



10th Anniversary of *Computation*—Computational Chemistry

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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

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