

## Special Issue

# Crystallography of Enzymes (2nd Edition)

### Message from the Guest Editors

Following the success of the first Edition, we are pleased to announce the launch of the second Edition of the Special Issue. In this second Edition, we particularly encourage contributions that expand the frontier of enzyme discovery and design. This includes studies on:

- Novel or uncharacterized natural enzymes, revealing new catalytic strategies;
- De novo designed enzymes and artificial biocatalysts, showcasing how structural insights guide structural or AI-assisted design;
- Ancestrally reconstructed enzymes, providing evolutionary perspectives on catalysis and stability;
- Engineered enzymes with improved selectivity, altered substrate scope, or novel functionality;
- Mechanistic and structural studies coupling crystallography with kinetics, spectroscopy or computation;
- Crystallization innovations enabling previously intractable enzyme targets.

We welcome original research articles, reviews and perspectives from structural biologists, biochemists, enzymologists and computational modelers. Together, these contributions will deepen our understanding of how structure encodes catalytic power and continue Francis Crick's timeless insight: "*If you want to understand function, study structure.*"

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### Guest Editors

Dr. Bo Liang

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### Deadline for manuscript submissions

20 August 2026



## Crystals

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CiteScore 5.0



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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.

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### Editor-in-Chief

Prof. Dr. Alessandra Toncelli  
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