Biomolecular Simulation: Methodology Advancements and Applications

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Molecular simulation has become an important tool in modern computational chemistry and biochemistry. Nevertheless, accuracy and efficiency of the approach still need further improvement to achieve the goal of robust and predictive simulation, particularly for large and complex biomolecular systems. The accuracy issue arises from the intrinsic limitations of classical models that have to be used to approximate the quantum molecular processes. The efficiency issue is a direct consequence of the high dimensionality of biomolecular systems: sophisticated molecular machines are complexes of thousands to millions of atoms. What further complicates the picture is the need to realistically model the interactions between biomolecules and their surrounding water molecules. In this talk, I will review our developments of biomolecular simulation models and methods and their applications to interesting biomedical systems from cancer biology and biosynthesis of natural products.

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