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# First-Principle Simulations of Crystalline Materials

Guest Editors:

**Dr. Giane B. Damas**

**Dr. Luciano Tavares Costa**

**Dr. Mahsa Ebadi**

**Dr. Mehdi Mahmoodinia**

Deadline for manuscript submissions:
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## Message from the Guest Editors

In recent decades, the higher accessibility to powerful computational resources has promoted the development of robust modelling techniques that have revolutionized the field of material science.

First-principle simulations constitute the core of computational chemistry, often relying on mathematical approximations to solve classical or quantum-mechanical expressions that do not require experimental information. For instance, density functional theory is appropriate for the investigation of electronic structure, as well as equilibrium and non-equilibrium processes at the zero-coverage limit. Moreover, the evaluation of diffusion and temperature effects over these properties could be assessed by means of molecular dynamics and kinetic Monte Carlo (KMC).

In this Issue, we invite the researchers from the community of material science to contribute to the understanding of atomic- and mesoscale-related processes, as well as material design and the prediction of relevant thermochemical and kinetic properties by means of first-principle simulations.

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## Editor-in-Chief

**Prof. Dr. Alessandra Toncelli**
Department of Physics, University of Pisa, 56126 Pisa, PI, Italy

## 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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## Contact Us

*Crystals* Editorial Office
MDPI, Grosspeteranlage 5
4052 Basel, Switzerland

Tel: +41 61 683 77 34
www.mdpi.com

mdpi.com/journal/crystals
crystals@mdpi.com
𝕏@Crystals_MDPI