# Special Issue

# Computational and Theoretical Methods in Environmental Catalysis

## Message from the Guest Editors

This Special Issue of "Computational and Theoretical Methods in Environmental Catalysis" focuses on advancing our understanding and application of computational and theoretical approaches in catalysis for environmental remediation. Specifically, it explores the utilization of advanced computational techniques to design and optimize catalysts for environmental applications, with a particular emphasis on catalytic processes aimed at mitigating environmental pollution and promoting sustainability.

Through a collection of original research articles, reviews, and perspectives, this Special Issue provides an opportunity for researchers to exchange ideas, share insights, and showcase the latest developments in the field. Topics covered include the computational modeling of catalytic mechanisms, structure–property relationships in catalytic materials, simulation of reaction kinetics and dynamics, and development of predictive models for catalyst design and optimization.

## Guest Editors


Dr. Sanja J. Armakovic

1. Department of Chemistry, Biochemistry and Environmental Protection, Faculty of Sciences, University of Novi Sad, Trg Dositeja Obradovića 3, 21000 Novi Sad, Serbia
2. Vice President of the Association for the International Development of Academic and Scientific Collaboration—AIDASCO, 21000 Novi Sad, Serbia

Dr. Stevan Armaković

1. Department of Physics, Faculty of Sciences, University of Novi Sad, Trg Dositeja Obradovića 4, 21000 Novi Sad, Serbia
2. President of the Association for the International Development of Academic and Scientific Collaboration—AIDASCO, 21000 Novi Sad, Serbia


## Deadline for manuscript submissions

closed (30 November 2024)


# Catalysts

an Open Access Journal by MDPI

Impact Factor 4.0
CiteScore 7.6

mdpi.com/si/205791

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

mdpi.com/journal/catalysts

# Catalysts

an Open Access Journal by MDPI

Impact Factor 4.0
CiteScore 7.6

mdpi.com/journal/catalysts

MDPI

# 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 16.6 days after submission; acceptance to publication is undertaken in 2.7 days (median values for papers published in this journal in the first half of 2025).