



Advances in Theoretical and Computational Chemistry

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Message from the Guest Editor

Dear colleagues,

In this Special Issue on “Advances in Theoretical and Computational Chemistry”, we will focus on achievements in the area of theoretical and computational chemistry. Theoretical chemistry develops theoretical generalisations. Theoretical chemistry models are turned into computation software, which can calculate the structures and properties of molecules and solids. At present, computational chemistry has a great predictive power and accompanies many experiments which are hungry for theoretical confirmation. It can—in some cases—reveal unobserved chemical phenomena. It is widely applied in the design of new drugs and materials. Suitable computational chemistry methods for molecular dynamics, electronic structure theory, and other theoretical chemistry areas can serve—if properly applied—as a tool for resolving various chemistry problems...





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Editor-in-Chief

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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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