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Advances in Computational Materials Science on Functional Interfaces and Surfaces

Guest Editor:

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Deadline for manuscript submissions:
closed (30 September 2022)

Message from the Guest Editor

Hybridization of heterogeneous materials or heterogeneous scales is a new materials technology that has been assessed as new technology to create various functional materials. Computational materials science enables the functional interface and surface to design, invent, and forecast nanomaterials properties using computer simulation techniques such as density functional theory (DFT), molecular dynamics (MD), Monte Carlo (MC) method, finite element methods (FEM), and machine learning (ML) approaches. All topics potentially falling into the category of computational materials science will be considered, including inorganic materials (metals, ceramics, composites, semiconductors, nanostructures, 2D materials, metamaterials, etc.), organic materials (polymers, liquid crystals, surfactants, emulsions, etc.) and hybrid materials of inorganic and organic components. Both original research articles, in the form of full papers or communications, and reviews are welcome.

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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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