Special Issue

Density Functional Theory: From Fundamentals to Applications

Message from the Guest Editor

Density Functional Theory (DFT) has emerged as a pivotal computational approach in quantum chemistry and condensed matter physics, bridging the gap between theoretical insights and practical applications. At its core, DFT provides a framework for understanding the electronic structure of many-body systems by expressing the energy of a system as a functional of its electron density. DFT has found extensive applications across various fields, including materials science, nanotechnology, and chemistry. It enables the prediction of molecular geometries, reaction pathways, and properties of solids, which are crucial for designing novel materials and understanding complex chemical processes. The aim of this Special Issue is to provide potential readers with an overview of recent challenges and developments in the fields of computational chemistry and molecular modeling, particularly those pertaining to gas sensing fundamental mechanism analysis and application upon 1D/2D nanomaterials. Reviews, full papers, and short communications covering the methodology, theory, and application aspects of molecular modeling are equally welcomed.

Guest Editor

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Message from the Editor-in-Chief

As the premier open access journal dedicated to molecular chemistry, now in its 30th 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 all major fields of molecular chemistry and multidisciplinary topics bridging chemistry with biology, physics, and materials science, as well as timely reviews and topical issues on cutting-edge fields in all of these areas.

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