Open Access

Catalysis Research

LIDSEN Publishing Inc.

Editorial

Opportunities and Challenges of Molecular Catalysts

Amarachi Nkwoada *

Department of Chemistry, School of Physical Sciences, Federal University of Technology Owerri, Imo State, PMB 1526, Nigeria; E-Mails: amarachi.nkwoada@futo.edu.ng; chemistryfrontiers@gmail.com

* **Correspondence:** Amarachi Nkwoada; E-Mails: amarachi.nkwoada@futo.edu.ng; chemistryfrontiers@gmail.com

Special Issue: Opportunities and Challenges of Molecular Catalysts

Catalysis Research
2024, volume 4, issue 4
doi:10.21926/cr.2404013

Received: November 28, 2024
Accepted: November 29, 2024
Published: December 02, 2024

Keywords
Molecular catalysis; energy conversion; green chemistry; machine learning; catalyst design; renewable fuels

Molecular catalysis remains a focus of contemporary chemistry as it offers opportunities to effectuate selective, efficient transformations crucial for various uses. From enzymatic-like reactions to large-scale synthesis, molecular catalysts are a perfect example of the marriage between basic research and application. Emerging trends like iron- and cobalt-based catalysts for water splitting [1] demonstrate advancements in the synthesis of catalysts for sustainable energy conversion and environmental cleaning.

Nonetheless, molecular catalysis has its drawbacks. In the past, challenges such as catalyst deactivation, low recyclability, and poor scalability have been major drawbacks that hindered industrial application. These challenges remain the same but are magnified by the requirement to use renewable resources and work under less severe conditions. For instance, the palladium-catalyzed cross-coupling reactions are very efficient; however, their reusability and substrate generality are still areas that need further enhancement [2]. Addressing these challenges will require invention at the interface of materials science and catalysis.

The design and synthesis of molecular catalysts are two fields that are currently in their state of development. In traditional synthetic strategies, the scale and cost of production may be issues. These include high-throughput screening and computational modelling to enhance the search of catalyst libraries [3]. Ligands that are designed to selectively coordinate to specific metals, for instance, those that mimic enzymatic active sites, are the future of higher selectivity and stability as observed in hydrogen evolution catalysts from earth-abundant metals [4].

There is a lot of potential in such applications as artificial photosynthesis, selective conversion of CO_2, and renewable fuel production. The use of molecular catalysts for the electrochemical reduction of CO_2 to methanol is a good example of how chemistry can support sustainable development [4]. Likewise, molecular catalysts developed for synthetic transformations in drug discovery underlines the industrial applicability of these catalysts.

The importance of molecular catalysis research is the fact that it seeks to respond to some of the most critical global concerns, including energy security and environmental cleanup. It also makes sustainable development a reality around the globe, while at the same time decreasing the use of nonrenewable resources. In the future, the applications of molecular catalysis are still enormous. The appearance of new approaches, for example, the use of artificial intelligence in the search for new catalysts, can help in the search for new generation catalysts. Molecular catalysis promises to revolutionize chemical transformations throughout sectors when implemented with the help of interdisciplinary cooperation and proper funding [6].

Author Contributions

The author did all the research work for this study.

Competing Interests

The author declares no conflict of interest.

References

1. Gu Y, Wang L, Xu BQ, Shi H. Recent advances in the molecular-level understanding of catalytic hydrogenation and oxidation reactions at metal-aqueous interfaces. Chin J Catal. 2023; 54: 1-55.
2. Zaera F. New challenges in heterogeneous catalysis for the 21st century. Catal Letters. 2012; 142: 501-516.
3. Wegener SL, Marks TJ, Stair PC. Design strategies for the molecular level synthesis of supported catalysts. Acc Chem Res. 2012; 45: 206-214.
4. Goswami N, Bhattacharya T, Maiti D. Transient directing ligands for selective metal-catalysed C-H activation. Nat Rev Chem. 2021; 5: 646-659.
5. Brands MB, Reek JN. Mechanistic insights into electrocatalytic hydrogen evolution by an exceptionally stable cobalt complex. Inorg Chem. 2024; 63: 8484-8492.
6. Mitchell S, Martín AJ, Pérez-Ramírez J. Transcending scales in catalysis for sustainable development. Nat Chem Eng. 2024; 1: 13-15.