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### *Explore and push the limits for next-generation catalysts using fundamental understanding*

Venerdì 17 giugno, ore 15, Aula A "Nasini", via Marzolo, 1

Catalysis has gained strongly growing interest for both a clean and a sustainable future in society. Catalysis is the key technology for emission control to remove CO, NO<sub>x</sub>, hydrocarbons and volatile organic compounds (VOCs). Furthermore, electro- and thermal catalysis are the crucial tools to convert wind and solar power to fuels and chemicals. In emission control and power-to-X processes the reaction conditions are very dynamic and we face the challenge that the catalysts themselves are also very dynamic (see e.g. perspective article, ref. [1]). In many of these cases, noble metal catalysts are indispensable. For next-generation catalysts, the scarce and expensive noble metal loading needs to be decreased as much as possible by discovering and developing new materials in a knowledge-based way. Hence, the understanding of the most active sites is crucial. Finally, the stability needs to be addressed and, preferentially, catalysts are to be reactivated in situ during operation.



In this respect, operando spectroscopy has gained a lot of attention, unravelling the dynamic structural changes of catalysts, even in a time and spatially resolved manner [2,3]. Furthermore, the dynamics can be exploited to reactivate the catalysts or improving their activity. In this seminar, case studies from emission control (single sites, clusters, particles, [4,5]) and CO<sub>2</sub>-hydrogenation (methanation, Fischer-Tropsch reaction on Ni and Co-based catalysts, [2, 6-8]) will be presented to show the current status and future opportunities in these fields. Prototype examples are Pt/CeO<sub>2</sub> catalysts for emission control, Cu/ZnO for methanol synthesis and Ni-Fe/Al<sub>2</sub>O<sub>3</sub> for CO<sub>2</sub>-methanation. The examples highlight the importance of operando spectroscopy, the dynamics of catalysts and the potential of hard X-ray based techniques as powerful tool to bridge the gap between applied and industrially oriented environments, recently even using in situ and operando X-ray tomography [9].

- [1] K.F. Kalz, R. Kraehnert, M. Dvoyashkin, R. Dittmeyer, R. Gläser, U. Krewer, K. Reuter, J.-D. Grunwaldt, *ChemCatChem* 9, 17-29 (2017).
- [2] J.-D. Grunwaldt, J.B. Wagner, R.E. Dunin-Borkowski, *ChemCatChem* 5, 62-80 (2013).
- [3] J.-D. Grunwaldt, D.E. Doronkin, In situ and Operando Analysis of Heterogeneous Catalysts in Chemical Energy Conversion, in: R. Schlögl (Ed.) *Chemical Energy Storage*, Walter de Gruyter GmbH, Berlin/Boston, 2nd edition, p. 369 - 392 (2022).
- [4] A.M. Gänzler, M. Casapu, P. Vernoux, S. Loridant, F.J. Cadete Santos Aires, T. Epicier, B. Betz, R. Hoyer, J.-D. Grunwaldt, *Angew. Chem.Int. Ed.* 56, 13078-13082 (2017).
- [5] F. Maurer, J. Jelic, J. J. Wang, A. Gänzler, P. Dolcet, C. Wöll, Y. M. Wang, F. Studt, M. Casapu, J.-D. Grunwaldt, *Nature Catal.* 3, 824-833 (2020).
- [6] M. A. Serrer, M. Stehle, M. L. Schulte, H. Besser, W. Pflöging, E. Saraci, J.-D. Grunwaldt, *ChemCatChem* 13, 3010-3020 (2021).
- [7] M. Loewert, M. A. Serrer, T. Carambia, M. Stehle, A. Zimina, K. F. Kalz, H. Lichtenberg, E. Saraci, P. Pfeifer, J.-D. Grunwaldt., *React. Chem. Eng.* 5, 1071-1082 (2020).
- [8] L. Pandit, A. Boubnov, G. Behrendt, B. Mockenhaupt, C. Chowdhury, J. Jelic, A. L. Hansen, E. Saraci, E. J. Ras, M. Behrens, F. Studt, J.-D. Grunwaldt, *ChemCatChem* 13, 4120-4132 (2021).
- [9] J. Becher, D. F. Sanchez, D. E. Doronkin, D. Zengel, D. M. Meira, S. Pascarelli, J.-D. Grunwaldt, T. L. Sheppard, *Nature Catal.* 4, 46-53 (2021).

La presenza della S. V. sarà molto gradita.

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