Special Issue

Computational Phase Stabilities and Phase Tailoring of Alternative and Sustainable Hard Magnetic Materials

Message from the Guest Editors

This Special Issue aims to provide a comprehensive platform for the latest research on computational approaches to understanding, predicting, and engineering the phase stability and magnetic properties of alternative hard magnetic materials.

We invite original research articles, reviews, and short communications that address, but are not limited to, the following topics:

- First-principles calculations and atomistic simulations of phase stability in hard magnetic materials;
- Computational discovery and screening of rare-earth-free or reduced-rare-earth magnetic compounds;
- Thermodynamic modelling and phase diagram calculations for novel magnetic systems;
- Machine learning and data-driven approaches for predicting magnetic properties and phase behaviour;
- Strategies for phase tailoring and microstructure optimization to enhance magnetic performance;
- Sustainable synthesis pathways informed by computational insights;
- Case studies on the computational design of new hard magnetic materials;
- Integration of computational and experimental approaches for accelerated materials development.

Guest Editors

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Deadline for manuscript submissions

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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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