

## Special Issue

# Catalysts and Modeling of Ammonia Synthesis Catalytic Reactions

### Message from the Guest Editor

The synthesis of ammonia has been one of the milestones of catalysis for over 100 years. It is a vital chemical compound that serves as a cornerstone in various industries, such as agriculture and the production of fertilizers and as a future fuel for the shipping industry, as well as a critical component in the manufacturing of various chemicals and materials. Within the realm of scientific exploration, the synthesis and characterization of ammonia synthesis catalysts play a pivotal role. We are seeking to collect manuscripts by leading researchers in the field that investigate how various formulations of ammonia synthesis catalysts have different catalytic activities. Also, manuscripts that focus on the mechanism for ammonia synthesis and the identification of intermediates are relevant to this Special Issue, especially with the use of in situ and operando techniques. Both experimental and computational studies are welcome. These catalyst studies may optimize the efficiency, sustainability and performance of ammonia synthesis.

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### Guest Editor

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### Deadline for manuscript submissions

20 September 2025



## Crystals

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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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