

Special Issue

Symmetry/Asymmetry in Computational and Theoretical Chemistry

Message from the Guest Editors

Theoretical chemistry significantly influences the understanding of molecular structures, predicts chemical reactions, simplifies chemical problems, and aids in predicting molecular behavior. Techniques like symmetry projection and spectral shift enhance the accuracy and efficiency of quantum calculations. In contrast, asymmetry introduces unique properties such as chirality, which is essential in chemical species and plays a vital role in designing selective catalysts and reagents. This balance between symmetry and asymmetry underscores their roles in addressing the complexity of chemical systems and offering valuable insights for advancements in chemical research. To highlight symmetry/asymmetry in computational and theoretical chemistry, we invite you to participate with a review or original research article in this Special Issue of the MDPI Symmetry journal. We believe that you would make an excellent contribution in this area. All contributions, including surface science, nanoscience, scanning tunneling microscopy, and experimental/theoretical studies, are welcome if they demonstrate significant innovation in chemical physics.

Guest Editors

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About the Journal

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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