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CatLab: Hydrogen and Beyond - Thin-film Catalysts for Sustainable Chemistry with Renewable Electricity

Catalysis – a key enabler for a climate neutral society

The transformation of an economy based on fossil fuels into a climate-neutral economy requires a radical change of existing energy concepts. The expansion of renewable energy sources and smart grid technologies, as well as the development of a global trading and distribution system for renewable energy are urgently needed for a successful transition. A global economy driven by renewable energy will rely on sustainability in production, transport and trade of synthesized chemicals and fuels. These new technologies and processes should be integrated into the existing energy infrastructure to avoid high investment costs.

Green hydrogen and its energy-efficient conversion into base chemicals and synthetic fuels on a global industrial scale is regarded as a building block of sustainable energy systems. Sustainably produced hydrogen-based chemical energy carriers are critical for long-term storage solutions, crucial as enablers for the transformation of the mobility sector, and a core component of the defossilization of industrial processes, especially in energy-intensive industries. However, such a hydrogen economy can only be achieved with innovation leaps in synthesis chemistry for the required conversion processes.

Three main challenges for the realization of H_2-based CO_2-neutral energy systems and the utilization of renewable electricity as a primary energy source on a global scale entail:

(1) the production of green hydrogen on a global scale;
(2) long-distance transport and storage of hydrogen using synthetic energy carriers (ammonia, methanol, methane, LOHC);
(3) energy-efficient conversions into synthetic fuels and base chemicals.

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DOI-Nr.: 10.26125/rabf-vw12

In order to meet these three challenges, chemical conversion processes based on novel tailor-made (thermo-, electro- and photo-) catalysts on an industrial scale are necessary. This not only includes the splitting of water as the only permanently sustainable way to obtain hydrogen, but also comprises processes for (de)hydrogenation. The latter is necessary for storing and transporting hydrogen in large quantities and represents the core process for a closed energy cycle.

Reinventing Catalysis

All dehydrogenation reactions are endothermic and must therefore be catalyzed in order to achieve useful kinetic parameters and keep the additional losses to the stored energy as small as possible. Current technologies in catalysis are not optimally suited for this purpose, since the catalyst´s so-called active centers represent the coldest areas of the catalyst. As a result, the reaction deactivates itself, leading to reduced conversion rates and considerable further deactivation effects due to the separation of reaction products - and eventually to the blocking of the active centers. If hydrogen is to be used (or transported) in a particularly versatile way, a small number of platform molecules, such as methanol, ethanol, propanol and butanol, are of particular importance. They can be used advantageously both as intermediates in the chemical industry or as fuels. Unfortunately, their catalytic production beyond biotechnology has not been sufficiently successful to date, either because the yields are very small or because significant amounts of hydrogen are converted to methane, an undesirable reaction for energy storage. Both challenges can be tackled by improving the synthesis of the active phase in novel catalysts. Thin film systems on supports with different functionalities, which can be synthesized individually and selectively, promises a completely new target-oriented approach with unprecedented opportunities. Thanks to advances in thin-film technologies e.g. for the production of high-efficiency thin-film solar cells, we now also have the possibility of producing catalysts at low cost on technologically relevant large areas.

The new research platform *CatLab*, which is currently being established at the Berlin science location Adlershof, is pursuing such a completely new approach for innovative catalysts and will cover large parts of innovation chain. The *Helmholtz-Zentrum Berlin* (HZB) and two Max Planck institutes – the *Fritz Haber Institute* (FHI) and the Max *Planck Institute for Chemical*

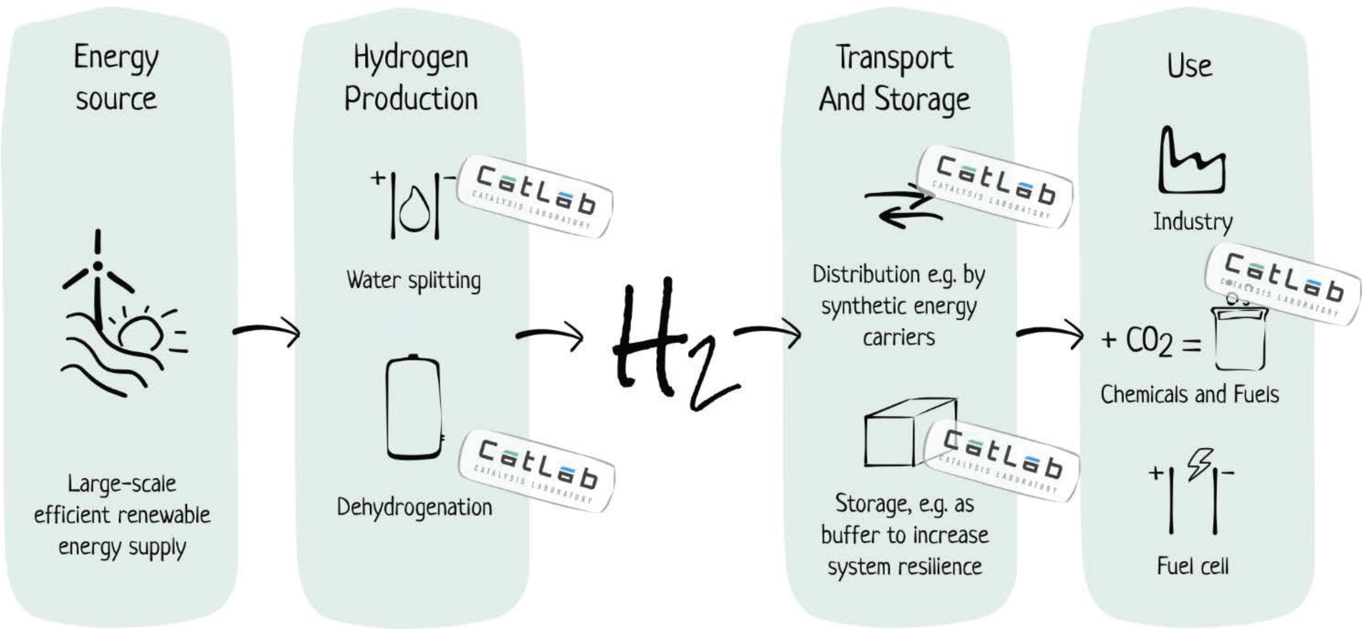

Fig. 1: Simplified illustration of the H_2 value chain and key areas of CatLab

Energy- Conversion (MPI CEC) – are combining their expertise in thin-film and nanotechnology as well as in catalysis to develop catalysts based on tailor-made functional thin films that can be specifically adapted as required for chemical reaction processes and scaled up to pre-industrial level. CatLab aims to reinvent catalysis and will serve as a bridge between fundamental research and industry. Synthesis and advanced analytical methods are coupled with new procedures for automated evaluation through machine learning to accelerate rational material design by means of digital catalysis. At the same time, disruptive concepts and technologies are scaled up for industrial application in collaboration with industrial companies.

The focal points of CatLab are the generation of green hydrogen and its selective conversion into easily transportable chemicals and synthetic fuels, such as various alcohols. Figure 1 depicts the links and high relevance of CatLab in a green hydrogen-based energy system (simplified representation).

With these unique selling points, CatLab also provides the strategic and structural framework for the long-term development of a new R&D area.

Key Ideas

The new knowledge-based approach of CatLab is based on a functional description of a catalyst by a support, a thermal stimulation layer, the active components as a layer and a mesoscopic structuring ("roughness") as building blocks. These are completely independent of the formation of chemical phases in almost any combination and can be assembled with each other in different and customized reaction processes. Subsequent steps in the activation of the active components (redox reactions; incorporation of light atoms such as atomic hydrogen, carbon, nitrogen, or oxygen) create a high density of catalytically active centers through the optimized adjustment of the structural dynamics of the active layer under catalytic reaction conditions. The introduction of the reaction energy by heating the corresponding layer with electricity from renewable energy and the contact with the reactants under optimized kinetic conditions in terms of pressure and mass transfer finally lead to a catalytic process characterized by:

(1) minimizing the volume to be stimulated,
(2) avoiding supercooling of the active centers on the catalyst through low-inertia energy supply and
(3) the possibility of using very reactive active phases that are very far away from thermodynamic equilibrium.

A Hub For Catalysis Research and Development (R&D)

CatLab is deeply embedded into the vibrant Berlin science ecosystem. Strategic partnerships with universities will contribute to strengthening an internationally renowned research hub. The unique constellation of the core partners HZB and MPG is poised to establish an international R&D network and drive catalysis R&D along the value chain. In particular, the involvement of industrial partners at an early phase of research and development allows CatLab to address industry-relevant processes and tremendously accelerate the innovation cycle. CatLab has a strong strategic partnership with BASF to design and establish chemical reactors and processes. In addition, the BasCat project between BASF, the TU Berlin and the Fritz-Haber-Institute provides direct access to industrial processes in which the functional interfaces of CatLab can be evaluated against current technologies.

Prof. Dr. Bernd Rech

Bernd Rech is Scientific Director of the Helmholtz-Zentrum Berlin für Materialien und Energie (HZB) and Professor in the Photovoltaics Department of the Faculty of Electrical Engineering and Computer Science at the Technische Universität Berlin.

photo credit: HZB/Phil Dera

He was head of the Institute Silicon Photovoltaics at HZB from 2006 to 2017. The focus of his research was on the development of both highly efficient and cost-effective thin-film silicon solar cells and new material combinations for the production of tandem solar cells. From 2008 to 2020, he was spokesman for the Helmholtz Association's Renewable Energies program. Bernd Rech and Robert Schlögl share Bavarian origins and enjoy thinking about and discussing science across disciplinary boundaries. This also gave rise to the joint idea for CatLab.

Bernd Rech also serves on numerous committees, such as the supervisory board of the Institute for Solar Energy Research in Hameln and the board of trustees of the Baden-Württemberg Center for Solar Energy and Hydrogen Research. Since 2017, he has been an elected member of the German Academy of Engineering Sciences (acatech). In 2018, he received the Apple of Inspiration, an award from the President of Slovenia.

Prof. Dr. Robert Schlögl

Robert Schlögl is Director at the Fritz Haber Institute of the Max Planck Society in Berlin as well as Founding Director at the Max Planck Institute for Chemical Energy Conversion in Mülheim a.d. Ruhr.

Robert Schlögl's research focuses primarily on the investigation of heterogeneous catalysts, with the aim to combine scientific with technical applicability as well as on the development of nanochemically-optimized materials for energy storage. The application of knowledge-based heterogeneous catalysis for large-scale chemical energy conversion summarizes his current research focus.

He is Vice-President of the National Academy Leopoldina as well as an Honorary Professor at Technical University Berlin, at Humboldt University Berlin, at University Duisburg-Essen, at Ruhr University Bochum as well as a Distinguished Affiliated Professor at TU Munich and an Honorary Professor of Boreskov Institute of Catalysis. He is member at acatech and BBAW and other numerous international organizations, received numerous national and international awards as well as is partner in numerous European and international joint projects.

He is Author/co-author of more than 1200 publications, more than 550 presentations and invited talks as well as inventor of more than 20 patent families.