Special Issue

Molecular Dynamics Simulations of Biomolecules

Message from the Guest Editors

Molecular dynamics (MD) computational studies have played a critical role in both detailed atomic-scale and coarse-grained level information of a physical system. The MD simulation techniques have established their relevance in modern drug development processes, all-atom simulations of protein folding, protein–ligand docking, and mechanisms of large biomolecular networks. With remarkable advances in computing hardware and theoretical advancement, it is now possible to run longer MD simulations and thus a highly promising future of MD simulations. The aim of this Special Issue is to present recent applications of MD simulations in life sciences, especially in the context of interactions and free energy landscapes. This Special Issue is open to researchers working with MD simulations at any of these levels: a) thermodynamics, b) dynamics, and c) structural or conformational transitions. Original research papers and review articles that address the MD simulations of biomolecules are all welcome.

Guest Editors

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The concept of entropy is traditionally a quantity in physics that has to do with temperature. However, it is now clear that entropy is deeply related to information theory and the process of inference. As such, entropic techniques have found broad application in the sciences.

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