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Theoretical Calculation and Molecular Modeling of Nanomaterials

Guest Editor:

Prof. Dr. Frederik Tielens
General Chemistry (ALGC), Materials Modelling Group, Vrije Universiteit Brussels, 1050 Brussels, Belgium

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Message from the Guest Editor

The success of computational chemistry and chemical modeling of materials is in line with the available computation power and techniques, evolving every day. This evolution has kept chemists' skills in the limelight. Indeed, Moore's law being respected or not, modeling has now shifted to the creation of the model itself. Of course, the accuracy of calculations can be still be improved, but the main chemical properties and their trends are relatively well reproduced today. One can say that DFT is now at a mature age, and that it can be used as a reliable prediction tool in material science applications. Classical molecular dynamics is indispensable for the study of large systems. Other methods are emerging, though, such as AI-based methods. We are entering an exciting era in which our own creativity will be the limit for understanding our environment—the era of multiscale modeling. In this Special Issue, we want to focus on the construction of pertinent models that can describe and predict, as accurately as possible with the available computation power and techniques, the chemistry of nanomaterials.

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Editor-in-Chief

Prof. Dr. Shirley Chiang
Department of Physics, University of California Davis, One Shields Avenue, Davis, CA 95616-5270, USA

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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Contact Us

Nanomaterials Editorial Office
MDPI, Grosspeteranlage 5
4052 Basel, Switzerland

Tel: +41 61 683 77 34
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𝕏@nano_mdpi