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

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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

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