https://doi.org/10.1038/s44286-023-00005-1

Transcending scales in catalysis for sustainable development

Sharon Mitchell, Antonio J. Martín & Javier Pérez-Ramírez

Heterogeneous catalysis will continue to be a fundamental pillar of chemicals manufacturing. The development of sustainable catalytic technologies requires a multidimensional approach, bridging atomic-level design with planetary impact considerations. Prioritizing sustainability metrics, industry partnerships and circular economy principles as well as raising public awareness are crucial.

Chemical engineering pioneers built the first large-scale plants, paving the way for the manufacturing of hundreds of thousands of products, including fuels, fertilizers and medicines, that have been fundamental to human development. However, the heavy reliance on fossil resources in these processes has resulted in severe environmental and health impacts. A recent analysis of around 500 chemicals revealed that the production of more than 99% of them transgresses the safe operating space of at least one of the seven planetary boundaries evaluated, particularly climate change, ocean acidification and change in biosphere integrity, and thus can be deemed unsustainable[1]. The current linear economy model, in which only approximately 7% of extracted resources from natural capital are recycled, compounds the environmental burden. These challenges have contributed to the transition into the Anthropocene epoch, characterized by human-induced environmental changes, and have made limiting global warming to 1.5 °C within this century a formidable challenge.

Heterogeneous catalysis, the science of developing selective paths to break and form desired bonds in a stable manner over solid materials, has been central to shaping the chemical industry in the past and will continue to do so. It will play a pivotal role in unlocking sustainable pathways for transforming renewable feedstocks, such as carbon dioxide, water, nitrogen and biomass, that are key to materializing the grand transition toward fossil resource independence in chemicals manufacturing. Chemical engineers are trained to think across scales, which is essential to developing catalytic processes that satisfy the

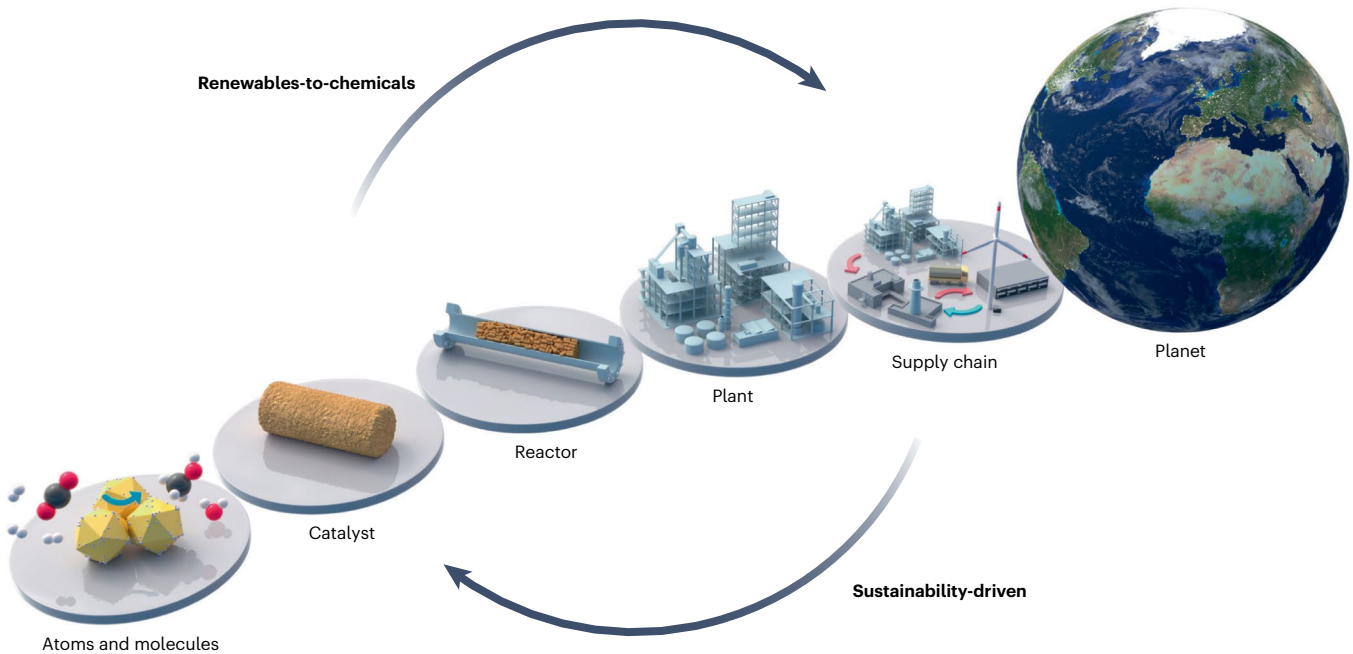

Fig. 1 | Concept for sustainable chemicals production. The integrated approach combines bottom-up optimization of atomic-scale catalytic routes for converting renewables into chemicals with top-down strategies that assess macroscopic impacts and guide catalyst design based on sustainability criteria. This provides a comprehensive framework for designing catalytic processes that can contribute to a more sustainable future.

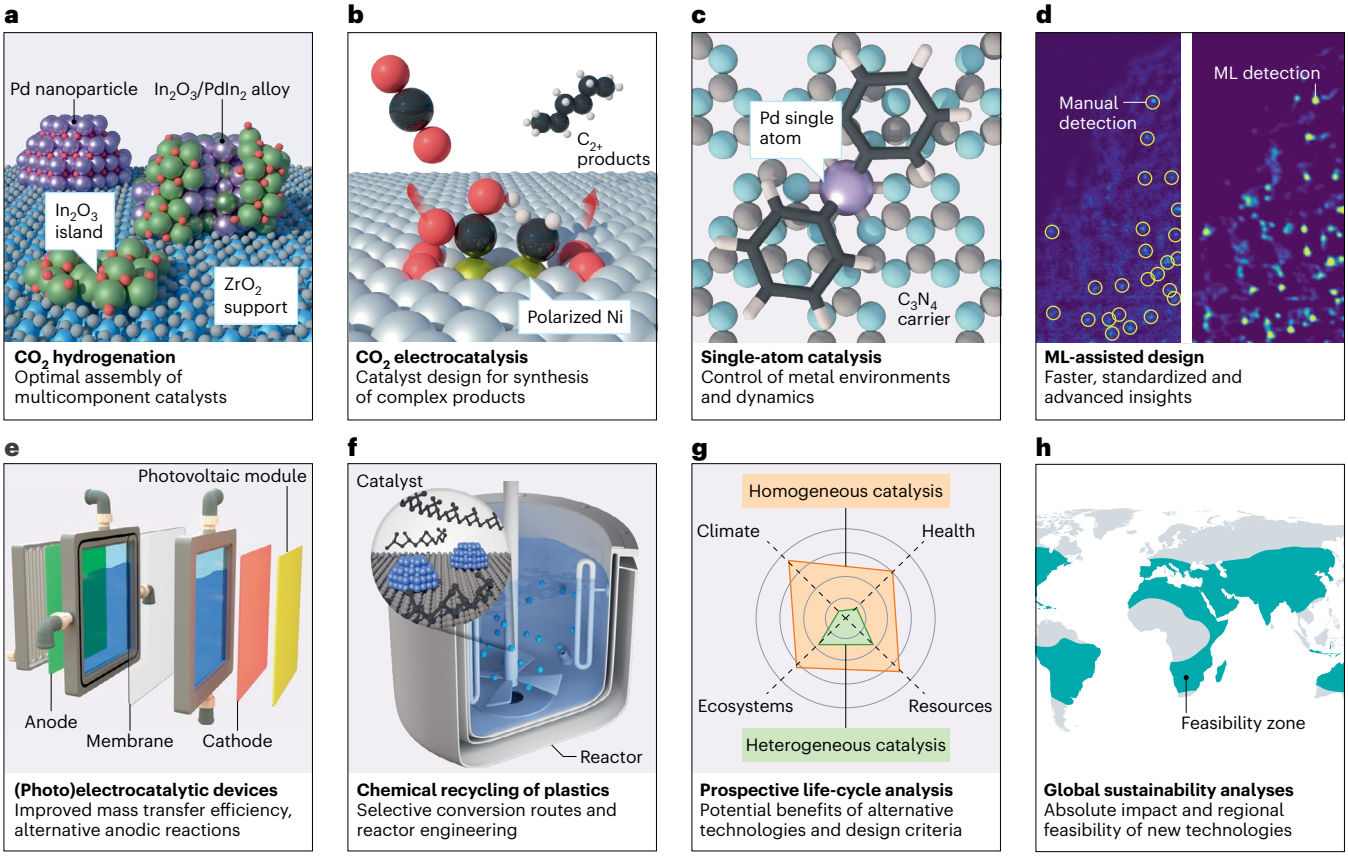

Fig. 2 | Priorities in heterogeneous catalysis. a–h, Case studies illustrate key areas for sustainable technology development and current challenges that may lead to breakthroughs. **a–c**, Precise control of active site architectures is crucial to unlock high performance and novel reactivity, as exemplified by the development of Pd–In_2O_3–ZrO_2 catalysts for CO_2 hydrogenation (**a**), Ni-based catalysts for producing C_{2+} products in electrocatalytic CO_2 reduction (**b**), and reusable $Pd_1@C_3N_4$ single-atom catalysts for organic synthesis (**c**). **d**, Machine learning (ML) can aid catalyst characterization, enabling rapid and standardized analysis as illustrated for atom detection in transmission electron microscopy images, providing advanced insights into single-atom organizations. **e**,**f**, Reactor design and mass-transport considerations will play a key role for improving the efficiency of (photo)electrocatalytic devices (**e**) and plastics recycling (**f**). **g**,**h**, Examples illustrating how life-cycle analysis can guide catalytic process design by quantifying potential environmental benefits of different processes for organic synthesis (**g**) and determine the regional feasibility for green ammonia synthesis (**h**).

environmental, social and economic dimensions of sustainability. Taking a multidimensional approach that integrates efforts from designing atomic-level reactions to evaluating their impact on the planet is paramount in this quest (Fig. 1).

Rapid progress in atomic- and molecular-scale engineering has opened new possibilities in various energy conversion processes involving catalysis[2,3]. For example, the effective nanostructuring of active phases with supports and promoters enabled the identification of new families of materials capable of transforming carbon dioxide, an inherently inert molecule, to methanol via thermocatalytic routes. This achievement has led to advanced architectures such as Pd–In_2O_3–ZrO_2 or Zn–ZrO_2 yielding industrially competitive productivity[2] (Fig. 2a). Optimizing the assembly of these multicomponent systems to deliver the desired functionality is challenging. Dedicated tools including operando methods are crucial for understanding the dynamic behavior of catalysts and identifying relevant performance descriptors[4].

Similarly, emerging technologies such as artificial leaves can revolutionize energy conversion and fertilizer production. By harnessing sunlight, water and abundant small molecules such as carbon dioxide and nitrogen, these technologies permit decentralized operation[3,5]. However, to demonstrate the industrial viability of this concept, it is essential to improve the efficiency of current electrocatalysts and expand the range of products they can generate. Recent breakthroughs, such as the use of polarized nickel centers for electrocatalytic carbon dioxide reduction, leading to long-chain hydrocarbons, highlight the potential for discovering new reactivity by moving beyond classical catalytic systems[6] (Fig. 2b). Bridging the knowledge gap at the atomic scale in electrocatalytic applications, including the active site structures and the effect of their environments, will undoubtedly push catalyst design forward.

At the frontier of nanostructuring, single-atom catalysts have emerged as an another advancement, offering uniform and tailorable structures that can enhance the utilization of scarce metals[7]. These catalysts show promise in replacing the non-recoverable homogeneous catalysts in organic synthesis[8] (Fig. 2c). However, challenges remain in controlling metal environments and dynamics during reactions, where

the coordination of active centers must be flexible enough to permit the catalytic cycle but constrained enough to ensure high stability. Designing new generations of carrier materials that go beyond the conventional carbon-based structures and tailoring their coordination sites and metal nuclearity will be crucial for increasing their applicability. As requirements to develop more precise architectures increase, advancements in characterization techniques are necessary to support their development. Existing techniques often face limitations in distinguishing different types of active site structure and determining their relative populations. To address this challenge, machine learning methods show promise in standardizing, accelerating and providing more quantitative insights during catalyst analysis[9] (Fig. 2d). By leveraging machine learning, we can enhance the reproducibility of catalyst synthesis and gain a deeper understanding of catalyst performance.

In conjunction with discovering and developing catalytic materials, the effective implementation of many emerging renewable-based technologies necessitates careful attention to reactor and process design (Fig. 1). For instance, the development of efficient membrane reactors can shift the thermodynamic equilibrium, improving the efficiency of carbon dioxide conversions[10]. Similarly, tandem reactor concepts are highly relevant for hybrid strategies integrating multiple catalytic approaches (for example, heterogeneous and enzymatic). Reaction engineering is particularly crucial in electrochemical devices (Fig. 2e), where enhancing energy efficiency and stability, exploring alternative reactions at the anode, and designing efficient electrolyzer structures and gas diffusion electrodes to minimize mass transport constraints are paramount[11]. Furthermore, catalysis can play a pivotal role in addressing complex waste management, particularly in the areas of biomass and plastics, requiring dedicated reactor designs driven by their rheological properties. Attention to mass and energy transfer, aspects that must be considered at any stage of development regardless of the process under consideration, will be of special relevance to develop catalytic processes that can enable effective chemical recycling strategies of polymers (Fig. 2f). A breakthrough toward achieving this circularity would involve the selective conversion of unfunctionalized polyolefins, which constitute two-thirds of plastic waste, using heterogeneous catalysts[12].

At the macroscale (Fig. 1), comprehensive evaluation of the environmental impact of catalytic processes requires a systems approach that incorporates tools such as life-cycle assessment and techno-economic analyses. These approaches can provide valuable insights into the environmental implications of emerging technologies through early-stage analyses. For instance, a preliminary comparison revealed the potential benefits of using heterogeneous palladium catalysts instead of homogeneous ones for cross-coupling reactions in fine chemical synthesis[8] (Fig. 2g). By employing life-cycle assessments, it is possible to evaluate specific catalytic processes and formulate future scenarios for the chemical sector. They help identify optimal supply chains that utilize renewable carbon sources, fostering the integration of sustainable chemical processes with decarbonized energy generation and promoting the transition toward a circular economy. These assessments also contribute to understanding the planetary-level impact and aid in identifying regionally specific criteria for sustainable development, which can guide policy development. For instance, a regional analysis of decentralized ammonia synthesis via solar-powered electrocatalytic nitrogen reduction indicated the feasibility of fertilizer production in many densely inhabited locations globally[5] (Fig. 2h). However, it is important to address the current challenges faced in sustainability assessments, such as the availability and reliability of data and the adoption of standardized metrics across the chemical industry.

Implementing a catalytic process is a complex and time-consuming endeavor, often taking more than a decade. To reduce this timeline, it is crucial to consider catalyst and process scalability aspects and reactor concepts that ensure safe and stable operation from early stages of development[13]. Collaborative efforts between academia and industry are essential, particularly in bridging gaps between emerging concepts and practical challenges in large-scale manufacturing, thereby accelerating the development of sustainable processes[14]. We believe that rapidly evolving machine learning methods hold substantial potential for expediting data extraction, analysis and learning across all scales. However, it is important to improve the interpretability of these algorithms to gain a fundamental understanding from their outputs[15]. Finally, the traditional model of 'take–make–dispose' must shift to a circular model that considers the entire life cycle of products. Achieving this transformation requires educational initiatives and public awareness campaigns to promote a different mindset toward sustainable practices among industry, government and consumers.

Enabling a sustainable chemical industry is paramount for the well-being of our planet. Heterogeneous catalysis is a crucial tool for achieving this goal. However, implementing sustainable catalytic processes requires a multifaceted approach considering technical, economic and social factors across various scales. Collaboration between stakeholders and public education are essential for promoting a cultural shift toward sustainability in the chemical industry. By prioritizing sustainability metrics and incorporating social science perspectives, we can ensure that chemical engineering continues to contribute to societal progress while safeguarding our planet for future generations.

Sharon Mitchell, Antonio J. Martín & Javier Pérez-Ramírez
Institute of Chemical and Bioengineering, Department of Chemistry and Applied Biosciences, ETH Zurich, Zurich, Switzerland.
e-mail: jpr@chem.ethz.ch

Published online: 11 January 2024

References

1. Tulus, V., Pérez-Ramírez, J. & Guillén-Gosálbez, G. *Green Chem.* **23**, 9881–9893 (2021).
2. Araújo, T. P. et al. *Nat. Commun.* **13**, 5610 (2022).
3. Ampelli, C. et al. *Energy Environ. Sci.* **16**, 1644–1661 (2023).
4. Hartman, T., Geitenbeek, R. G., Whiting, G. T. & Weckhuysen, B. M. *Nat. Catal.* **2**, 986–996 (2019).
5. D'Angelo, S. C. et al. *Energy Environ. Sci.* https://doi.org/10.1039/D2EE02683J (2023).
6. Zhou, Y. et al. *Nat. Catal.* **5**, 545–554 (2022).
7. Hai, X. et al. *Nat. Nanotechnol.* **17**, 174–181 (2022).
8. Faust Akl, D. et al. *Green Chem.* **24**, 6879–6888 (2022).
9. Mitchell, S. et al. *J. Am. Chem. Soc.* **144**, 8018–8029 (2022).
10. Hyeon, M. H. et al. *Nat. Commun.* **14**, 1673 (2023).
11. Liu, X. et al. *Adv. Energy Sustain. Res.* **3**, 2200005 (2022).
12. Martín, A. J., Mondelli, C., Jaydev, S. & Pérez-Ramírez, J. *Chem* **7**, 1487–1533 (2021).
13. Martín, A. J., Mitchell, S., Mondelli, C., Jaydev, S. & Pérez-Ramírez, J. *Nat. Catal.* **5**, 854–866 (2022).
14. Godineau, E. et al. *Chimia* **77**, 159–159 (2023).
15. Esterhuizen, J. A., Goldsmith, B. R. & Linic, S. *Nat. Catal.* **5**, 175–184 (2022).

Acknowledgements

We acknowledge funding from NCCR Catalysis (grant no. 180544), a National Centre of Competence in Research funded by the Swiss National Science Foundation.

Competing interests

The authors declare no competing interests.