“Large-scale correlated calculations with fragment molecular orbital scheme”

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The fragment molecular orbital (FMO) scheme invented by Kitaura et al., a decade ago [1,2], is one of promising recipes to treat large scale molecules such as proteins in a fully quantum mechanical (QM) framework, where the introduction of environmental electrostatic potential (ESP) is a key factor to maintain chemical reliability. Not only HF method but also various correlated methods such as MP2 are straightforwardly usable in the FMO context. An additional attractive point of FMO should be an inherent affinity with parallelism. In fact, a number of practical applications to bio-chemically relevant proteins had been reported [3,4]. The largest FMO-MP2/6-31G* calculation was performed on the influenza antigen-antibody system consisting of more than 900 residues by using a small cluster computer with 16 cores [3].

Recently, we have been promoting the next-generation FMO calculations in which (1) higher-order correlated methods would be adopted and (2) factorization-based integral approximations would also be introduced. Along the direction of (1), a parallelized coupled cluster (CC) [5,6] module has been developed, where approximated treatments such as CEPA-1 or MP4 could also be supported. The parallelization would be done in two compatible ways of flat MPI and hybrid MPI/OpenMP. The direction of (2) should correlate with the speed-up of FMO calculations for statistical discussion through multiple structure sampling of protein. In order to factorize integrals, we have adopted the Cholesky decomposition (CD) [7,8] and then FMO-MP2 calculations would be accelerated by about 10 times [9]. On the poster, I will present the recent topics of (1) and (2) as well as a brief review of our FMO calculations published to date.

[1] Kitaura et al. *Chem. Phys. Lett.* **312** (1999) 319. [2] Kitaura et al., *Chem. Phys. Lett.* **313** (1999) 701. [3] Fedorov et al. *J. Phys. Chem.* A **111** (2007) 6904. [4] Ed. by Fedorov & Kitaura, “The Fragment Molecular Orbital method”, CRC press (2009). [5] Cizek, *J. Chem. Phys.* **45** (1966) 4256. [6] Bartlett et al., *Rev. Mod. Phys.* **79** (2007) 291. [7] Beebe et al. *Intern. J. Quant. Chem.* **12** (1977) 683. [8] Pedersen et al., *Theor. Chem. Acc.* in press. [9] Okiyama et al., ICQC2009, C98.