Special Issue

Recent Advances in DFT: Theory, Simulations and Applications

Message from the Guest Editor

DFT methods have become very popular today and have become an invaluable tool for many researchers across a range of disciplines. This is due to the pragmatic observation that it is less computationally intensive than other methods with similar accuracy, or even better in some cases, such as in the theoretical prediction of vibrational spectra. Thus, DFT methods have widespread applications for the investigation of the electronic structure and chemical processes of many systems, in special molecules and condensed phases, which is crucial for molecular design and chemical synthesis. DFT methods provide invaluable information, complementary to the experimental data, about molecular systems and processes, and thus they represent very powerful tools for the interpretation and understanding of experimental results. Due to the importance of DFT methods and their extensive applications, unpublished manuscripts that report these applications to any organic, inorganic or organometallic system and their experimental values are welcome for this Special Issue. In addition, advances in theoretical methods will also be accepted.

Guest Editor

Dr. Mauricio Alcolea Palafox
Departamento de Química-Física, Facultad de Ciencias Químicas, Universidad Complutense de Madrid, 28040 Madrid, Spain

Deadline for manuscript submissions

closed (30 November 2019)

Molecules

an Open Access Journal by MDPI

Impact Factor 4.6
CiteScore 8.6
Indexed in PubMed

mdpi.com/si/20300

Molecules
Editorial Office
MDPI, Grosspeteranlage 5
4052 Basel, Switzerland
Tel: +41 61 683 77 34
molecules@mdpi.com

mdpi.com/journal/molecules

Molecules

an Open Access Journal by MDPI

Impact Factor 4.6
CiteScore 8.6
Indexed in PubMed

mdpi.com/journal/molecules

MDPI

About the Journal

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.

Editor-in-Chief

Prof. Dr. Thomas J. Schmidt
Institute of Pharmaceutical Biology and Phytochemistry, University of Münster, Corrensstrasse 48, D-48149 Münster, Germany

Author Benefits

High Visibility:

indexed within Scopus, SCIE (Web of Science), PubMed, MEDLINE, PMC, Reaxys, CaPlus / SciFinder, MarinLit, AGRIS, and other databases.

Journal Rank:

JCR - Q2 (Biochemistry and Molecular Biology) / CiteScore - Q1 (Organic Chemistry)

Rapid Publication:

manuscripts are peer-reviewed and a first decision is provided to authors approximately 16.1 days after submission; acceptance to publication is undertaken in 2.6 days (median values for papers published in this journal in the first half of 2025).