

Special Issue

Progress in Quantum-Computer Calculations

Message from the Guest Editor

Electronic structure calculations have become an indispensable theoretical tool in physics, chemistry, and materials science. After four decades of rapid development, these calculations now allow us to study systems consisting of up to a few thousands of atoms. Further upscaling to yet bigger systems, such as those encountered in nanoparticles and other nanosystems, is all too often hindered by limited computer power of classical (super-)computers. Fortunately, there is a newly emerging class of quantum computers that should soon provide an exponentially higher computer power. Albeit promising, quantum computers are still in their infancy, and basic algorithms need to be developed. This Special Issue welcomes submissions focused primarily (but not solely) on recent developments in the broad field of quantum computers and their applications, especially software tools allowing for electronic structure calculations on quantum computers in physics, chemistry or materials science, as well as calculations on (i) either classical computer simulators of quantum processors or (ii) actual quantum computers.

Guest Editor

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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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