

Special Issue

First-Principles Prediction of Structures and Properties in Crystals

Message from the Guest Editors

This Special Issue aims at taking stock of the current state of the field, highlighting the capabilities (and perhaps, current shortcomings or future opportunities) of first-principles prediction methods of crystal structures and properties. Scientists across a range of disciplines are invited to contribute to this collection. The topics presented in the keywords cover broadly the scope of this Special Issue, but do not restrict it; innovative contributions are particularly welcome.

- crystal structure prediction techniques
- high-throughput screening
- constraint sampling
- fitness functions
- materials properties
- low-dimensional materials and interfaces
- new chemistry
- extreme conditions

Guest Editors

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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

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