catalysts

MDPI

Editorial

Spectroscopy in Catalysis

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Knowledge-based catalyst development is always an interaction between preparation, analysis and catalytic testing. Only if these three factors fit together can success be expected. For the analytic side of this triangle, spectroscopic methods play a crucial role. Whereas with diffraction, scattering and microscopy, decisive insights into the structure and morphology of the catalysts can be obtained, spectroscopy produces new knowledge about the chemical nature of the catalyst, e.g., its bonding and valence states.

Since the beginning of the century, operando, or in-situ, spectroscopy has played an increasing role in the analysis of catalysts [1,2]. This development makes it possible to "see catalysis in action" [3]. Whereas in-situ methods work under catalytic conditions, operando combines in-situ spectroscopy with catalytic activity [1], or, in other words, analytics and catalytic testing. Obviously, compromises must be made, because the ideal conditions for spectroscopic measurements with good signal/noise ratios do not fit with real catalytic conditions, comprising high pressure, high temperature and sometime aggressive compounds which could destroy the sensitive parts of the spectroscopic equipment. Starting several years ago, electrocatalysis and, herewith, investigations at the liquid/solid interface, have become more and more important [4–6]. This development is reflected in this Special Issue.

In their contribution, Kutin, Cox, Kubitz, Schnegg and Rüdiger presented a new spectroelectrochemical cell, which allows monitoring of the oxidation states and structural changes depending on the electrode potential of an electrodeposited cobalt/phosphate derivative, with promising properties for the water [7]. The applied technique, electron paramagnetic resonance (EPR), is extremely sensitive to oxidation state changes and is, therefore, a powerful tool for such electron transfer reactions [8].

Another promising field in catalysis, especially in photocatalysis, is the removal of pollutants from water [9]. Al-Kandari, Kasak, Abdullah et al. stressed out how important the evaluation of separation steps is to obtain accurate catalytic results and not to overestimate the activity of a catalyst [10]. Such considerations are important for the reproducibility and comparability of catalytic tests.

A major subject of this Special Issue is the investigation of the influence of the support on the catalytic system. It can be shown that the support is not an inactive material which holds the active center of the catalyst. In contrast, the support can play a vital role in the catalytic system. Lin, Zhang, He, Liu and Guo investigated defective ZSM-5 zeolite-supported Zn catalysts used for n-hexane transformation. [11] With operando FT-IR, the role of "hydroxyl-nest defects", consisting of four silanol as substitute for the usual [AlO_4] tetrahedron, can be elucidated. Zn grafted over such hydroxyl-nest defects shows a better dehydrogenative aromatization performance than Zn species over Si(OH)Al groups.

Redox active supports (e.g., TiO_2, CeO_2 and ZrO_2) are widely used in heterogeneous catalysis, and their beneficial effect on catalytic performance is known in many cases. [12] A review in this Special Issue by Wang, Jian and Wang summarize the latest developments in the application of in-situ/operando spectroscopy to metal catalysts with reducible metal oxides as supports. The strong

metal–support interaction leads to an encapsulation of the active center by the metal oxide and, as a result, to deactivation. In contrast, the electronic metal–support interaction, with charge transfer between a support and an active center, can have a beneficial effect on the performance, as is shown for several reactions, e.g., CO oxidation, the water-gas shift reaction, and CO_2 hydrogenation.

A further contribution by Bansmann, Abdel-Mageed, Behm et al. shows how suitable operando investigations can help to answer questions discussed controversially over a long period [13]. With in-situ/operando XANES (X-ray absorption near-edge spectroscopy) it was possible to obtain the Ce^{3+}/Ce^{4+} ratio at CeO_x-supported Au catalysts used in CO oxidation. Oxygen vacancies created in the pretreatment have only a weak effect on the activity because they are rapidly re-oxidized by the gas mixture. Thus, the influence of the support on the catalytic system could be clarified.

All the contributions in this Special Issue show how important spectroscopy is for the understanding of catalysts, which is the basis for the development of new effective catalysts or for the improvement of established systems. New opportunities for the understanding of catalysts are offered by computational modelling [14], which will give the analytical scientist the possibility or the challenge to design experiments with a much higher data volume, which must be machine-readable data. In such experiments, the accuracy of the data and the documentation and the reproducibility of the experiments are critical and must be taken into account with great care.

Conflicts of Interest: The authors declare no conflict of interest.

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