Special Issue

Density Functional Theory (DFT) in Crystalline Material

Message from the Guest Editors

The density functional theory (DFT) has become a cornerstone in computational materials science, providing insights into the electronic, structural, and thermodynamic properties of crystalline materials. With advancements in computational power and algorithms, DFT enables accurate predictions of material behavior, facilitating innovations in energy storage, catalysis, semiconductors, and beyond. This Special Issue of *Crystals* aims to highlight recent breakthroughs and challenges regarding the application of DFT to crystalline systems, thereby fostering interdisciplinary collaboration among theorists and experimentalists. This Special Issue seeks to publish state-of-the-art research and reviews on DFT applications in crystalline materials, aligning with the journal scope of computational and theoretical materials science. We encourage contributions that address methodological advancements, novel applications, or the validation of DFT predictions against experimental data.

Guest Editors

Prof. Dr. Tarciso Silva Andrade-Filho

Prof. Dr. Rodrigo Gester

Prof. Dr. Mateus Ribeiro Lage

Deadline for manuscript submissions

10 February 2026

Crystals

an Open Access Journal by MDPI

Impact Factor 2.4
CiteScore 5.0

mdpi.com/si/248174

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)