doi:10.2533/chimia.2024.384 Chimia 78 (2024) 384–389

NCCR Catalysis at a Glance: A National Research Program on Sustainable Chemistry

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Abstract: Curious about how chemistry can contribute to sustainable development? In this overview, we explain the essence of NCCR funding, the research focus and structural goals of NCCR Catalysis, and how these align with the sustainable development goals (SDGs). Additionally, we highlight opportunities for getting involved with our program.

Keywords: Catalysis · Research program · Sustainability assessment · Sustainable chemistry

Marie-Francine Lagadec has been the Program Officer of the Swiss National Centre of Competence in Research (NCCR) Catalysis since 2020. Her background is in Materials, Mechanical, and Electrical Engineering, and she completed her PhD on lithium-ion battery technology at ETHZ in 2018. She then worked as a CNRS postdoctoral researcher at Collège de France, Paris on battery technology concepts for green hydrogen production before joining the NCCR Catalysis Management Team shortly after the program's start.

1. NCCRs, Unique Frameworks in Swiss Research

The National Centers of Competence in Research (NCCRs) are long-term research programs for advancing science in areas of strategic importance for Switzerland and society. Each program is supported and hosted at one or more Federal Institutes of Technology and/or universities. The programs are funded for a maximum of three phases of four years (*i.e.* 12 years at most). The first round of programs was launched in 2001, and the evaluation of 79 outline proposals submitted to the 6th round of applications is ongoing, as of April 2024.

For each funding round, the Swiss Federal Department of Economic Affairs, Education and Research (EAER, headed by Federal Councilor Guy Parmelin) and State Secretariat for Education, Research and Innovation (SERI, headed by Dr. Martina Hirayama) announce the number of NCCRs envisaged, available funding and, if applicable, thematic priorities. The Swiss National Science Foundation (SNSF) conducts the call for proposals, evaluates the submitted (outline and full) proposals, and shortlists outstanding applications. These are then presented to the EAER/SERI, which select programs that best fit strategic research and higher education policies. Successful programs are then funded through SNSF, the supporting institution(s), and, if applicable, third parties. Their mission is to conduct transformative research of international visibility and standing; to promote young scientists and gender equality; to promote knowledge and technology transfer (KTT) and science communication; and to strengthen and (re-)structure the Swiss research landscape. These long-term structure-related areas (SRAs) are embedded in the NCCR's DNA and are essential for its success within the respective research community. NCCRs are thus testbeds for innovative approaches and are given great freedom to provide blueprints for approaches that individual groups or institutions could not pursue. They strengthen areas of societal importance through valuable long-term funding. Each NCCR is evaluated and audited extensively almost yearly by experts in the relevant research fields and the SNSF.

2. NCCR Catalysis

Despite the importance of chemistry for the Swiss economy and research community, no NCCR or larger-scale collaboration in the field of chemistry and sustainability had emerged before 2017, when SNSF issued the call for the 5th series of NCCRs. The seed for NCCR Catalysis was planted in 2016 through discussions between Javier Pérez-Ramírez and Christophe Copéret (both at ETHZ) and Cristina Nevado (University of Zurich) on one side and Jérôme Waser and Nicolai Cramer (both at EPFL) on the other side. Javier Pérez-Ramírez and Jérôme Waser (EPFL) gathered support from colleagues, ETHZ and EPFL, and interested research groups in the chemical sciences and engineering disciplines for an NCCR on the development of sustainable technologies for chemicals production accelerated by data-driven approaches. After passing the competitive two-stage application process with 54 outline proposals, the program's **Phase I** (August 2020 through July 2024) launched with a total funding of CHF 32M and 29 participating research groups across Switzerland, and a Management Team currently consisting of Prof. Javier Pérez-Ramírez and Prof. Jérôme Waser as directors; Dr. Marie-Francine Lagadec as Program Officer; Dr. Sharon Mitchell as Program Advisor; Annabelle Kin as Finance Officer; Lauren Gamp as KTT Officer; and Romain Graux as Data Officer.

To bring in members of the sustainable chemistry community with the necessary skills and expertise and thus encourage research in key areas, we organized a competitive open call, broadly advertised to relevant research institutions, as well as further internal and invited calls. As of April 2024, NCCR Catalysis has grown to include 48 contributing research groups and teams at relevant Swiss institutions (Fig. 1). With more than 250 members, it is the largest NCCR to date, and, to our knowledge, the broadest research program on sustainable chemistry and related metrics worldwide. Of these groups, students and researchers associated with the proposed research projects (paid through the program or

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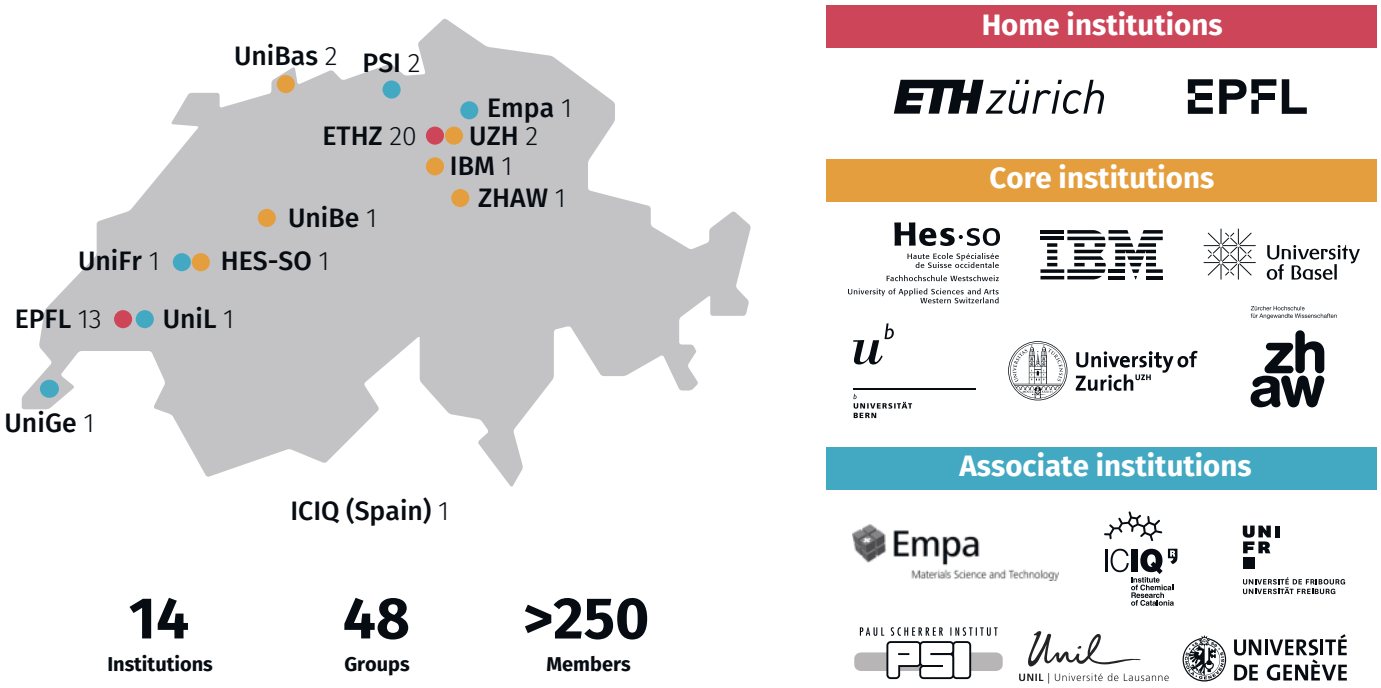

Fig.1. Team composition as of April 2024, with the number of research groups and teams indicated per institution. The NCCR Catalysis project team is based at the home institutions ETHZ and EPFL.

in-kind) are members of our consortium. We are thrilled to announce that the continuation of our program for **Phase II** has been recently confirmed (August 2024 through July 2028).

As a globally recognized research program, NCCR Catalysis strengthens Switzerland's scientific research landscape, fosters innovation, and increases the number of skilled workers in the chemical sciences in public and private research and development (**SDG Target 9.5**). Our mission of establishing circular chemical value chains based on renewable feedstocks and waste minimization (**SDG Targets 12.2**, **12.4-6**) aligns with efforts to continue Switzerland's leading role in chemistry but with more sustainable practices (**SDG Target 8.4**) and to strengthen urgently needed climate action and sustainability education (**SDG Targets 12.8** and **13.3**).

NCCR Catalysis is well embedded into the broader Swiss ecosystem of sustainable chemistry, *see the SCNAT perspective in this issue*, and is strengthening its ties with industry, ranging from small-size organizations to large conglomerates, *e.g.* through SusChem Switzerland. In combination with the program's unique approach and long-term funding – contrasting international schemes and initiatives focused on specific feedstocks or having less diverse team compositions – this creates excellent conditions for a significant and enduring impact towards sustainability in the chemical sciences.

2.1 *Research Activities*

Since August 2023, research activities in NCCR Catalysis have been structured into five work packages (WPs) as shown in Fig. 2. Within these, we pursue technology development, primarily driven by fundamental science from highly exploratory (low) to commercially promising (high) technology-readiness levels (TRLs).

WP1 *focuses on the discovery of innovative catalytic concepts and the development of optimized synthesis routes for the sustainable production of platform chemicals from renewable sources.*

Small molecule activation. Building on promising insights from **WP5**, we tackle strategic routes for the activation of abundant molecules like CO_2, H_2O, and N_2, target valuable products from CO_2 and strengthen activities on sustainable NH_3 production by exploring novel catalytic processes and considering also nitrate conversion. Additionally, we aim to improve the efficiency of H_2 production, which is essential for the feasibility of many other processes.

Complex feedstocks. Biomass and waste plastics are also anticipated to be key carbon sources of a post-petrochemical industry. Building on the success of producing green solvents and polymers from lignocellulosic biomass in **Phase I**, we are looking at new routes for biomass utilization. Additionally, we focus on the development of selective routes for chemically recycling large-volume plastic wastes.

WP2 *aims at discovering and implementing new methods and approaches for sustainable chemical transformations that valorize the renewable platforms of natural origin and/or prepared in **WP1** into customized products.*

Sustainable inputs and products. We develop sustainable synthetic strategies of industrial relevance in two key areas of industrial manufacture, polymer production and complex chemical synthesis, and aim to integrate a circular approach. We harness data-driven strategies to optimize synthetic methods for the construction of complex molecular structures of commercial relevance from renewable building blocks.

Novel strategies. Here, we develop sustainable chemical methods that minimize reliance on finite resources. We focus on the activation of strong bonds, using earth-abundant metals to form novel synthetic connections, leveraging engineered enzymes and small molecule ligands towards this goal. We explore different catalysis modes (homogenous, heterogenous, photo, bio, and electro) and evaluate their comparative sustainability.

WP3 *is dedicated to advancing the design of catalysts and unraveling the intricacies of active site structures and reaction dynamics, a crucial endeavor for the rational development of sustainable catalytic processes and the understanding of catalyst behavior across relevant temporal and spatial scales, and the interplay between local structure, kinetics, mass, heat, and charge transport.*

Innovative catalyst synthesis. While the precision achieved in designing molecules for homogeneous and biocatalysis is evident, the complex multicomponent nature of heterogeneous

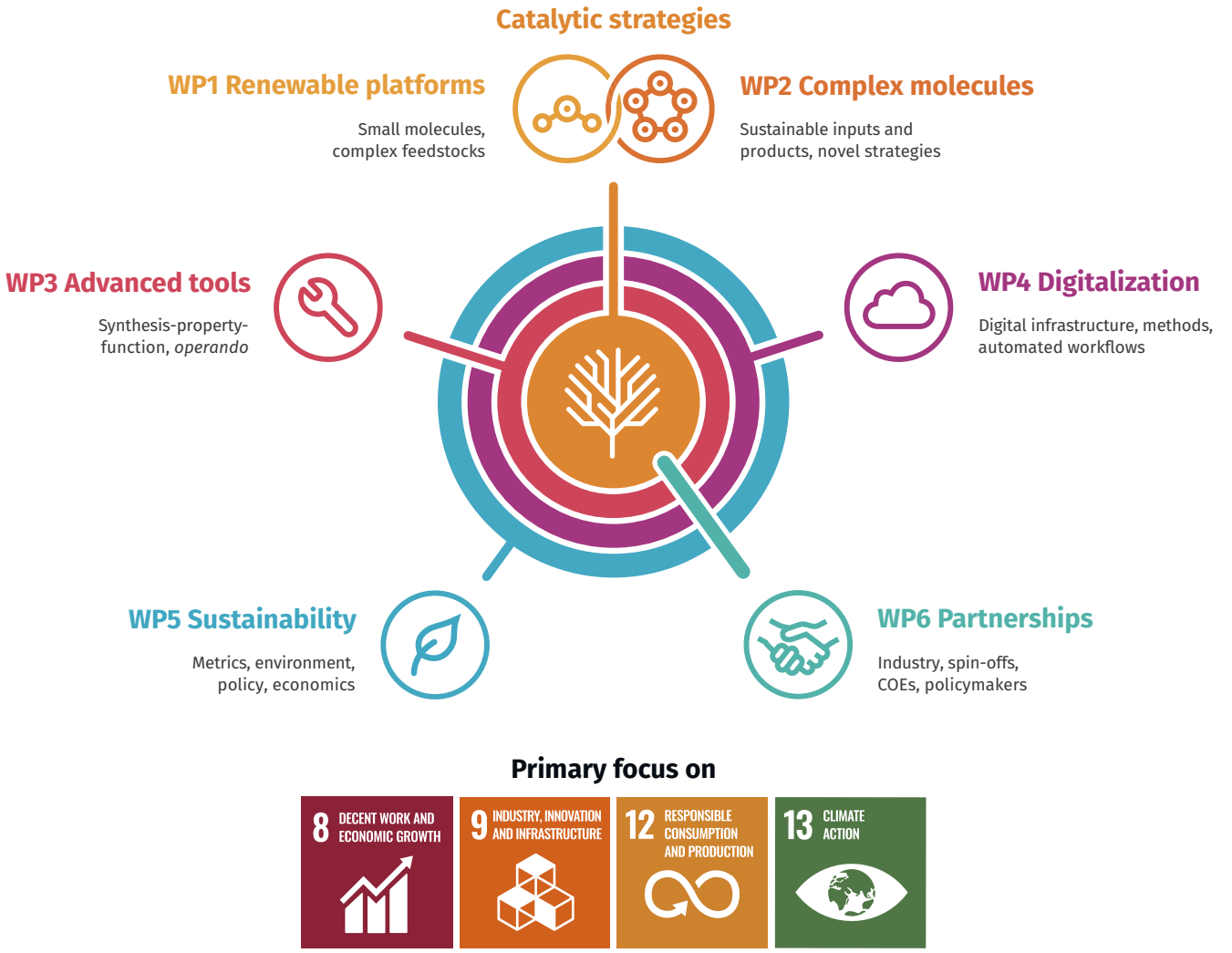

Fig. 2. Research structure of NCCR Catalysis with five WPs as of April 2024 and primary SDGs addressed by the program. Our research journey centers on catalytic strategies for producing Renewable Platforms (**WP1**) and their subsequent transformation into tailored Complex Molecules (**WP2**). Progressing our fundamental science is reinforced by Advanced Tools (**WP3**) and Digitalization (**WP4**), which are versatile components intersecting all aspects of our work. The principles of Sustainability (**WP5**) underpin all our activities, guiding research decisions. We aspire to build strong Partnerships (**WP6**) with industry, spin-offs, centers of excellence, and policymakers in the next phase.

catalysts introduces inherent complexities. To close this gap, we further pioneer robust synthesis routes for atomic-scale design of heterogeneous catalysts, investigating a broad range of catalyst families, and evaluate their potential for improved sustainability in **WP1** and **WP2** applications in collaboration with **WP5**.

Novel approaches for characterization and evaluation. Here, we focus on further developing advanced microscopic and spectroscopic approaches, supported by computational modeling, to understand the geometric and electronic structure of complex systems on a broad range of length scales from angstroms to millimeters. With a strong emphasis on real-time monitoring of reactions and catalysts, we identify the structure and dynamics of catalysts in relation to the activity, selectivity, and stability under realistic operating conditions.

WP4 *is dedicated to the strategic integration of digital solutions within the core of NCCR Catalysis, speeding up sustainable technology development. Through a combination of big data analysis, statistical learning insights, and AI, our mission is to enhance catalyst discovery and deepen insights while optimizing experimental and theoretical efforts*.

Automated exploration of catalysts and reactions. We aim to accelerate catalyst and process discovery and optimization in other WPs through cutting-edge computational techniques, ML algorithms, and quantum-chemical combined uncertainty quantification. Through systematic exploration and analysis, we uncover novel catalyst candidates, key reaction pathways, and optimal conditions. Automating this exploration process enhances the efficiency, productivity, and sustainability of chemical synthesis, propelling groundbreaking advances.

Modeling of chemicals and processes. We perform molecular simulations of catalysts and reactions, providing novel atomic-level insights into complex transformations and driving a deep comprehension of catalytic mechanisms, enabling the design of more efficient and benign processes. Modeling reactions and processes across scales facilitates a comprehensive understanding of chemical systems, aiding in predicting their behavior under varying conditions and optimizing processes while conserving resources. The use of AI models facilitates environmental impact assessments of chemical processes and of the sustainability of the developed computational technologies (with **WP5**).

WP5 *is designed to integrate sustainability assessment seamlessly as a guiding principle of our research structure towards achieving an ecologically conscious chemical industry. We concentrate on developing robust methodologies to evaluate the sustainability impact of both the catalytic processes to synthesize renewable platforms (**WP1**) and complex molecules (**WP2**) and the tools developed to accelerate this process in **WP3** and **WP4***.

Sustainability of chemicals and processes. We pioneer the establishment of comprehensive and standardized metrics to quantify the sustainability of novel chemical processes and technologies. These metrics, designed to be accessible and universally applicable, fuel discussions with industry partners, playing a key role towards framing umbrella projects in **WP6**. We embark on broad environmental assessments, envisioning potential circular chemicals production scenarios. By considering life cycle impacts, resource utilization, and potential risks, we guide research trajectories in **WP1** and **WP2**. We extend our efforts towards a complete sustainability assessment, including indicators from all three pillars of sustainability (environmental, social, and economic; Fig. 3), crucial dimensions that are often overlooked in chemical research. By analyzing the economic viability and societal implications of emerging technologies, we ensure that research priorities align with real-life constraints that are dictated by the economic or institutional environment in which the chemical industry operates.

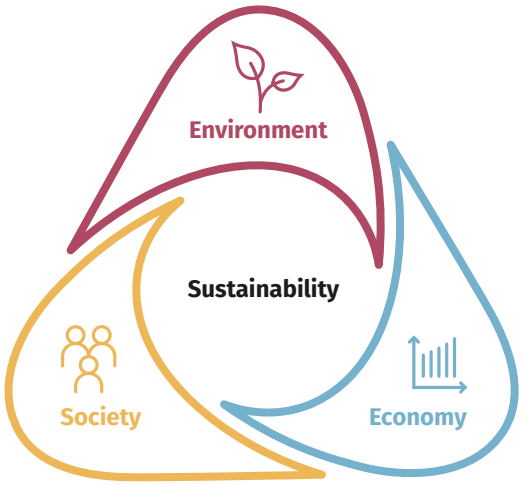

Fig. 3. Holistic approach to sustainability assessments, integrating all dimensions: environment, society, and economy.

Through **WP6**, *dedicated to nurturing multilateral collaborative projects and fostering interactions, we build relationships with key partners in our community. We are working to develop strategic programs with partners in the chemical industry*.

Individual research groups cannot tackle the broad scientific challenges we address in NCCR Catalysis. Therefore, we invested a major effort in connecting our many members through scientific meetings and encouraging them to develop common languages across communities. We aim to accelerate all facets of our research through standardized data-driven approaches and to remain as open as possible to technologies until we have proof that a particular direction should be pursued.

Key aspects of our program's success in **Phase I** have been the ability to flexibly allocate funds and the fluidity of our program's structure. We started the program with 29 topically diverse core research groups and soon identified areas that required strengthening and specific expertise needed to unlock new research directions through collaborations. In response to an open call, 13 research groups joined our community in 2021 as associate members. In 2022, we launched an internal data-driven research call to foster connections between experimental and computational research groups; these projects were designed to be inherently collaborative and have served as a blueprint for the multi-group multi-WP projects we will launch in **Phase II**. Several projects triggered by this call have resulted in self-reinforcing collaborations and high-impact outcomes. In 2023, after the reorientation of **WP5** on sustainability and in preparation for strategic research directions in **Phase II**, we reinforced selected topical areas and launched new ones, through which another four research groups joined our program.

2.2 *Structural Activities*

To strengthen the Swiss catalysis and sustainable chemistry community, ETHZ and EPFL support three professorships, two of them in Digital Chemistry. As a program, we pursue Structure-related areas (SRAs) in five categories (see Fig. 4). For each SRA, we have developed strategies to address the most relevant topics in our field and community.

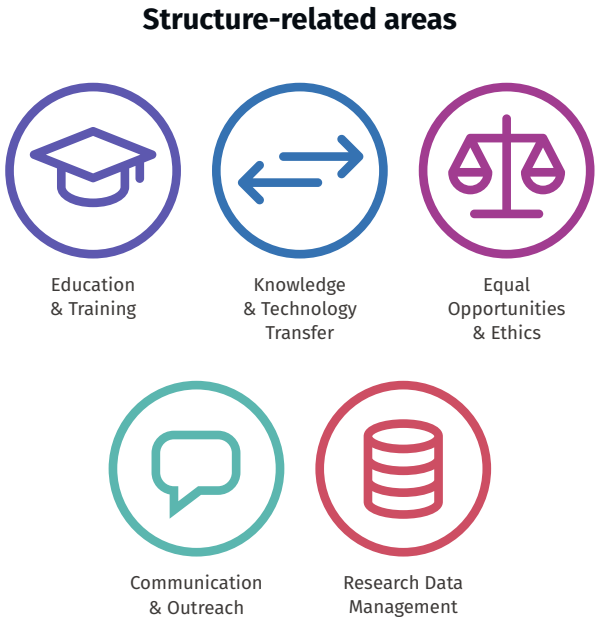

Fig. 4. SRAs covered within NCCR Catalysis and the SDGs they primarily address.

Our **Education & Training** activities focus on developing a catalysis education program, conveying 21st-century competencies, and fostering lifelong learning. Key targets here are to mainstream sustainability education at higher and continuing education levels (**SDG Target 13.3**) and to equip an increasing number of adults with the relevant knowledge and skills for employment and entrepreneurship in the sustainable chemistry field (**SDG Target 4.4**). Upon recognizing a crucial gap in the integration of sustainable development within the chemistry and chemical engineering master's programs at ETHZ and EPFL, we introduced

new sustainability courses that aim to provide students with the necessary knowledge and skills to be at the forefront of the future of the sustainable chemical industry. These address sustainability in all dimensions (Fig. 3) and strongly involve industry practitioners. These pioneering courses were spearheaded and designed by NCCR Catalysis, working in coordination with the relevant departments at ETHZ and EPFL. The courses should, therefore, continue beyond NCCR Catalysis, as integrated parts of the curriculum, and efforts are continuing to further strengthen the offer.

Our **Knowledge & Technology Transfer** activities target relationship building, consolidating KTT initiatives, and providing support for KTT to our members with the ultimate goal of fostering adoption of technologies, tools and methods by industry (**SDG Target 9.4**). To foster trust and allow for confidential disclosure of as-yet-unpatented and unpublished work while protecting the patentability of inventions, we initiated a confidentiality agreement covering interactions between NCCR Catalysis members from all our institutions. With it in place, we see improved awareness of confidentiality among our members, and more open interactions due to this layer of safety. Crucially, the confidentiality agreement has unleashed the potential for researchers to discuss cutting-edge research findings safely, nurturing a dynamic environment for groundbreaking ideas across disciplines and institutions. It opens the door for sharing unpublished data among members. We hope that the current and future agreements result in stronger patents, due to increased exchange among researchers at early stages of innovation.

In **Equal Opportunities & Ethics**, we focus on attracting, preserving, and supporting talents from diverse backgrounds with the long-term vision of increasing the female share of graduates from STEM fields at the tertiary level and providing equal access for all to affordable and quality education in sustainable chemistry (**SDG Target 4.3**). Through the SNSF Flexibility grant, we provide support for unpaid care work (**SDG Target 5.4**) for junior researchers. Inspired by the Academic Wheel of Privilege, we conceived, organized, and implemented our own version of it as a multifaceted educational, monitoring, and decision-making tool, empowering and promoting the social, economic and political inclusion of all, irrespective of status (**SDG Target 10.2**). The creation and presentation of our Wheel of Privilege helped us to clearly define terminology with respect to underrepresented groups, both for leadership and for our members. We use it to guide our decisions and actions in equal opportunities and community support and adapted it to the context of our Young Talents Fellowship.

Our **Communication & Outreach** activities range from establishing our brand to the community, building, increasing (inter) national visibility of sustainable chemistry research, and primarily outreach towards children in primary schools on sustainability and chemistry (**SDG Target 13.3**), with the goal of reducing gender disparities and ensuring access to education for vulnerable groups (**SDG Target 4.5**). We launched *Sustainability Day* as an initiative co-organized with **WP5**, in the form of a biannual event that provides an exciting opportunity for our researchers and invited guests to interact and exchange on sustainability topics. The first edition in 2022 centered around the topics of sustainability assessments and their challenges, as well as how each of our WPs addresses and assesses sustainability. The first *Sustainability Day* helped to foster discussions among our members and improve understanding of sustainability assessment, and ultimately led to reorienting **WP5** towards its current focus. The theme of *Sustainability Day* 2024 is *Expanding the horizon of sustainable chemical research*, and we highlight recently onboarded and incoming **WP5** Principal Investigators (PIs) whose research addresses socioeconomic, policy, and corporate sustainability topics.

Last but not least, our **Research Data Management** activities address the digitalization, automation, centralization and standardization of research data across our members, with the ultimate goal of modernizing and accelerating sustainable chemistry research and fostering digital competencies among our member groups. After our first year, we identified a critical opportunity to amplify synergies between **WP4** groups and those in other WPs. Our data-driven research call emerged as a pioneering initiative, demonstrating our commitment to data-driven research by funding nine additional projects for collaborative **WP4-WPX** projects. In bringing experimentalists and computationalists together, we have catalyzed a deeper understanding of what constitutes high-quality datasets, as well as of the effort necessary to craft such a resource, and of one another's science. This has fostered robust relationships and interdisciplinary collaborations, exemplified by an increase in tandem **WP4-WPX** presentations at NCCR Catalysis events. Tools developed in these projects have been translated into user-friendly web apps, which are accessible to the whole community.

Through the program and the participating institutions, we provide learners with the knowledge and skills required for sustainable practices. We encourage women's access to leadership positions and gender equality in STEM. Our focus on cultural diversity will ultimately contribute to a more sustainable and equitable society (**SDG targets 4.7** and **5.5**).

3. Conclusions and Outlook

Since its inception and start in 2020, NCCR Catalysis has taken us on an exciting ride, shaping and rethinking Swiss catalysis and sustainable chemistry research. Designed to foster collaboration among diverse research communities, our program faces the continuing challenge of bridging gaps in understanding and terminology across disciplines. Despite relatively modest funding levels due to the breadth of our community, our research teams demonstrate an unwavering commitment to investing resources beyond the allocated funding, contributing to collective growth.

In **Phase I**, our program prioritized dynamism and flexibility to strengthen our community and address emerging research directions through collaborative efforts. With the recent approval of **Phase II** (2024–2028), we will intensify these efforts and pursue a holistic approach towards sustainability assessments through the integration of social scientists, as initiated in our program's fourth year. Through collaborative projects and ideas for spin-offs, we will take more risks in developing and advancing cutting-edge technologies.

We're grateful to our program's Review Panel for their support and valuable suggestions which have also helped us sharpen the program; to SNSF, ETHZ and EPFL for their continued support and the freedom to shape our program; and to all supporters who have allowed us to embark on and successfully navigate this journey.

We welcome inquiries if you are interested in becoming involved in our program or are seeking further information. Research group leaders are encouraged to contact the relevant WP Coordinators indicated on our website to learn more about specific WP aims. We also encourage students and researchers to directly contact relevant PIs listed on our website, as funding is allocated to them in accordance with SNSF regulations, rather than on an individual basis.

To stay informed on our activities, please follow us on our website and social media channels:

https://nccr-catalysis.ch
https://twitter.com/NCCR_Catalysis
https://linkedin.com/company/nccr-catalysis
https://www.instagram.com/nccr_catalysis/

Acknowledgments

The descriptions of the WPs are adapted from the NCCR Catalysis **Phase II** Full Proposal, which were co-drafted initially by Peter

Broekmann and Kevin Sivula (**WP1** *Renewable platforms*), Rebecca Buller and Bill Morandi (**WP2** *Complex molecules*), Raffaella Buonsanti and Christophe Copéret (**WP3** *Advanced tools*), Teodoro Laino (**WP4** *Digitalization*), Gonzalo Guillén-Gosálbez and Stefanie Hellweg (**WP5** *Sustainability*) and the NCCR Catalysis Management Team for **WP6** *Partnerships*. The descriptions of the SRAs are adapted from the NCCR Catalysis Y3 Report, and were originally drafted by Sharon Mitchell (E&T), Lauren Gamp (KTT), Marie-Francine Lagadec (EOE, C&O) and Romain Graux (RDM).

This publication was created as part of NCCR Catalysis (grant number 180544), a National Centre of Competence in Research funded by the Swiss National Science Foundation.

Received: April 30, 2024