

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-cellular signaling.

Guest Editor

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