Special Issue

New Horizons in Metal–Organic Frameworks: Fundamentals, Characterization, and Molecular Modeling

Message from the Guest Editors

Metal-Organic Frameworks (MOFs) have emerged as a revolutionary class of materials, captivating interest due to their versatile structures and tunable properties. This topic delves into the latest advancements in MOFs, emphasizing fundamental principles, characterization techniques, and the role of molecular modeling in their development. MOFs consist of metal ions or clusters coordinated with organic ligands, forming crystalline frameworks with immense surface areas and pore volumes. These characteristics enable applications in various fields, such as energy conversion, catalysis, and health applications. The synthesis of MOFs involves precise control over metal–ligand interactions, allowing for the customization of pore size and functionality. Characterization techniques such as X-ray diffraction (XRD), nuclear magnetic resonance (NMR) spectroscopy, and electron microscopy are pivotal in elucidating their structural and chemical properties. Molecular modeling, including density functional theory (DFT) and molecular dynamics (MD) simulations, plays a crucial role in predicting the behavior and stability of MOFs and guiding experimental efforts.

Guest Editors

Prof. Dr. Jesus Baldenebro-López

Faculty of Engineering Mochis Autonomous, University of Sinaloa Los Mochis, Sinaloa 81210, Mexico

Prof. Dr. Vladimir P. Fedin

Nikolaev Institute of Inorganic Chemistry, Siberian Branch of the Russian Academy of Sciences, 630090 Novosibirsk, Russia

Deadline for manuscript submissions

20 November 2025

Crystals

an Open Access Journal by MDPI

Impact Factor 2.4
CiteScore 5.0

mdpi.com/si/212667

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

mdpi.com/journal/crystals

Crystals

an Open Access Journal by MDPI

Impact Factor 2.4
CiteScore 5.0

mdpi.com/journal/crystals

MDPI

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)