



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

Guest Editors:

**Dr. Muhammad Khalid**

Department of Chemistry,  
Khwaja Fareed University of  
Engineering & Information  
Technology, Rahim Yar Khan  
64200, Pakistan

**Dr. Muhammad Nadeem  
Arshad**

Department of Chemistry, King  
Abdulaziz University, Jeddah  
21589, Saudi Arabia

Deadline for manuscript  
submissions:

**closed (30 April 2024)**

### 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.





an Open Access Journal by MDPI

## Editor-in-Chief

### Prof. Dr. Thomas J. Schmidt

Institute of Pharmaceutical  
Biology and Phytochemistry,  
University of Münster,  
Corrensstrasse 48, D-48149  
Münster, Germany

## 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.

## Author Benefits

**Open Access:** free for readers, with [article processing charges \(APC\)](#) paid by authors or their institutions.

**High Visibility:** indexed within [Scopus](#), [SCIE \(Web of Science\)](#), [PubMed](#), [MEDLINE](#), [PMC](#), [Reaxys](#), [CaPlus / SciFinder](#), [MarinLit](#), [AGRIS](#), and [other databases](#).

**Journal Rank:** JCR - Q2 (*Chemistry, Multidisciplinary*) / CiteScore - Q1 (*Chemistry (miscellaneous)*)

## Contact Us

*Molecules* Editorial Office  
MDPI, St. Alban-Anlage 66  
4052 Basel, Switzerland

Tel: +41 61 683 77 34  
[www.mdpi.com](http://www.mdpi.com)

[mdpi.com/journal/molecules](http://mdpi.com/journal/molecules)  
[molecules@mdpi.com](mailto:molecules@mdpi.com)  
[X@Molecules\\_MDPI](https://twitter.com/X@Molecules_MDPI)