# Theoretical studies on oxidation of molecules by combining MD and QM/MM calculations

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Oxidation-reduction (Redox) reaction in protein complex, which is caused by an electron transfer between metal-containing active sites, occurs in the photosynthesis and metabolism in *vivo*. Since the redox reaction can be applied to the development of high performance fuel bio-cell, the understanding of redox mechanism of solute should be important in both industry and biology. In the experimental study, the redox potential of several organic molecules and metalloproteins have been estimated so far. The difference of redox potential between oxidant and reductant $\Delta E_0$ has been shown to be correlated with the thermodynamic free energy of formation $\Delta G_0$ [1-3]. In the computational study, this difference of redox potential can be calculated by summing the free energy difference of the oxidant and reductant in solution. The oxidation/reduction potential has been estimated by quantum chemical calculation with PCM method [4]. However, due to the poor treatment of solvent in the calculation, the resultant redox potential has shown to be in disagreement with experimental observation.

In this study, we thus carry out the molecular dynamics simulations of oxidant and reductant of organic molecule and metalloprotein in explicit water solvent and estimate the difference of redox potential $\Delta E_0$ of the reactions by using hybrid quantum/molecular-mechanics (QM/MM) calculations. The evaluated difference of oxidization/reduction potentials is compared with the experimental data. We discuss the reaction directionality from these results.

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