

# 日本生物物理学会北海道支部講演会

講師：John E. Straub 氏

Boston University, Department of Chemistry



日時：平成24年5月14日（月）15:00-16:15

場所：理学部5号館5-206室

講演題目：*Dynamics of methionine ligand rebinding in cytochrome c*

講演要旨：

Geminate recombination of the methionine ligand to heme iron in ferrous cytochrome c protein following photodissociation displays a rich kinetics. It is of particular interest to develop an understanding of “fast” and “slow” rebinding timescales, observed in experimental studies, in terms of features of the underlying complex energy landscape. Using classical molecular dynamics, an algorithm based on the Landau-Zener non-adiabatic transition theory has been employed to model the electronic surface hopping between two spin states during the process of ligand dissociation and recombination. Multiple conformational substates of the dissociated methionine ligand are found to participate in the reaction dynamics. Varying timescales for interconversion between substates lead to a mechanism elucidating the “fast” and “slow” rebinding time scales. The reaction system may be understood in terms of a two-dimensional reaction coordinate distinctly separated from the coupled bath of surrounding protein and solvent degrees of freedom. Insights into the reaction dynamics provided by this study lead to suggestions for future experiments to further probe the role of dynamic heterogeneity in the kinetics of ligand-protein binding.

ボストン大学化学科 John E. Straub 先生は Journal of Chemical Physics の Associate Editor を務められている方で、化学反応から蛋白質のダイナミクス全般を対象に精力的に研究を進めてこられています。今回、日本に訪問される機会を利用して、北海道大学にもお越しいただきました。上記のとおり講演会を開催致しますので、皆様奮ってご参加下さい。

連絡先：北海道大学電子科学研究所

小松崎民樹

電話&FAX 011-706-9434

電子メール tamiki@es.hokudai.ac.jp