Special Collection: Catalysts and Reactors under Dynamic Conditions for Energy Storage and Conversion

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Power-to-Chemical, power-to-fuels or power-to-gas are nowadays more than ever important cornerstones on the way to decarbonize the industry. The German Energy Transition ("Energiewende")[1,2,3] aims at decreasing the net emissions of CO_2 by 65% in 2030, 88% by 2040 and CO_2-neutrality in 2045.[4] Similar targets are set in Europe (CO_2-neutrality in 2050), and other countries around the globe.

Dominant sources of renewable electricity are wind and photovoltaic solar power. In contrast to fossil resources, the availability of both renewables fluctuates on time scales of minutes to days.[7] The necessity for a stable electricity grid posts new demands on rapid storage of large amounts of excessively generated energy – a completely new technological challenge since many ideas are still very new, immature and inefficient for application on the required technical scale. In addition, this opens new pathways to sustainable production of chemicals and brings together two areas that traditionally have only had few links: (1) solar and wind power including grids and (2) conversion to chemicals and fuels. In other words: physics, chemistry and engineering are combined to master the energy transition. At the core is catalysis which allows to transform the electrical energy and low-energy molecules such as water and CO_2 into high-energy reactive molecules: hydrogen, hydrocarbons and fuels. These conversions rely on electrocatalysis and (mainly) heterogeneous catalysis. Application areas in focus are water

electrolysis into hydrogen and oxygen as well as conversion of CO_2 into hydrocarbons, especially methane, methanol, and CO.

Up to now, technical catalysis in both electrochemical and conventional chemical processes has been conducted at steady-state operation. However, these processes need to be considered under dynamic conditions that better represent the availability fluctuations of renewable power. From a scientific point of view this is very attractive, since the mechanism of catalytic processes at the molecular level is mostly unknown under transient reaction conditions.[5,6,7] New methods have to be developed that allow describing the molecular processes theoretically, understand them by *operando* spectroscopic methods and develop appropriate and adaptive catalytic materials. Hence, it requires an interdisciplinary scientific approach, involving chemistry, theoretical approaches including quantum mechanics, spectroscopy including photon science, mathematics, reactor modelling, and machine learning. New materials as well as (electro-)catalytic processes have to be predicted and then developed using a knowledge-based materials design. While this approach is promising and attractive, it also poses a challenge to the next generation of scientists, who need a deep interdisciplinary knowledge in addition to their specialized skills in physics/chemistry/engineering. In fact, also a recent DFG Priority Program (SPP 2080) on “Catalysts and reactors under dynamic conditions for energy storage and conversion” focuses on this topic (for details, see website: <url href="https://www.spp2080.org">www.spp2080.org</url>).

The topical collection of “Catalysts and reactors under dynamic conditions for energy storage and conversion” aims at presenting the current state of research in these technologies, as well as the potential contribution of all scientific disciplines in the dynamic operation of catalytic energy conversion systems. A significant focus is given to the following advanced research approaches:

- *Operando* spectroscopy, using for instance synchrotron radiation for X-ray based and advanced photon-in-photon-out methods as well as vibrational spectroscopies,
- *In situ* and high-resolution electron microscopy and X-ray imaging
- Synthesis of novel catalysts
- Process and reactor design based on chemical engineering combined with physical chemistry
- Theory and kinetic modelling
- Digitalization in modern catalytic processes from research data management, *via* a digital twin of the experimental facility to machine learning, by using realistic inputs from data and experiments.

The importance of the data obtained from those advanced characterization and theoretical methods is the basis for a rational design of improved catalysts for the dynamic processes of renewable energy storage (Figure 1).

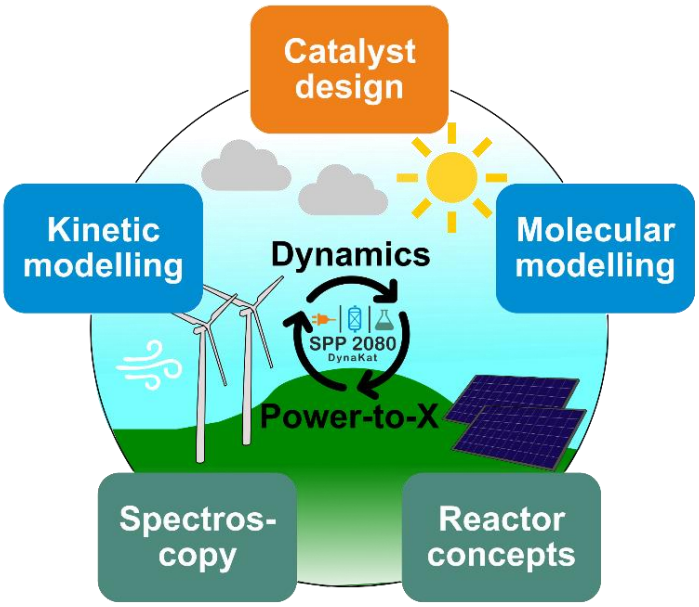

Figure 1. Knowledge-based rational design of (electro-)catalytic processes for the renewable energy storage applications, achieved by combining the contribution of different disciplines, with in-depth characterization and theoretical modelling of the systems under dynamic conditions.

In particular, this collection aims to connect practical engineering solutions with the fundamental approach of physical sciences and builds bridges between thermal and electrocatalysis. Catalysis stands at the core of 90% of all industrial processes, including the highly-relevant renewable energy storage ones. In order to make rational advancements in the field of energy storage, a deep understanding of the underlying physical processes involved in the catalysis of the process is crucial. Therefore, this special collection provides insight into the state-of-the art of conventional and novel methods for understanding the (electro-)catalytic systems under dynamic conditions. The fundamental studies based on physical methods have a major impact on the final design of the catalytic systems. Thus, a link between the application of these methods with deeper fundamental understanding will provide a valuable toolbox to scientists working in the field of catalysis in general and those who focus on energy storage in particular. This gives the basis for discussing future concepts for the energy transition strategy.

In this topical collection of *ChemCatChem* and *ChemElectroChem* on the dynamics of catalysts and reactors, international authors report on their recent progresses in overall 27 research articles. Among them, 21 publications cover the topic of thermal catalysis, while six deal with electrocatalysis. In both equally important fields, novel characterization, preparation, reactor design, simulation or molecular/kinetic modeling approaches were applied in order to further elaborate the Power-to-X concept in reactions such as Fischer-Tropsch synthesis or CO_2 methanation.

The newest developments were presented during EUROPACAT 2023, held from date to date in Prague (27.08.-01.09.23), in two sessions with 12 talks and many posters, all dedicated to catalysts and reactors under dynamic conditions for energy storage and conversion. Next

year, the discussion on this topic can be continued at the EUROPACAT 2025 (31.08.-05.09.25 in Trondheim, Norway).

DynaKat – It's catalysis' hour to efficiently use dynamic wind and solar power.

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