Special Issue

Charge Density for Physical Properties in Crystals

Message from the Guest Editor

We warmly invite experts in the field to submit manuscripts related to theoretical and/or experimental aspects of charge density in both organic and inorganic solid-state materials. The focus should preferentially be on correlations among crystal/defect structure, charge density, and measurable properties, including chemical reactivity and molecular recognition. See the keyword list below for further information on the covered topics; feel free to contact us if more details are needed.

- Advances in experimental and theoretical charge density methods
- Charge density and molecular recognition, including application in crystal structure prediction and drug design
- Charge density as a tool to explain and predict measurable physical and chemical properties
- Charge density and correlated responses (thermoelectricity, piezoelectricity, pyroelectricity, shape-shifting materials)
- Spin-resolved charge density and magnetism
- Charge density for nonlinear optical applications
- Charge density and properties of complex nets, such as metal organic frameworks and supramolecular assemblies
- Charge density for biological and pharmacological applications
- Charge density in defective solids

Deadline for manuscript submissions

closed (20 January 2021)



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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

Prof. Dr. Alessandra Toncelli
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