

Special Issue

Crystallization Processes and Simulation Calculations, Fourth Edition

Message from the Guest Editors

The inherent challenges of strong coupling, nonlinearity, and large lagging in crystallization processes make designing robust, well-characterized processes for high-quality products demanding. The development of process analytical technology (PAT) for rapid, accurate inline/online measurements, alongside simulation technologies (e.g., molecular dynamics, hydrodynamics), provides multiscale insights. The integration of artificial intelligence (AI) and machine learning (ML) also offers powerful new approaches for process design and control, enabling advanced modeling, optimization, and real-time decision-making. These combined experimental, simulation, and AI/ML tools offer innovative strategies for designing and controlling crystallization processes, enabling the production of products with target quality attributes and predictable performance. This Special Issue, titled “Crystallization Processes and Simulation Calculations, Fourth Edition”, serves to provide a platform for researchers to report results and findings regarding AI-enhanced crystallization process technologies, simulation and process analytical technologies, and relevant crystallization studies.

Guest Editors

Dr. Mingyang Chen
Prof. Dr. Jinbo Ouyang
Dr. Mingxuan Li

Deadline for manuscript submissions

20 September 2026



Crystals

an Open Access Journal
by MDPI

Impact Factor 2.9
CiteScore 5.4



mdpi.com/si/246716

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 2.9
CiteScore 5.4



[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 crystal, 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, CAPus / SciFinder, and other databases.

Journal Rank:

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