# Special Issue

# Advances in Computational Materials Science on Functional Interfaces and Surfaces, Volume II

## Message from the Guest Editor

Based on the successful Special Issue “Advances in Computational Materials Science on Functional Interfaces and Surfaces”, we have set up a second volume. Computational materials science enables a functional interface and surface in order to design, invent, and forecast nanomaterials’ properties by using computer simulation techniques such as density functional theory (DFT), molecular dynamics (MD), the Monte Carlo (MC) method, finite element methods (FEMs), 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 as well as organic components. Original research articles, in the form of full papers or communications, and reviews are both welcome.

## Guest Editor

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## Deadline for manuscript submissions

closed (30 November 2023)

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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

Prof. Dr. Eugenia Valsami-Jones
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