Special Issue

First-Principles Simulation—Nano-Theory

Message from the Guest Editors

First-principles calculation is based on quantum mechanics, which was established in 1930s but is still undergoing evolution, thanks to the rapid development of supercomputers and new theories for the treatment of numerous electron systems at the desired accuracy and within reasonable computation times. First-principles calculation is rapidly broadening its application fields and enabling study of several kinds of material and nanostructure which, until recently, had been impossible to simulate. We invite researchers to contribute to the Special Issue “First-Principles Simulation—Nano-Theory”, which intends to serve as a unique multidisciplinary forum covering broad aspects of the science, technology, and applications of first-principles simulations.The potential topics include, but are not limited to:- New theory of first-principles simulation- Development of first-principles calculation code- Computer science of first-principles calculation- Simulation of molecules, solid, condensed matter, mineral, surface, and nanostructure- Simulation of nanodevice- Simulation of soft matter- Chemical and pharmaceutical application of first-principles simulation

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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