Special Issue

Insights into the Development of Molecular Simulations in Chemical Physics

Message from the Guest Editor

Dear Professor,

Molecular simulation in chemical physics is a vital field that provides significant insights into molecular behavior. Hydrogen bonds are key interactions that significantly influence the structure and properties of many substances. The integral equation theory and Wertheim's theory offer powerful frameworks for describing molecular distributions and addressing complex interactions, including hydrogen bonds. Phase diagrams are essential tools for predicting phase transitions and understanding the stability of different phases under varying conditions. Computational methods such as Monte Carlo and molecular dynamics enable the simulation of molecular systems over time, providing detailed insights into dynamic processes and energy landscapes.

This Special Issue invites the submission of original research articles and reviews that contribute to advancing the field of chemical physics. We welcome contributions that explore these areas, driving further advancements and applications. Submission guidelines and deadlines are available on the journal's online platform.

Guest Editor

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Message from the Editor-in-Chief

As the premier open access journal dedicated to experimental organic chemistry, and now in its 25th year of publication, the papers published in *Molecules* span from classical synthetic methodology to natural product isolation and characterization, as well as physicochemical studies and the applications of these molecules as pharmaceuticals, catalysts and novel materials. Pushing the boundaries of the discipline, we invite papers on multidisciplinary topics bridging biochemistry, biophysics and materials science, as well as timely reviews and topical issues on cutting edge fields in all these areas.

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