

# CORRELATING STRUCTURE AND REACTIVITY ON ENERGY MATERIALS BY IN SITU SPECTROSCOPY

C. Rameshan

*Institute of Materials Chemistry, TU Wien, Getreidemarkt 9, 1060 Vienna, Austria*

In heterogeneous catalysis surfaces decorated with uniformly dispersed, catalytically highly active particles are a key requirement for excellent performance. One of the main tasks in catalysis research is the continuous improvement or development of new catalytically active materials and the search for efficient catalyst synthesis routes.

Based on model catalysts we present different innovative approaches in catalyst design that allow precisely tuning the complexity of the surface structure. Furthermore, characterization under catalytically relevant reaction conditions (operando studies) with simultaneous gas analysis allows obtaining correlations between structure and reactivity.

Atomic layer deposition (ALD) can be utilized for controlled synthesis of catalysts with various surface structures (e.g. from small particles up to closed coatings) and the process can be easily scaled [1]. We present results on supported Pt model catalysts with different surface morphology and the resulting impact to catalytic reactivity.

Alternatively, an emerging concept in catalyst design is to selectively and reversibly tune and modify the surface chemistry by either electrochemical polarization or reductive treatment. Perovskite-type catalysts raise the opportunity to incorporate guest elements as dopants. Upon reduction (or in reducing reaction environment) these dopants emerge from the oxide lattice to form catalytically active clusters or nanoparticles on the surface (by exsolution). In consequence, this leads to a strong modification or enhancement of catalytic selectivity and activity.

Highlighted are studies for Pt/ZrO<sub>2</sub> model systems and different acceptor doped perovskite-type catalysts, which can be applied for CO<sub>2</sub> utilization via rWGS or dry reforming. We show a direct correlation of surface chemistry with catalytic activity, selectivity.

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## References

- [1] J. Lu, J.W. Elam, P.C. Stair, ACCOUNTS OF CHEMICAL RESEARCH, 46, (2013), 1806
- [2] V. Pramhaas, M. Roiaz, N. Bosio, M. Corva, C. Rameshan, E. Vesselli, H. Grönbeck, G. Rupprechter, ACS Catal. 2021, 11, 1, 208–214
- [3] L. Lindenthal, J. Popovic, R. Rameshan, J. Huber, F. Schrenk, T. Ruh, A. Nenning, S. Löffler, A.K. Opitz, C. Rameshan, Applied Catalysis B: Environmental, 292 (2021) 120183

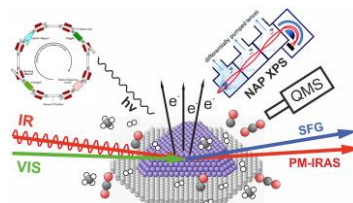


Fig. 1: Well-defined model catalysts were characterized in terms of structure, adsorbed molecules, and catalytic reactivity simultaneously.