Special Issue

Advances in Computer-Aided Drug Design and Molecular Dynamics Simulations

Message from the Guest Editors

With the rapid advancement of science and technology, computer-aided drug design (CADD) and molecular dynamics (MD) simulations have become increasingly prominent in drug development.

This Special Issue aims to compile the latest research findings related to CADD and MD simulations, particularly their innovative applications in biomolecular crystal studies. We welcome submissions in the following areas:

Computer-Aided Drug Design: Including structure-based drug design, virtual screening, quantitative structure-activity relationship (QSAR) models, etc.

Molecular Dynamics Simulations: MD simulations, free energy calculations, and large-scale molecular simulations et.al.

Biomolecular Crystal Studies: Involving the analysis of biomacromolecular crystal structures, growth mechanisms, and the interactions between drugs and biomolecular crystals.

Multiscale Simulations and Integrated Methods: Combining quantum mechanics, molecular mechanics, and coarse-grained models et.al.

Case Studies and Applications: Demonstrating the successful applications of CADD and MD simulations in actual drug development, including the design and optimization of anticancer, antiviral, and antibacterial drugs et.al.

Guest Editors

Dr. Xueping Hu

Prof. Dr. William J Welsh

Dr. Shaoqing Du

Deadline for manuscript submissions

closed (28 February 2025)

Crystals

an Open Access Journal by MDPI

Impact Factor 2.4
CiteScore 5.0

mdpi.com/si/212656

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)