Special Issue

Experimental and Computational Design of Novel Structural and Functional Materials for Energy and Sustainability

Message from the Guest Editors

The search for advanced technologies to convert and store renewable energies remains a hot but challenging topic in revolutionizing the energy system. Catalysis will be an essential and powerful tool in making the shift from a fossil-fuel-based to a greener and more sustainable society. However, our understanding of the fundamental catalysis mechanism and our ability to achieve a rational design of highly efficient catalysts are still facing many problems, such as linking catalyst activity to 'turnover frequency' and explaining catalytic performance in terms of 'structure sensitivity' or 'structure insensitivity'. The 'structure–property' relationship should be well understood to guide experimental synthesis. The combination of state-of-the-art theory modeling and experiments provides an ideal approach to address the issues. The present Special Issue on "Experimental and Computational Design of Nanocatalysts for Renewable Energy Conversion" will serve as a platform to report or summarize the progress achieved in this field.

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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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