Special Issue

Synthesis, Characterization, Applications and Computational Studies of Nanomaterials

Message from the Guest Editor

Advances in the green chemical industry and sustainable energy production depend on the development of novel nanomaterials that can be used as adsorbents, catalysts, sensors, and electrodes. In this Special Issue, many fundamental aspects are discussed, such as pore size, surface area, and ligand functionalization of nanomaterials for adsorption, catalysis, and sensing. Promising energy storage systems are also included, which usually work on the principle of adsorption. Furthermore, the study of nanomaterials using computational approaches, such as ab initio, DFT, molecular dynamics, Monte Carlo, and machine learning methods, is a rapidly developing field that provides a solid foundation for understanding the structure and functional applications of nanomaterials. This Special Issue, therefore, brings together synthesis, characterization, applied and computational studies of nanomaterials, including experimental and computational results on nanomaterials and original research contributions in the fields of environmental remediation, chemical industry, sensors, biosensors, nano-drug delivery systems (NDDSs), electrochemical energy storage and conversion, etc.

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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