

Special Issue

Crystal Structures and Electronic Properties Under High Pressure

Message from the Guest Editor

High-pressure crystal structure prediction and the study of structural phase transitions have become key frontiers in condensed matter physics and materials science. Advanced computational methods, including first-principles calculations and intelligent search algorithms, can now accurately predict novel high-pressure structures. The focus of research has shifted from discovering new phases to understanding transition pathways, mechanisms, and their dynamics, supported by in situ diffraction and X-ray spectroscopy techniques. The physical properties of materials are often determined by their crystal structures, and some novel phenomena, such as charge density wave order, are related to structural distortions or lattice modulations. The purpose of this Special Issue is to provide a platform for recent developments in the field of new crystal structure discussed in the context high-pressure, novel structure prediction methods, X-ray experiments, and current work in material properties and its applications.

Guest Editor

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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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