Special Issue

Computational Materials Design for Band Gap Engineering

Message from the Guest Editor

Band gap engineering is an attractive area for computational materials design, and addresses the control of multiscale material features to achieve superior optical, thermal, and electronic properties. This Special Issue considers all manuscripts addressing the band gap design of crystalline materials (0d, 1D, 2D, 3D) in multiple length scales and multiple material models for a wide range of applications in energy, electronics, optoelectronics, biomedical, and aerospace industries. The current Special Issue covers all manuscripts utilizing first-principles computations, atomistic simulations, and meso-, macro-, and multi-scale algorithms to understand and design band gap in all crystalline materials, including multifunctional nanomaterials, metamaterials, heterostructures, and interfaces. We welcome all submissions from all studies dealing with computational approaches for band gap engineering.

Guest Editor

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Deadline for manuscript submissions

closed (30 August 2019)

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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.

Editor-in-Chief

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