Special Issue

Recent Advance in Molecular Modeling and Simulation of Nanomaterials

Message from the Guest Editors

We showcase computational studies of diverse nanostructures, where atomistic simulations decode structure-property relationships, stability, and interfacial behavior. Concurrently, molecular simulations of adsorption and membrane materials enable precise prediction of critical performance metrics—selectivity, adsorption capacity, diffusion kinetics, and permeance—for applications like CO_2 capture, hydrogen purification, and water desalination. Critically, the issue explores integrating machine learning (ML) in material design. Deep learning, generative models, and high-throughput screening synergistically optimize nanostructures, predict properties, and guide synthesis, transcending conventional computational limits. By bridging nanoscale insights with performance simulations and data-driven innovation, this collection demonstrates how computational strategies overcome experimental bottlenecks, unlock novel materials, and deliver scalable, sustainable solutions to global challenges. We invite original research, reviews, and perspectives advancing these frontiers.

Guest Editors

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About the Journal

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

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