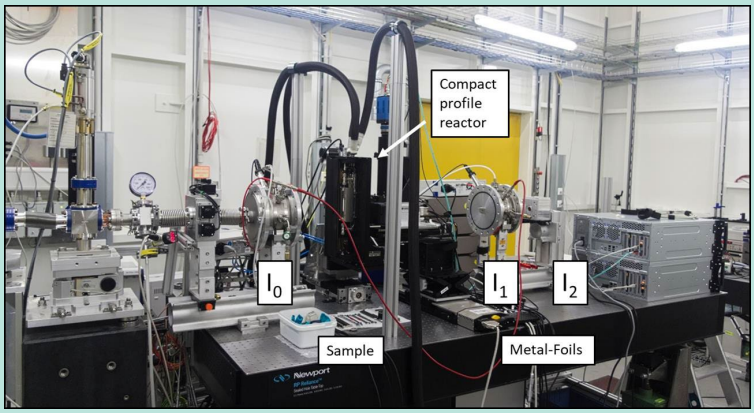
Looking Into Catalytic Reactors at Work: Profile Measurements, Modeling & Operando Spectroscopy

Heterogeneous catalytic reactors are the workhorses in chemical industry and play a prominent role in storage and conversion of renewable energy. Despite their rather simple mechanical design, these reactors show a complex behavior resulting from the interplay between linear transport processes, nonlinear reaction kinetics and dynamic changes of the catalyst inside the reactor. Our research work at the Institute of Chemical Reaction Engineering at TU Hamburg and at Reacnostics aims at understanding the dynamic behavior of catalysts, single porous catalyst pellets and catalytic reactors under industrial conditions. We develop novel experimental methods to “look inside” catalytic reactors and catalyst pellets at work and combine them with numerical simulations to improve catalysts and catalytic processes by knowledge instead of trial and error. In this talk I will give an overview of correlative concentration, temperature- and spectroscopic profiling in catalytic reactors and introduce the concept of iso-potential spectroscopy. It will be shown how spatial reactor profiling can be done for gas and liquid phase reactions in catalytic reactors and in single porous catalyst pellets and how kinetic models and model parameters can be quickly determined from the resulting profile data [1,2,3]. Results for spatially resolved XRD, XANES/EXAFS and Raman spectroscopy will be shown to illustrate how oxidation state and crystalline phase composition of a catalyst changes along the reactor coordinate due to gradients in chemical potential [1,4]. The novel concept of iso-potential spectroscopy [5] will be introduced to show how operando spectroscopy can be done quasi “inside” catalytic reactors of arbitrary size, viz. potentially also in industrial reactors. By means of isopotential DRIFTS spectroscopy it will be illustrated how profiles of surface adsorbates can be measured along a catalytic fixed bed reactor under reaction conditions aiding the development of microkinetic reaction models.





Experimental setups for correlative operando spectroscopy in a catalytic fixed-bed reactor. Left: X-Ray Diffraction (XRD). Right: X-Ray Absorption Spectroscopy (XAS).

[1] B. Wollak et al., J. Catal. 408 (2022) 372-387
[2] A. Aquino et al., Ind. Eng. Chem. Res. 62 (2023) 3098-3115
[3] B. Sosna et al., J. Catal. 381 (2020) 285-294
[4] B. Wollak et al., J. Synch. Rad. 30 (2023) 571-581
[5] R. Horn, Device and method for determination of a catalyst state in a chemical reactor, PCT/EP2020/079663

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