

## Special Issue

# Catalytic Reaction Mechanics of Enzymatic Reactions

### Message from the Guest Editors

Theoretical methods (molecular docking, molecular dynamics simulation, quantum mechanical/molecular mechanics, and so on) are a new cross-biological means with the development of biological science and computer science technology. They have been applied to the research of biological macromolecular catalytic mechanism, protein conformation change between enzyme and ligand, which can affect the catalytic efficiency of the enzyme, and rational design of enzyme. Hence, in order to better explore the catalytic reaction mechanism of many macromolecules, it is necessary to introduce relevant research into the Special Issue to promote the development of this field. In this Special Issue, original research articles and reviews are welcome. Research areas may include (but are not limited to) the following: structure–activity relationship between protein and ligand, QM/MM enzyme catalytic reaction mechanism, structural modification of enzymes, and rational design of enzymes. We look forward to receiving your contributions.

### Guest Editors

Prof. Dr. Weiwei Han  
Prof. Dr. Minghui Li  
Prof. Dr. Lihong Hu

### Deadline for manuscript submissions

closed (10 April 2022)



## Catalysts

an Open Access Journal  
by MDPI

Impact Factor 4.0  
CiteScore 7.6



[mdpi.com/si/98401](https://mdpi.com/si/98401)

*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).