第 5 回量子生命科学セミナー

日時：　2003 年 11 月 14 日（金）10：50〜12：20

場所：　理学部 E002 室

講演題目：　Quantum Chemical Studies Relevant to Biochemistry:
Electron Transfer in Ifc3 Cytochrome and Clustered Damages in DNA

講演者：　Dr. Michel Dupuis
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内容：

We will illustrate the application of quantum chemical approaches to the molecular-level characterization of the structure and mechanisms of biochemical interest. Ifc3 is a four heme cytochrome that plays a key role in bacterial respiration toward, for example, reduction of soluble metals to insoluble form. Large-scale DFT calculations in connection with Marcus's model provide detailed insight in the mechanism of electron transfer. Cluster damages in DNA are usually associated with low dose ionizing radiation. Large-scale DFT calculations provide detailed structural and energetic information about base damages in DNA.