

Looking at heterogeneous liquid-phase catalysts at work – An ATR-IR approach

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- Inhalt* UHV studies on single crystals and model catalysts still represent an extremely valuable approach for gaining fundamental insight into the functioning of heterogeneous catalytic systems. However, particularly in the case of liquid phase reactions the interpretation of the data requires extrapolation to normal pressure and a new medium, which is often connected with great uncertainty. Due to the development of adequate spectroscopic techniques overcoming problems related to the presence of the solvent, studies of heterogeneous liquid-phase catalysts under working conditions are receiving increasing interest. Observation of processes *during* the catalytic event is of primary importance to better design the catalytic material and the environment in which it operates.
- Attenuated total reflection infrared spectroscopy (ATR-IRS) is a tool of choice to follow surface processes at solid-liquid interfaces and recent studies demonstrated its potential for catalytic applications.
- The complex reaction mechanism involved in alcohol oxidation over Pd/Al₂O₃ is chosen as an example of the use of this technique for the investigation of catalytic interfaces. Although the reaction is largely applied on the industrial scale, information on the catalytic processes at the real catalyst-liquid interface have been extrapolated from UHV studies. It will be shown how the reaction mechanism can be corroborated using ATR-IRS in combination with GC and online FTIR for simultaneous activity measurements. Monitoring the evolution of surface species and differentiating active metal sites for dehydrogenation and decarbonylation can be achieved *during* reaction. Moreover, important differences in the abundance of surface species in presence of bismuth reveal the likely origin of the promoter effect on Pd. Combination with other spectroscopic techniques such as XAS is also discussed.

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