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Mathematical and Computational Modeling for Nanohybrids

Guest Editor:

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Deadline for manuscript submissions:
closed (10 January 2024)

Message from the Guest Editor

Dear Colleagues,

The Special Issue, entitled "Mathematical and Computational Modelling for Nanohybrids ", welcomes the numerical research of nanohybrids by means of computation, numerical analyses, modeling, and the interplay of modeling and computational mathematics. Nanohybrids are materials with organic and inorganic components that are linked together at the nanometer scale. All numerical investigations are encouraged, including first-principles calculations, molecular dynamics simulations, Monte Carlo simulations, tight-banding, phase fields, finite element methods, multiscale modeling, and other mathematical and computational models. This Special Issue will especially focus on the studies of various properties (structural, mechanical, electrical, thermal, optical, acoustic, chemical, etc.) of nanohybrids for diverse applications in energy, catalysis, electronics, optoelectronics, advanced functionals, and so on. Advanced algorithms and methods for nanohybrids from all disciplines are also desirable.

Dr. Qing Peng

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Editor-in-Chief

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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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