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Modeling of Complex Interfaces: From Surface Chemistry to Nano Chemistry

Guest Editor:

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Message from the Guest Editor

Quantum chemical modeling of materials has experienced a tremendous boost, which is in line with the available computational power. The accuracy of the calculations can be still be improved, but the main chemical properties and their trends are relatively well reproduced nowadays. 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. Nevertheless, DFT is especially efficient describing chemical phenomena at the molecular level, the systems studied increases continuously in size and complexity. The size of the system is directly related to the computation power, and the complexity is related to the quality of the calculation method and the representation of the chemical environment in the model. It is the latter property that brings the computational chemist's chemical intuition and general chemistry knowledge the forefront. In this Special Issue we want to focus on the construction of pertinent models that are able to describe and predict as accurately as possible with available computational power, the chemistry of materials.

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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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