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First Principles Calculation for Crystalline Materials

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Deadline for manuscript submissions:
closed (31 August 2023)

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.

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.

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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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