Special Issue

DFT Applications to Biomolecules and Complex Reactions

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 are the best combination of accuracy and efficiency, and they are extensively used today in the prediction of biomolecular structure and the electronic properties of many systems, in computer-aided drug design, in catalysis and chemical reactivity, in surfaces and periodic solids, in transport, and in 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.

This Special Issue seeks to collect papers related to any aspect of DFT applications to biomolecules and complex reactions, including molecular simulations, structure predictions, inter-molecular interactions, and spectroscopic calculation, as well as theoretical developments and experiments.

Guest Editor

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

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

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The International Journal of Molecular Sciences (*IJMS*, ISSN 1422-0067) 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, molecular biophysics, molecular medicine, and all aspects of molecular research in chemistry. *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.

Editor-in-Chief

Prof. Dr. Maurizio Battino
Department of Odontostomatologic and Specialized Clinical Sciences, Sez-Biochimica, Faculty of Medicine, Università Politecnica delle Marche, Via Ranieri 65, 60100 Ancona, Italy

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