Special Issue

Design and Structure of Electrocatalytic Materials

Message from the Guest Editor

This Special Issue, titled “Design and Structure of Electrocatalytic Materials”, aims to collate innovative research across material science, chemistry, and engineering, focusing on precise structural modulation strategies—from atomic-scale tailoring to macrostructural engineering—and elucidate fundamental structure–performance relationships.

Key topics of interest include the following: 1, Novel Material Design: emerging systems such as single-atom catalysts, 2D materials, alloys, and defect-engineered architectures; 2, Advanced Characterization and Simulation: applications of “in situ”/operando techniques, machine learning-guided design, and multiscale computational modeling; 3, Structure–Function Correlations: dynamic surface reconstruction, the evolution of active sites, and synergistic mass–charge transport mechanisms; and 4, Scalable Synthesis Strategies: industrial-scale catalyst fabrication and stability enhancement approaches.

We invite the submission of original research articles, reviews, and perspectives, particularly those integrating interdisciplinary methodologies and addressing real-world applications.

Guest Editor

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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.

Editor-in-Chief

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