Special Issue

Theoretical Chemistry and Computational Simulations in Nanomaterials

Message from the Guest Editors

With the rapid advancement of nanoscience and nanotechnology, researchers increasingly rely on theoretical and computational approaches for the design, prediction of properties, and optimization of nanomaterials. Theoretical chemistry and computational simulations play a pivotal role in elucidating fundamental principles, in explaining experimental phenomena, and in guiding the synthesis and applications of nanomaterials. This Special Issue provides a platform for researchers to exchange ideas, showcase cutting-edge research findings, and discuss methodological developments. This Special Issue aligns closely with the scope of the journal *Nanomaterials*, which focuses on the publication of research papers addressing both scientific and applied aspects of nanomaterials. It offers an excellent opportunity to present the latest advancements in theoretical chemistry and computational simulations within the field of nanomaterials. We welcome original research articles and reviews that cover a wide range of topics.

Guest Editors

Dr. Dashuai Wang

1. Institute of Zhejiang University-Quzhou, Quzhou 324000, China
2. Key Laboratory of Biomass Chemical Engineering of Ministry of Education, College of Chemical and Biological Engineering, Zhejiang University, Hangzhou 310027, China

Dr. Xianyun Peng

1. Institute of Zhejiang University-Quzhou, Quzhou 324000, China
2. College of Chemical and Biological Engineering, Zhejiang University, Hangzhou 310027, China

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Editorial Office
MDPI, Grosspeteranlage 5
4052 Basel, Switzerland
Tel: +41 61 683 77 34
nanomaterials@mdpi.com

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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.

Editor-in-Chief

Prof. Dr. Eugenia Valsami-Jones
School of Geography, Earth and Environmental Science, University of Birmingham, Birmingham B15 2TT, UK

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