Special Issue

Computational Research on Crystals

Message from the Guest Editor

We are pleased to invite you to submit your ground-breaking research to this Special Issue of *Crystals*, "Computational Research on Crystals". This Special Issue aims to gather the results of applications of molecular modeling methods in the study of crystalline materials or those that are based on the molecular structures derived from corresponding crystal structures. Articles dealing with predicting the physicochemical and structural properties of materials and molecules, explaining the experimentally obtained results, or predicting the conditions required to obtain the new forms of already known materials, in order to minimize the number of experiments or optimize the experimental conditions, are especially welcome. Furthermore, as calculated properties, such as NMR shielding constants or Raman/IR frequencies, may greatly facilitate the creation of future solid-state analysis articles, presenting such results is of particular interest for this Special Issue. In this Special Issue, original research articles and reviews are very welcome

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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