



DFT Applications in Molecular Biology and Biophysics

Guest Editor:

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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





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Message from the Editor-in-Chief

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