

Tuning Catalyst's Performance via Optimizing Particle Size, Composition and Support: The Role of *in Situ* Techniques in Catalysis Studies

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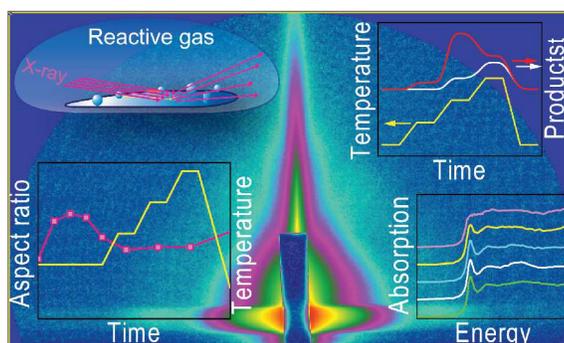
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The elucidation of the size, composition, shape, structure and function relationship, the effect of support along with the determination and control of the nature of the catalytic particles under reaction conditions are instrumental for addressing fundamental aspects of catalysis on the way to the design of new classes of catalysts. Highly uniform particles on technologically relevant supports are prerequisites for such studies, hand-in-hand with the characterization of the working catalyst under realistic reaction conditions.

Our experimental studies are based on 1) the use of technologically relevant oxide and carbon based supports, 2) size- selected cluster deposition with atomic precision control of cluster size as well as composition, 3) *ex situ* and *in situ* microscopies and 4) *in situ* synchrotron X-ray characterization of cluster size, shape and oxidation state under realistic working conditions, combined with mass spectroscopy analysis of the reaction products. The experimental studies are complemented with DFT calculations.

The first part of the lecture will focus on the understanding and optimization of catalyst function in oxidative reactions such as the dehydrogenation of propane or cyclohexane and cyclohexene and the selective partial oxidation of propylene on size-selected clusters and their assemblies.

As time shall allow, in the second part of the presentation the strongly size-dependent performance of sub-nanometer clusters in water splitting and Li-air batteries will be discussed.



References

- [1] S. Vajda, M. J. Pellin, J. P. Greeley, C. L. Marshall, L. A. Curtiss, G. A. Ballentine, J. W. Elam, S. Catillon-Mucherie, P. C. Redfern, F. Mehmood and P. Zapol, *Nat. Mater.*, 2009, 8, 213
- [2] Y. Lei, F. Mehmood, S. Lee, J. P. Greeley, B. Lee, S. Seifert, R. E. Winans, J. W. Elam, R. J. Meyer, P. C. Redfern, D. Teschner, R. Schlögl, M. J. Pellin, L. C. Curtiss, and S. Vajda, *Science*, 2010, 328, 224
- [3] L. M. Molina, S. Lee, K. Sell, G. Barcaro, A. Fortunelli, B. Lee, S. Seifert, R. E. Winans, J. W. Elam, M. J. Pellin, I. Barke, A. Kleibert, V. von Oeynhausen, Y. Lei, R. J. Meyer, J. A. Alonso, A. Fraile-Rodríguez, S. Giorgio, C. R. Henry, K.-H. Meiwes-Broer and S. Vajda, *Catal. Today* **160** (2011) 116
- [4] S. Lee, M. Di Vece, B. Lee, S. Seifert, R. E. Winans and S. Vajda, *Chem. Cat. Chem.* 4 (2012) 1632
- [5] G. Kwon, E. C. Tyo, C. Yin, G. A. Ferguson, J. DeBartolo, S. Seifert, R. E. Winans, A. J. Kropf, C. J. Heard, R. L. Johnston, J. P. Greeley, L. A. Curtiss, M. J. Pellin, and S. Vajda, *ACS Nano* 7, (2013) 5808