

Editorial



NCCR

Catalysis

Sustainable production of chemicals



Dear reader,

In this special issue of CHIMIA, we are pleased to introduce our program, the National Center of Competence in Research, **NCCR Catalysis** (nccr-catalysis.ch). Funded by the Swiss National Science Foundation (SNSF), our home institutions ETH Zurich and EPFL, and other contributions, our goal is to identify and develop sustainable routes for manufacturing chemicals from renewable platforms across the value chain. Our team brings together top scientists with diverse expertise combining advanced approaches in chemistry with modern tools like digitalization to accelerate the discovery, understanding, and implementation of novel catalysts and processes. Since launching in August 2020, our consortium has grown to 47 Principal Investigators across 13 institutions, with over 200 members. This issue collects selected collaborative projects from our portfolio that illustrate the diverse areas we are working on:



Towards the defossilization of the chemical industry, the valorization of CO₂ and sustainable production of H₂ are key examples of our small molecule activation portfolio. Here, the groups of **Senocrate/Battaglia** (Empa) and **Broekmann** (UniBe) present advances on improving the stability of electrochemical CO₂-to-CO converters. The **Luber** (UZH) and **Sivula** (EPFL) groups combine experimental and computational methods to investigate alternative oxidation reactions on WO₃ anodes for photoelectrochemical H₂ production.



Catalytic strategies are also crucial in developing more atom-efficient routes for the elaboration of complex molecules. Here, the **Buller** group (ZHAW) highlights successful algorithm-aided protein engineering examples and computational methods developed to improve enzyme properties for organic synthesis. The **Coskun** (UniFr) team discusses the suitability of porous organic polymers for selective palladium recovery for waste reduction. The **Guillén-Gosálbez** and **Pérez-Ramírez** (ETH Zurich) and **Marti** (HES-SO) groups explore reusable single-atom catalysts on scale for more sustainable cross-coupling chemistry.



Tools play a crucial role in advancing our understanding of catalytic systems. The group of **Bodi/Hemberger** (PSI) applies *operando* photoelectron photoion coincidence spectroscopy, a versatile tool capable of detecting elusive intermediates, to deepen the understanding of catalyst synthesis and catalytic reaction mechanisms investigated by experimental groups.



The integration of digital methods with chemistry provides new opportunities for accelerating and automating catalyst discovery and optimization. The groups of **Reiher** (ETH Zurich) and **Corminboeuf** (EPFL) overview a computational pipeline for model testing and refining for *in silico* catalyst optimization in collaboration with the **Cramer** (EPFL) group. The **Laino** (IBM Research) team addresses the role of artificial intelligence in driving the sustainability of the chemical industry with respect to estimating sustainability metrics and designing more sustainable chemical processes.

The development and application of sustainability assessments plays a key role in guiding catalytic process design for emerging technologies. The teams of **Guillén-Gosálbez** and **Pérez-Ramírez** (ETH Zurich) reveal the conditions under which small-scale decentralized ammonia-leaf systems become an environmentally competitive technology.

Swiss CAT+ is a complementary initiative on data-driven infrastructure for heterogeneous and homogeneous catalyst discovery and optimization funded by the ETH Domain, and **Laveille** (ETH Zurich) and **Miéville** (EPFL) provide an overview on its centers and activities with strong ties to NCCR Catalysis. This issue concludes with a contribution from **SusChem.CH** and **invited industry representatives** on how academia can help industry reduce the footprint of chemicals manufacture, and on unmet scientific needs serving as inspiration and guidance for researchers in the field of sustainable chemistry.

We are grateful to all authors and their teams for their time and efforts towards preparing the contributions, and to SNSF, ETH Zurich and EPFL for funding and support. We thank CHIMIA for this opportunity to highlight sustainable chemistry and catalysis.

In order to transition to a net-zero society, chemical value chains must become sustainable, and the vast and exciting field of catalysis will play a key role in attaining this goal. We hope that you enjoy this snapshot of our activities and would be happy to hear from you at info@nccr-catalysis.ch.

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The Editorial Board of CHIMIA thanks the guest editors for providing this extensive overview of the NCCR Catalysis and we look forward to following the progress of this vital field of research in the future.