

Exploring guest dynamics in nanoporous host materials

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Diffusion is an omnipresent phenomenon in nature. In the world of molecules, it describes their irregular thermal motion. The interplay of diffusion and interaction of molecules with pore walls of nanoporous materials constitutes the benefit of using such materials in applications of separation and catalysis. The need for understanding the rate-limiting mechanisms, further optimization and development of new processes makes this topic subject of continued fundamental research [1].

The recently introduced techniques of microimaging by infrared (IR) and interference microscopy provide insights on molecular mass transfer, which are inaccessible via commonly used techniques [2]. Examples are the direct quantification of surface barriers, new aspects of multicomponent guest diffusion (including the detection of a reversal in the preferred diffusion pathways), imaging of guest-induced phase transitions in nanoporous materials and matching the results of diffusion studies under equilibrium and non-equilibrium conditions [1-3].

Recently, the potential of IR microimaging in characterizing chemical reactions was highlighted [4-5]. From the time evolution of the local concentration of reactant and product molecules, reaction rates and “effectiveness factors” (a key number for the efficiency of a catalyst in a given reaction) can be estimated [4]. Its determination was until now based on a series of experiments with purposefully varied catalyst particles and required additional assumptions. The “one-shot determination” of effectiveness factors by IR microimaging provides new options to overcome these limitations [5].

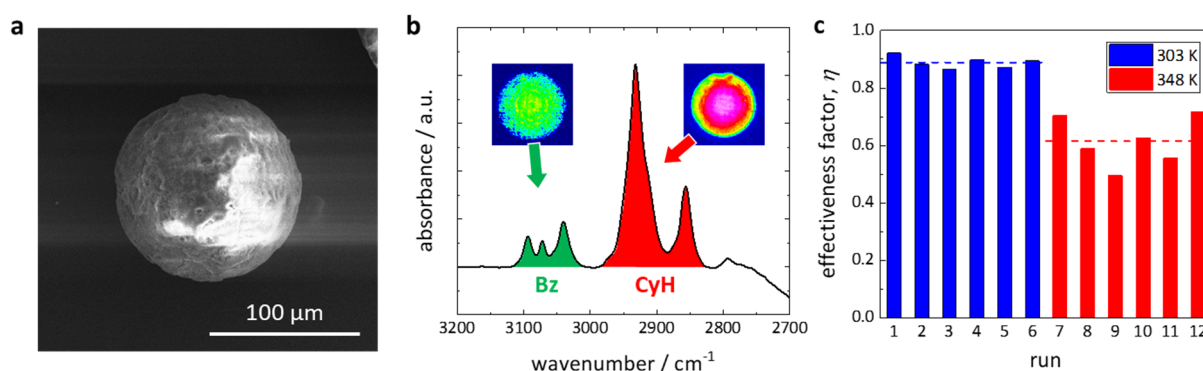


Figure 1: One-shot measurements of effectiveness factors of chemical conversion in porous catalysts. a) SEM-image of a representative catalyst particle and b) IR-spectrum showing the bands exploited for determining the concentrations of benzene (Bz, green) and cyclohexane (CyH, red). c) These concentrations were used to calculate the effectiveness factor of this reaction in different catalyst particles.

References

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Christian Chmelik got his PhD degree in 2008 at the Leipzig University in the group of Jörg Kärger on establishing IR microimaging as a new tool for diffusion measurements in nanoporous materials. He continued to work at the Faculty of Physics and Earth Science in the Department of Interface Physics as a Postdoc and headed the working group microscopy and recently moved to the office for study affairs.

His work is dedicated to the investigation of mass transfer in nanoporous materials by IR microscopy and IR micro-imaging. The interplay of host structure and transport properties was in the focus of his recent investigations, as well as new options to measure key quantities in chemical conversions in porous catalysts.

Dr. Chmelik is a member of the editorial board of the online journal “Diffusion Fundamentals” and co-chaired the “Diffusion Fundamentals III” conference in Athens, 2009 and the “Diffusion Fundamentals VI” conference in Dresden, 2015. Since 2015, he is also member of the structure-related commission “Spreading in Nature, Technology and Society” of the Saxonian Academy of Sciences. He co-authored more than 75 publications and has an h-index of 28.

