Special Issue

Computational Chemistry and Catalysis: Prediction and Design

Message from the Guest Editors

Combining both experimental and computational methods is an interdisciplinary approach of great benefits to explain the main features of complex molecular systems involved in chemical areas at the frontiers of chemical sciences, including homogeneous and heterogeneous transition metal catalysis and organo-, photo- and photoredox catalysis. The present Special Issue intends to publish original research and review articles on the state-of-the-art of experimental and computational synergy in accounting for and exploring reactivity, selectivity, stability and mechanisms in transition metal, organo-, organic photo-, and photoredox catalysis in homo- and heterogeneous phases. Submission of articles combining experimental and theoretical approaches are particularly encouraged. Purely computational studies providing new methodologies to be used in synergy with experimental techniques and improving the current mechanistic understanding of catalytic processes will be also considered.

Guest Editors

Prof. Dr. Salah-Eddine Stiriba

- Dr. Mar Ríos-Gutiérrez
- Dr. Roberto Schimmenti
- Dr. Saurabh Bhandari
- Dr. Lahoucine Bahsis

Deadline for manuscript submissions

closed (10 February 2022)



Catalysts

an Open Access Journal by MDPI

Impact Factor 4.0 CiteScore 7.6



mdpi.com/si/26078

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



catalysts



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).

