



crystals



an Open Access Journal by MDPI

First Principles Calculation for Crystalline Materials

Guest Editors:

Dr. Mingqing Liao

Dr. Xiaoqiang Liu

Prof. Dr. Yingchun Ding

Dr. Zheng Chang

Dr. Jintong Guan

Dr. Fei Zhou

Dr. Xin Liu

Message from the Guest Editors

Dear Colleagues,

As an important part of the Materials Genome Initiative (MGI), the computational design of materials is gaining increasing attention. Among different computational methods, first principles calculation has rapidly developed for its accuracy and lack of dependence on empirical parameters. The method has been applied in various materials (solid, surface, 2D materials, etc.) and various properties (mechanical, optical, electronical, etc.) can be accessed by it. However, much remains to be done in the first principles community, such as the development of new theory and the design of new materials.

Deadline for manuscript
submissions:
closed (31 August 2023)

Hence, we set up a Special Issue entitled “First Principles Calculation for Crystalline Materials”, which intends to serve as a high-quality, high-speed and high-impact platform covering broad aspects of first principles simulations for communication within the first principles community.



mdpi.com/si/157753

Special Issue



crystals



an Open Access Journal by MDPI

Editor-in-Chief

Prof. Dr. Alessandra Toncelli

Department of Physics, University
of Pisa, 56126 Pisa, PI, Italy

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.

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](#), [CAPus](#) / [SciFinder](#), and [other databases](#).

Journal Rank: JCR - Q2 (*Crystallography*) / CiteScore - Q2 (*Condensed Matter Physics*)

Contact Us

Crystals Editorial Office
MDPI, St. Alban-Anlage 66
4052 Basel, Switzerland

Tel: +41 61 683 77 34
www.mdpi.com

mdpi.com/journal/crystals
crystals@mdpi.com
[X@Crystals_MDPI](https://twitter.com/Crystals_MDPI)