Special Issue

Density Functional Theory (DFT) and Beyond for Crystalline Materials

Message from the Guest Editors

We cordially invite you to submit a manuscript to a Special Issue of the journal Crystals, which focuses on density functional theory (DFT)-based studies of crystalline materials. The aim of this Special Issue is to present recent exciting developments and applications of DFT covering a wide variety of methodologies, including, but not limited to, ab initio molecular dynamics, relativistic DFT, many-body theory extensions (e.g., GW, DMFT), new advances in exchange–correlation functionals, time-dependent DFT, and applications related to equations of state, phase transitions, and excited state phenomena. In particular, the goal of this Special Issue is to focus on cases where standard or conventional DFT treatments fail to properly describe the relevant physics of a system, but some new or non-conventional treatments improve or resolve the issues. We aim to showcase a diverse cross section of studies spanning development methods for applications with an emphasis on improving our ability to predict real material properties.

Guest Editors

Dr. Danny A Rehn

Dr. Ann E. Mattsson

Dr. Roxanne Tutchton

Dr. Jian-Xin Zhu

Dr. Christopher Lane

Deadline for manuscript submissions

closed (20 December 2023)

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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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