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Quantum and Molecular Mechanic Analysis of Crystalline Materials

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Message from the Guest Editor

The Special Issue on “Quantum and Molecular Mechanic Analysis of Crystalline Materials” is intended to provide an opportunity for interdisciplinary and international exchange, covering a broad description of a variety of methods for modeling the structures and properties of crystalline materials and of results obtained by these methods. Having both quantum and molecular mechanic methods for analysis on board allows scientists working in a wide range of disciplines to contribute to this cause.

The topics summarized under the keywords broadly cover examples of the large number of sub-topics in mind. The volume is especially open for any innovative methodical contributions involving new programmatic developments, allowing to include unusual types of bonding, as well as aspects of bonding analysis tools and nonstandard properties.

Keywords

- crystal structure
- quantum mechanical modeling
- molecular mechanical modeling
- electronic structure methods
- force fields
- structure-properties relations

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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.

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