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Theoretical Investigation on Non-covalent Interactions

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Deadline for manuscript submissions:
closed (25 May 2023)

Message from the Guest Editors

Dear Colleagues,

The problem of non-covalent interactions in crystals is one of the paradigms for computer modelling and theoretical studies in chemistry and related fields of knowledge (crystallography, biology, physics, mathematics, and computer science). Modern methods of data science, artificial intelligence, and quantum and computational chemistry are widely used for the investigation of nature and various properties of different non-covalent interactions (hydrogen, halogen, chalcogen, pnictogen, tetrel, and semi-coordination bonds; agosic and anagosic interactions; stacking, anion/cation–**π** interactions; metallophilic interactions, etc.).

Our Special Issue welcomes contributions from researchers focused on this subject to highlight and overview modern trends and attract the attention of the scientific community to the problem of theoretical investigation on non-covalent interactions.

All types of papers (reviews, full papers, communications, technical notes, highlights, etc.) are welcome for consideration.

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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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