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Modeling, Simulation and Optimization of Nanomaterials

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Deadline for manuscript submissions:
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Message from the Guest Editors

Dear Colleagues,

This Special Issue aims to compile cutting-edge research in the broad arena of simulation of nanomaterials, covering a wide array of state-of-the-art techniques, from density functional theory to coarse-grained molecular dynamics, and beyond. This Special Issue will not only explore mechanical behaviors but also electronic, thermal, optical, and chemical properties of nanostructured materials. We invite submissions of original research articles, reviews, and short communications that delve into any aspect of modeling, simulation, and property optimization in the context of nanomaterials. Papers employing interdisciplinary approaches, integrating insights from material science, physics, chemistry, and engineering, and those that aim to optimize material properties through either fundamental or data-driven techniques are especially welcome.

Please see more details at the following link: mdpi.com/si/184185

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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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