Special Issue

10th Anniversary of *Computation*—Computational Chemistry

Message from the Guest Editors

Computational chemistry is crucial for understanding the relationship between atomic structure and material properties. Many papers, including in this journal, have been published on this topic. Simulations often simplify computations through idealizations. Methodology analysis is critical for enhancing computation quality, particularly for electronic structure using density functional theory (DFT) based on functionals. Determining which functionals align with experimental data is crucial. Additional important factors include temperature, pressure, magnetism, substitutions, and relativistic effects (for heavy elements). Accuracy is essential for evaluating similar cases like magnetic anisotropy. Improving efficiency enables exploration of complex structures representing real systems. Systematic studies unveil trends, enhancing structure-property relations with new insights. We plan to publish a Special Issue addressing current challenges and future innovations. Solid-state research, numerical analysis, machine learning, AI, computational biology, and bioinformatics are also significant in computational chemistry.

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Message from the Editor-in-Chief

You are invited to submit the results of your research for consideration and publication in *Computation,* an international open access journal, which is published monthly online by MDPI.
The editorial board and staff of *Computation* are dedicated to establishing a benchmark journal for the world scientific and engineering communities for original research articles, reviews, conference proceedings (i.e., peer reviewed full articles), and communications, in the cutting-edge areas of computational biology, computational chemistry, computational social science and computational engineering.

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