Frontier Chemistry Center
フロンティア化学教育研究センター 講演会

演 題：**Motion of Nuclei and Motion of Electron**

講 師：**Prof. Nikita Matsunaga**

Department of Chemistry & Biochemistry,

Long Island University, Brooklyn, NY 11201, USA

日 時：2013 年 1 月 8 日（火）14:30~15:30

場 所：理学部 7 号館 7-2-19 室

要旨：

It has become possible to incorporate anharmonic effect in the calculations of molecular vibration beyond harmonic approximation. If the molecule of interest is moderate size, one can approach molecular vibration through vibrational self-consistent field approach. If, however, the molecule is diatomic, it is possible to perform spectroscopic accuracy calculations using latest ab initio potential. In this talk, development of perturbation theory based on vibrational self-consistent field theory, as well as the ro-vibrational spectra of F_2 at spectroscopic accuracy are presented.

Moore's law, which states that the speed of the computer doubles every 18 months, has been already no longer applicable since the dimension of individual transistor size is near molecular dimension. Electronic devices of near future must be designed by fully incorporating quantum mechanics. Single-molecule electronic device would be the ultimate goal. Electron conduction mechanisms of molecules in nano-pore device will be elucidated. From this, possibility of single-molecule diode has emerged.

本講演は、大学院総合化学院『化学研究先端講義／総合化学特別研究第二』の一部として認定されています。

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