Special Issue

Computational Chemistry and Theoretical Catalysis for Nanomaterial-Catalyzed Chemical Conversion and Energy Storage

Message from the Guest Editors

This Special Issue of *Nanomaterials* focuses on showcasing the current state of the art in the application of computational chemistry, theoretical catalysis, and machine learning for designing and understanding catalytic materials. By compiling research that integrates these advanced methodologies, this Special Issue aims to provide fundamental insights into catalytic systems, facilitating the rational design of high-performance nanoscale catalysts. Research areas may include (but are not limited to) the following:

- Molecular insights into active sites, reaction mechanisms, and kinetics via advanced characterization, computational modeling, and experiments.
- Design and synthesis of catalyst materials guided by structure–activity relationships and machine learning.

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Message from the Editor-in-Chief

Nanoscience and nanotechnology are exciting fields of research and development, with wide applications to electronic, optical, and magnetic devices, biology, medicine, energy, and defense. At the heart of these fields are the synthesis, characterization, modeling, and applications of new materials with lower nanometer-scale dimensions, which we call “nanomaterials”. These materials can exhibit unusual mesoscopic properties and include nanoparticles, coatings and thin films, metal–organic frameworks, membranes, nano-alloys, quantum dots, self-assemblies, 2D materials such as graphene, and nanotubes. Our journal, *Nanomaterials*, has the goal of publishing the highest quality papers on all aspects of nanomaterial science to an interdisciplinary scientific audience. All of our articles are published with rigorous refereeing and open access.

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