Fragment molecular orbital calculations with ABINIT-MP(X)

Yuji Mochizuki[1,2]
[1]*Department of Chemistry, Faculty of Science, Rikkyo University, Japan*
[2]*Institute of Industrial Science, The University of Tokyo, Japan*

I. Introduction

The fragment molecular orbital (FMO) scheme proposed by Kitaura [1] has been one of promising recipes to treat large scale molecules such as proteins in a quantum mechanical manner with practical costs of computation through the natural parallelism. FMO-related methodological developments and associated applications have been achieved in diverse ways during this decade [2]. This presentation will cover various topics of FMO calculations performed with our original program, ABINIT-MP(X) [3,4].

II. Correlated calculations

Higher-order treatments up to CCSD(T) have been available with a hybrid parallelization of OpenMP/MPI. The FMO-CCSD(T)/6-31G job for a complex between HIV-1 protease (198 residues) and lopinavir could be processed in 9.8 h on the Earth Simulator (ES2) with 512 processors. The largest target was an influenza hemagglutinin trimer (HA3) with two Fab fragments (total 2351 residues) at the FMO-MP3/6-31G level, where this job was completed in 5.8 h with 1024 processes of ES2.

CIS(D) type calculations incorporating some higher-order effects have been used to evaluate the electronic transition energies of photoactive proteins as well as the hydrated molecules. The excitation energies of yellow- and blue fluorescent proteins (YFP and BFP) were estimated to be 2.53 and 3.36 eV, respectively, being in good agreement with the corresponding experimental values of 2.41 eV and 3.21/3.25 eV [5].

III. Molecular dynamics

Molecular dynamics (MD) calculations could be performed with the FMO-based energy gradients straightforwardly [6]. Several organic reactions in water were analyzed by FMO-MD, and the dynamical features such as diversity of pathway were revealed. The hydration structures of metal ions were simulated as well.

YM thanks Dr. Tatsuya Nakano, Prof. Shigenori Tanaka, Dr. Kaori Fukuzawa, Dr. Yuto Komeiji, Mr. Katsumi Yamashita and others for collaborative works. YM is also indebted for supports by JST-CREST project, MEXT-Kakenhi and Rikkyo SFR-aids.

[1] K. Kitaura, et al., *Chem. Phys. Lett.* **313** (1999) 701.
[2] D.G. Fedorov, K. Kitaura, ed. "*Fragment Molecular Orbital Method*", CRC (2009).
[3] T. Nakano et al., *Chem. Phys. Lett.* **351** (2002) 475.
[4] Y. Mochizuki et al., *Chem. Phys. Lett.* **493** (2010) 346.
[5] N. Taguchi et al., *Chem. Phys. Lett.* **504** (2011) 76.
[6] Y. Komeiji et al., *J. Mol. Struct.* (*THEOCHEM*) **898** (2009) 2.