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Molecular simulations of biological molecular functions

生体分子機能の分子シミュレーション

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Protein functional processes involve dynamic molecular conformational changes of complex protein systems which often correlate with enzymatic chemical reactions. Hence molecular mechanism of enzymatic activities and coupling of the chemical reactions with protein molecular dynamics underlying functional processes need to be revealed for understanding of molecular nature of protein functions. For the purpose, hybrid quantum mechanical/molecular mechanical (QM/MM) methods have been widely utilized. The methods allow one to perform quantum chemistry for chemical reactions at reaction centers in large surrounding molecular environments of proteins described with molecular mechanics and molecular dynamics approaches. In this lecture, theoretical background of the QM/MM methods along with their several applications to enzymatic reactions and dynamics will be presented.

Keywords: enzymatic activity, protein dynamics, rational design of molecular function, hybrid QM/MM method, molecular dynamics method