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## Computational Chemistry in Bionanotechnology

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Deadline for manuscript  
submissions:

**closed (10 March 2024)**

### Message from the Guest Editor

Dear Colleagues,

Computational chemistry techniques range from first-principle approaches, such as ab initio methods and density functional theory (DFT), which are based on quantum chemistry, to semi-empirical methods, such as density functional tight binding (DFTB), which facilitate simulations using pre-fitted parameters, to molecular mechanics (MM) and molecular dynamics (MD) calculations, which are based on approximate classical potentials.

The recent combination of nanotechnology and biology has led to the development of vital systems, both in biology and in nanoengineered materials. Bionanotechnology is today an established and cutting-edge interdisciplinary research area that is located at the interface between chemistry, physics, biology, materials science, engineering, and medicine, and that finds application in numerous technological fields.

The purpose of this Special Issue, entitled “Computational Chemistry in Bionanotechnology”, is to focus on the biomedical, food, agricultural, energy, and environmental fields.

You can see more details at the following link:  
<https://www.mdpi.com/si/180350>

Dr. Emiliano Laudadio  
Guest Editor



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# Special Issue



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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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