Special Issue

DFT Applications in Molecular Biology and Biophysics

Message from the Guest Editor

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.

Guest Editor

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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.

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