International Journal of
Molecular Sciences

IMPACT FACTOR 4.9 | Indexed in: PubMed | CITESCORE 9.0

an Open Access Journal by MDPI

DFT Applications in Molecular Biology and Biophysics

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 (20 February 2025)

Message from the Guest Editor

Dear Colleagues,

Density functional theory (DFT), in its various forms, is a computational quantum method that has become an invaluable tool for many researchers across a range of disciplines. DFT methods provide the best combination of accuracy and efficiency, and they are extensively used today in the prediction of the biomolecular structure and electronic properties of many systems, in computer-aided drug design, in catalysis and chemical reactivity, in surfaces and periodic solids, in transport, optical and magnetic properties, etc. The combination of DFT calculations with molecular dynamics promises to provide an efficient way to study structures and reactions in molecules and extended systems. They are less computationally demanding than other computational methods, and have a similar accuracy.

This Special Issue aims to collect papers related to any aspect of DFT Applications in Molecular Biology and Biophysics, including molecular simulations, structure predictions, and inter-molecular interactions, in computer-aided drug design and in all biomolecules more generally.

Dr. Mauricio Alcolea Palafox
Guest Editor

International Journal of
Molecular Sciences

IMPACT FACTOR 4.9 | Indexed in: PubMed | CITESCORE 9.0

an Open Access Journal by MDPI

Editor-in-Chief

Prof. Dr. José L. Quiles
Department of Physiology, Institute of Nutrition and Food Technology "Jose Mataix", Biomedical Research Center, University of Granada, Avda. Conocimiento s/n, 18100 Armilla, Granada, Spain

Message from the Editor-in-Chief

The *International Journal of Molecular Sciences* (*IJMS*) is an open access journal, which was established in 2000. The journal aims to provide a forum for scholarly research on a range of topics, including biochemistry, molecular and cell biology, and molecular biophysics. *IJMS* publishes both original research and review articles, and regularly publishes special issues to highlight advances at the cutting edge of research. We invite you to read recent articles published in *IJMS* and consider publishing your next paper with us.

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, PMC, MEDLINE, Embase, CAPlus / SciFinder, and other databases.
Journal Rank: JCR - Q1 (Biochemistry and Molecular Biology) / CiteScore - Q1 (Organic Chemistry)

Contact Us

International Journal of Molecular Sciences Editorial Office
MDPI, Grosspeteranlage 5
4052 Basel, Switzerland

Tel: +41 61 683 77 34
www.mdpi.com

mdpi.com/journal/ijms
ijms@mdpi.com
𝕏@IJMS_MDPI