Special Issue

AI-Enhanced Study of Biomolecular Dynamics with Molecular Dynamics Simulations

Message from the Guest Editors

Dynamics in biomolecules play an essential role in various biological processes such as enzymatic reactions, protein folding, and molecular recognition. Dynamics study in biomolecules combines computational modeling, experimental techniques, and theoretical approaches to enhance our understanding of the intricate workings of life at a molecular level. As a computational technique for studying biomolecular dynamics, molecular dynamics (MD) simulation applies principles of classical physics to simulate the motions and interactions of atoms in a biomolecule over time. With the recent success of artificial intelligence (AI) in protein structure prediction, the potential of AI to revolutionize the study of biomolecular dynamics with MD simulations has been demonstrated in many recent publications. We look forward to collecting research reporting advances in the AI-enhanced study of biomolecular dynamics with MD simulations.

Guest Editors

Dr. Wenjin Li
Institute for Advanced Study, Shenzhen University, Shenzhen, China
Dr. Muhammad Junaid
Institute for Advanced Study, Shenzhen University, Shenzhen 518060, China

Deadline for manuscript submissions

closed (30 April 2024)

Crystals

an Open Access Journal by MDPI

Impact Factor 2.4
CiteScore 5.0

mdpi.com/si/184866

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

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)

MDPI