# Special Issue

# Analysis of Halogen and Other σ-Hole Bonds in Crystals (2nd Edition)

## Message from the Guest Editor

This Special Issue of Crystals reflects the very significant role that crystallography has played in recognizing the existence of halogen bonding and arriving at an understanding of what has sometimes been described as an enigma. While halogen bonds were already observed in the 19th century, a major advance was the series of crystallographic studies by Hassel et al. in the 1960s. They characterized complexes between covalently bonded halogen atoms and oxygen/nitrogen Lewis bases, i.e., attractive interactions between two ostensibly negative sites.

The importance of halogen bonding and other sigma–hole interactions (which include hydrogen bonding) in biological systems and in areas such as the design of new materials is now well established and continues to increase.

This Special Issue intends to provide an overview of current activity. While emphasis is placed upon such interactions in crystals, related theoretical and computational analyses have also played a key part in the development of this field, which this Special Issue aims to reflect.

## Guest Editor

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## Deadline for manuscript submissions

closed (20 July 2025)

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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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