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a perspective

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Molecular Catalysis for the Chemistry of the future: a perspective

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The chemistry of the future will have to find solutions for the societal challenges of tomorrow (and today) and undoubtedly, catalysis will play a central role. Molecular catalysis for the chemistry of the future will openly face significant challenges for present and future generations including: 1) scarcity of resources (food, water, fossil resources etc.) combined with 2) an ever increasing degradation of the environment, 3) a "new life" for plastics and particularly plastic waste that is not recycled, and 4) the development of a circular economy based on the use of renewable energies limiting or ideally reversing CO_2 emissions.

All types of catalysis are profoundly linked with each other at the molecular level. However, they are mostly studied by different communities at present with little scientific exchange between them. It is important to develop unifying concepts of catalysis (thermal-, bio-, photo- and electro-catalytic pathways) by using state-of-the-art techniques from different subdisciplines. In this manner, new understandings will be generated on important design parameters in catalysis including solvent and pH effects, synergies between metals in alloy catalysts, synergy between metals and ligands and support in heterogeneous catalysts. The vision is to achieve fundamental understanding of catalytic processes culminating in a great unifying theory of catalysis.

To elucidate the catalytic mechanism at the atomic and molecular level and predict the catalytic activity and stability before trial-and-error based experiments to work out sophisticated catalyst designs, computational approaches are also essential. Over the last two decades, the computer-aided design of catalysts has been very successful owing to the prosperous establishment of computational methodologies accompanied with tremendous progress of computing power. Many examples can be found, in which computational screening has played a major role in experimentally finding a new class of molecular catalysts and computational analyses could be successfully explained for the underlying mechanism of catalysts' behaviours. However, there are still many challenges to overcome for the use of these approaches, and continuous efforts on this research field are further necessary.

As editors of *Molecular Catalysis*, we feel in an advantageous position to directly follow (and impact) various academic trends and industrial realities to deal with such problems administrating different contributions submitted to our journal. This privileged position allowed us to visualize a number of hot areas (Figure 1) currently under development for a more sustainable future:

a) *Establishing new chemistries for safe-by-design/benign-by-design products*, not only comprises synthesis methods avoiding immediate hazards for the environment such as emissions and wastes generated as well as safety issues of the production process. More importantly, it will also yield safer products. Safer in the sense that they will exhibit only the desired properties in human use and further on if exposed to the environment, i.e. bio-degradable by design. [1]
b) *Highly selective catalytic transformations.* Reducing the amount of wastes formed in chemical transformations is key to reducing the environmental impact of the chemical industry. This comprises, but is not limited to: more selective transformations (avoiding undesired side products), avoidance of protection group chemistry and reduction of the energy demand of chemical transformations (reducing energy-linked CO_2 emissions). Biocatalysis will play a central role here.[2] When it comes to selectivity, enzymatic methods are unparalleled. Further exploring this catalytic wealth and designing reaction concepts compatible with

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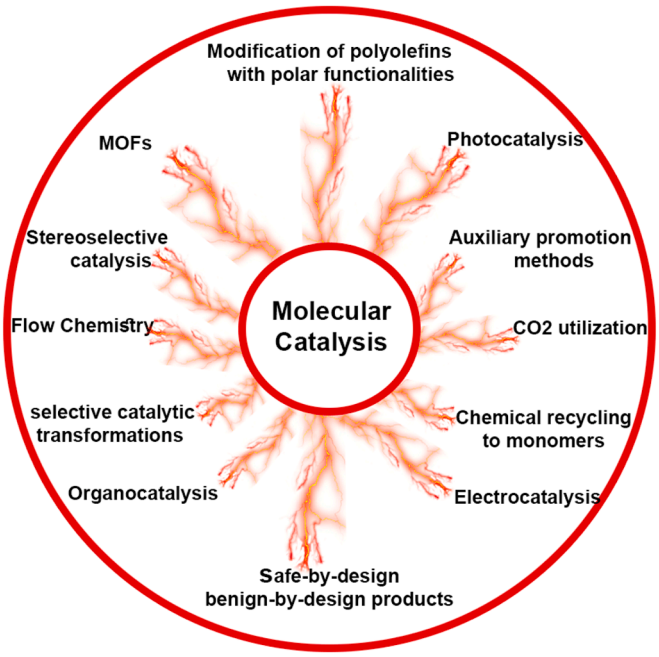

Figure 1. Impact of Molecular Catalysis in the chemistries of the future

the current chemical industry will represent one of the challenges for future White Biotechnology.

c) *A more general and widespread attention to Metal Organic Frameworks* (MOFs) as practical catalysts not only for the synthesis of specialty and fine chemicals but also for other relevant environmental-related applications in photocatalysis, the design of bionanoMOF hybrids and related topics. [3].

d) *Stereoselective catalysis of monomers obtained by renewable resources and biomass-derived.* An interesting example is the stereoselective ring opening polymerization (ROP) of lactide. The polylactides (PLAs) found important industrial applications and their mechanical and thermal properties are strongly depending on the microstructures. [4].

e) *CO_2 utilization as a C1-feedstock* by incorporating into suitable products (e.g. stereoselective CO_2/epoxide copolymerization) and/or CO_2 catalytic transformation into biosourced organic carbonates. Both aspects are combined with the primary task to develop selective, fast and efficient reduction processes of CO_2 into valuable products in a sustainable manner (e.g. carbon monoxide, formic acid, methanol, methane and so on). [5]

f) *The development of chemical recycling to monomers (CRM)* where the final polymers are transformed back into monomers and the monomers are reconsidered for repolymerization without loss in properties. This process, although at an early stage, creates an ideal circular polymer economy pushing the necessary economic and environmental synergies for a circular economy. [6]. Efficient catalytic synthesis of monomers building up biodegradable polymers, ideally from renewable resources in a carbon neutral manner, is also a key target.

g) *Modification of polyolefins with polar functionalities*. The controlled incorporation of polar monomers into the polyolefins backbone chain strongly enhances the polymer properties. The copolymerization of α-olefins with polar monomers catalyzed by late transition metals achieved significant breakthroughs in the academia although no commercial process currently exists for such reactions due to the lack of high-performance heterogeneous catalysts. [7]

h) *The design of single-atom based systems for advanced catalytic prospects,* potentially applicable to industrial premises [8].

i) *Living cells as chemical factories* with unprecedented flexibility with respect to the source of energy and material input [9]. Photoautroph organisms for example can build up complex molecules from CO_2 using visible light as energy source. To fully explore this potential, combined efforts of metabolic-, protein- and reactor engineering will be needed. Similarly, electrotroph organisms principally can utilise electrical energy to build complex products from simple carbon sources.

j) *Organocatalysis,* following up the steps of the recently granted 2021 Nobel Prize will play a fundamental role, particularly enantioselective organocatalysis in the advance synthesis of drugs and pharmaceuticals (e.g. greener enantioselective halogenations) for a more sustainable future. [10].

k) *Electro- and photo-catalysis* for the catalytic synthesis of the molecules of the future, with the potential to be extended to selective functionalisations (e.g. electro/photochemical upgrading), synthesis of pharmaceuticals and relevant high added value chemicals. [11, 12].

l) *Auxiliary promotion methods* including mechanochemistry, microwaves, ultrasound, electric and magnetic fields, and electric potentials, have all shown promise in tuning the adsorbate–active size interactions, thereby increasing the reactivity. These strategies should be widely tested in promoting various types of catalytic reactions, in particular those that are notoriously difficult to occur under mild conditions. [13, 14].

m) *The combination of Flow Chemistry and Catalysis* as a valuable tool for more scalable catalytic applications able to bring us one step closer to industrial premises [15].

The main question is which of the above lines will be predominant as the way forward in Molecular Catalysis for the Chemistry of the future? There is not an unique answer and we believe that the near future will see a flourishing demand of all identified research topics. Certainly, chemistry papers will show even more a combination of experimental and theoretical aspects with the recent input of machine learning techniques for fast catalyst screening. The combination of these key identified topics/areas (and various others) hint how chemists are preparing themselves for the challenges to come of a still undisclosed and uncertain future. At *Molecular Catalysis*, we will certainly welcome contributions providing alternatives and solutions to some of the highlighted future challenges that we hope to be enjoying for the journal in the years to come.

CREDIT AUTHOR Statement

All authors contributed to writing, revising and editing of the manuscript including conceptualization and overall shown ideas/topics.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper

References

[1] J.F.M. van der Waals, A. Falk, P. Fantke, P. Filippousi, R.C.H. Flipphi, D. Mottet, X. Trier (2019). Safe-by-design for materials and chemicals: Towards an innovation programme in Horizon Europe.
[2] U. Hanefeld, F. Hollmann, C.E. Paul, Chem. Soc. Rev. 51 (2022) 594–627.
[3] K. Shen, L. Zhang, X. Chen, L. Liu, D. Zhang, Y. Han, J. Chen, J. Long, R. Luque, Y. Li, B. Chen, Science 359 (2018) 206–210.
[4] X. Zhang, M. Fevre, G.O. Jones, R.M. Waymouth, Chem. Rev. 118 (2018), 839885.
[5] A. Akhundi, A. Badiei, G.M. Ziarani, A. Habibi-Yangjeh, M.J. Muñoz-Batista, R. Luque, Mol. Catal. 488 (2020), 110902.
[6] Y. Jing, Y. Wang, S. Furukawa, J. Xia, C. Sun, M.J. Hülsey, H. Wang, Y. Guo, X. Liu, N. Yan, Angew. Chem. Int. Ed. 60 (2021) 5527–5535.
[7] S.L.J. Luckham, K. Nozaki, Acc. Chem. Res. 54 (2021) 344–355.

[8] R. Ciriminna, M. Gharemani, B. Karimi, M. Pagliaro, R. Luque, Current Op. Green Sust. Chem. 25 (2020), 100358.
[9] M. Eisenstein, Nature 531 (2016) 401–403.
[10] A. Carlone, L. Bernardi, P. McCormack, T. Warr, S. Oruganti, C.J. Cobley, Org. Process Res. Dev. 25 (2021) 2795–2805.
[11] C. Zhu, N.W.J. Ang, T.H. Meyer, Y. Qiu, L. Ackermann, ACS Cent. Sci. 7 (2021) 415–431.
[12] S. Song, J. Qu, P. Han, M.J. Hülsey, G. Zhang, Y. Wang, S. Wang, D. Chen, J. Lu, N. Yan, Nat. Commun. 11 (2020) 4899.
[13] K. Kubota, Y. Pang, A. Miura, H. Ito, Science 366 (2019) 1500–1504.
[14] M.J. Hülsey, C.W. Lim, N. Yan, Chem. Sci. 11 (2020) 1456–1468.
[15] G. Laudadio, Y. Deng, K. Van der Wal, D. Ravelli, M. Nuño, M. Fagnoni, D. Guthrie, Y. Sun, T. Noel, Science 369 (2020) 92–96.