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Application of Symmetry in In-Silico Studies of Materials

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Message from the Guest Editors

This Special Issue's objective is to compile recent developments in the theoretical investigations of the structural, electronic, vibrational, optical, and mechanical properties of atomic and molecular clusters of different crystal symmetry using first-principle calculations. It is evident that in silico methods that involve density functional theory (DFT) can be used to research significant materials in real-world applications and can also be utilized to create new compounds. The investigation of a variety of properties, including structural, electronic, optical, mechanical and vibrational properties, greatly benefits from the use of DFT computations. A thorough grasp of their characteristics is required to enhance the attributes of materials. In silico investigations make it possible to considerably simplify the interpretation of experimental data. It is, thus, without a doubt one of the most popular methods in materials science. It is now possible to work with complicated structures that contain numerous atoms in each cell and produce more realistic simulation results, due to the ongoing advancements in computational methods and codes, as well as increased processing capacity.

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Message from the Editor-in-Chief

Symmetry is ultimately the most important concept in natural sciences. It is not surprising then that very basic and fundamental research achievements are related to symmetry. For instance, the Nobel Prize in Physics 1979 (Glashow, Salam, Weinberg) was received for a unified symmetry description of electromagnetic and weak interactions, while the Nobel Prize in Physics 2008 (Nambu, Kobayashi, Maskawa) was received for the discovery of the mechanism of spontaneous breaking of symmetry, including CP symmetry. Our journal is named *Symmetry* and it manifests its fundamental role in nature.

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