Special Issue

Molecular Dynamics Simulation of Biomolecules

Message from the Guest Editor

Biomolecules play a big role in serving life functions. Understanding how they function can help us not only understand disease mechanisms and potential novel therapeutics, but also design new materials and industrial processes that can be more environmentally friendly and efficient. While many experiments can describe and elucidate what we observe on the macroscopic level, it does not explain microscopic phenomena in atomistic or molecular detail. Therefore, molecular dynamics simulations can be a tool to supplement experiments to help us understand and elucidate biochemical reactions, processes, biomolecular properties, and supramolecular assemblies of biomolecules. Starting from quantum calculations and scaling up into hybrid quantum mechanics/molecular mechanics and classical molecular mechanics simulations, we would like to understand biochemical processes and biomaterial properties more adequately at the molecular level. Topics can include but are not limited to photosynthesis, carbohydrates, lipids, combustion, nucleic acids, protein synthesis, metabolite self-assembly, protein folding, metabolite self-assembly, inter-cellular signaling, and intra-celluar signaling.

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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