Special Issue

Recent Advancements in Density Functional Theory (DFT) and beyond for Computational Chemistry

Message from the Guest Editors

Density functional theory (DFT) has shown unsurpassed influence in computational chemistry in terms of its performance, compared to wave-function-based electron correlation methods. However, narrow computational intricacy leads to limited DFT applications. Hence, developing new accelerating computational algorithms to obtain coherent results for complex systems at a feasible computational price is imperative. At present, technical and fundamental research surrounds excitations in solids and molecules by employing theoretical methods. Further, DFT-based analysis has been one of the most basic and important strategies for drug discovery, allowing the prediction of molecular interactions that hold together a protein and a ligand in the bound state.

The present Special Issue aims to examine new techniques such as combining computational chemistry and machine learning methods, mechanistic study, chemosensor behavior, photovoltaic and opto-electronic properties (NLO and solar cells), to obtain insightful information from DFT methods that are applicable to molecules.

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Message from the Editor-in-Chief

As the premier open access journal dedicated to molecular chemistry, now in its 29th 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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