

## Special Issue

# Computational Catalysis for Sustainability

### Message from the Guest Editors

The past decade has seen exponential progress in computational speed and the development of robust software tools. Incorporating cutting-edge machine learning and descriptor-based methods has further propelled the exploration of catalyst screening, enabling the identification of promising candidates for sustainable catalysis with unparalleled efficiency. As computational catalysis continues to evolve, its impact on clean energy solutions and sustainability is expected to become ever more profound. This Special Issue aims to publish original computational-based investigations and reviews within the broad field of catalysis. This includes the development of new computational techniques and screening methods, as well as the rigorous application of current computational tools for discovering new catalysts, reaction mechanisms, or catalytic processes. All fields of catalysis that are driven by a substantial computational component, including, but not limited to, heterogeneous, homogeneous, organocatalysis, biocatalysis, photocatalysis, electrocatalysis, and environmental catalysis, will be considered.

---

### Guest Editors

Prof. Dr. Igor A. Pašti  
Dr. José R. B. Gomes  
Prof. Dr. Kai S. Exner

---

### Deadline for manuscript submissions

closed (30 June 2024)



## Catalysts

---

an Open Access Journal  
by MDPI

---

Impact Factor 4.0  
CiteScore 7.6



[mdpi.com/si/191447](https://mdpi.com/si/191447)

*Catalysts*  
Editorial Office  
MDPI, Grosspeteranlage 5  
4052 Basel, Switzerland  
Tel: +41 61 683 77 34  
[catalysts@mdpi.com](mailto:catalysts@mdpi.com)

[mdpi.com/journal/  
catalysts](https://mdpi.com/journal/catalysts)





# Catalysts

---

an Open Access Journal  
by MDPI

---

Impact Factor 4.0  
CiteScore 7.6



[mdpi.com/journal/  
catalysts](https://mdpi.com/journal/catalysts)



## About the Journal

### Message from the Editor-in-Chief

---

#### Editor-in-Chief

Prof. Dr. Keith Hohn  
Carl R. Ice College of Engineering, Kansas State University, Manhattan,  
KS, USA

---

#### Author Benefits

##### High Visibility:

indexed within Scopus, SCIE (Web of Science), Inspec, Ei Compendex, CAPlus / SciFinder, CAB Abstracts, and other databases.

##### Journal Rank:

JCR - Q2 (Chemistry, Physical) / CiteScore - Q1 (General Environmental Science )

##### Rapid Publication:

manuscripts are peer-reviewed and a first decision is provided to authors approximately 15.9 days after submission; acceptance to publication is undertaken in 3.5 days (median values for papers published in this journal in the second half of 2025).