

Special Issue

Design and Structure of Electro catalytic Materials

Message from the Guest Editor

This Special Issue, titled “Design and Structure of Electro catalytic Materials”, aims to collate innovative research across material science, chemistry, and engineering, focusing on precise structural modulation strategies—from atomic-scale tailoring to macrostructural engineering—and elucidate fundamental structure–performance relationships.

Key topics of interest include the following: 1, Novel Material Design: emerging systems such as single-atom catalysts, 2D materials, alloys, and defect-engineered architectures; 2, Advanced Characterization and Simulation: applications of “in situ”/operando techniques, machine learning-guided design, and multiscale computational modeling; 3, Structure–Function Correlations: dynamic surface reconstruction, the evolution of active sites, and synergistic mass–charge transport mechanisms; and 4, Scalable Synthesis Strategies: industrial-scale catalyst fabrication and stability enhancement approaches.

We invite the submission of original research articles, reviews, and perspectives, particularly those integrating interdisciplinary methodologies and addressing real-world applications.

Guest Editor

Dr. Riming Hu

Institute for Smart Materials & Engineering, University of Jinan, Jinan 250022, China

Deadline for manuscript submissions

closed (15 October 2025)



Crystals

an Open Access Journal
by MDPI

Impact Factor 2.4
CiteScore 5.0



mdpi.com/si/232839

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

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





Crystals

an Open Access Journal
by MDPI

Impact Factor 2.4
CiteScore 5.0



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



About the Journal

Message from the Editor-in-Chief

Welcome to *Crystals*, the journal dedicated to the fascinating world of crystallographic research! Crystals are more than mere decorative elements; they hold the key to understanding the fundamental structure of matter. Our mission is to explore the crucial significance of this research across various fields. From medicine to technology, chemistry to geology, crystals play a vital role. Their structure provides insights into new advanced materials, innovative drugs, and groundbreaking technologies. Through *Crystals*, we delve into the microscopic world to discover solutions that will shape the future. Join us on a journey through the *Crystals*, where science merges with beauty and innovation.

Editor-in-Chief

Prof. Dr. Alessandra Toncelli
Department of Physics, University of Pisa, 56126 Pisa, PI, Italy

Author Benefits

Open Access:

free for readers, with article processing charges (APC) paid by authors or their institutions.

High Visibility:

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

Journal Rank:

JCR - Q2 (Crystallography) / CiteScore - Q2 (Condensed Matter Physics)