C-1-03

FMO calculations for nano-biotechnology

Yuji Mochizuki[1,2] **Yoshio Okiyama**[2] **Kaori Fukuzawa**[2,3]
fullmoon@rikkyo.ac.jp okiyama@iis.u-tokyo.ac.jp kaori.fukuzawa@mizuho-ir.co.jp

Chiduru Watanabe[2] **Kouichiro Kato**[3] **Takayuki Tsukamoto**[3]
chiduru@iis.u-tokyo.ac.jp kouichiro.kato@mizuho-ir.co.jp takayuki.tsukamoto@mizuho-ir.co.jp

Tatsuya Nakano[4] **Shigenori Tanaka**[5]
nakano@nihs.go.jp tanaka2@kobe-u.ac.jp

[1] Department of Chemistry & Research Center for Smart Molecules, Faculty of Science, Rikkyo University, 3-34-1 Nishi-ikebukuro, Toshima-ku, Tokyo 171-8501, Japan
[2] Institute of Industrial Science, University of Tokyo, 4-6-1 Komaba, Meguro-ku, Tokyo 153-8505, Japan
[3] Mizuho Information & Research Institute Inc., 2-3 Kanda-nishiki-cho, Chiyoda-ku, Tokyo 101-8443, Japan
[4] Division of Medicinal Safety Science, National Institute of Health, 1-18-1 Kamiyoga, Setagaya-ku, Tokyo 158-8501, Japan
[5] Graduate School of System Informatics, Department of Computational Science, Kobe University, 1-1 Rokkodai, Nada-ku, Kobe 657-8501, Japan

Keywords: four-body corrected fragment molecular orbital (FMO4) method, solid, peptide

The fragment molecular orbital (FMO) method [1] has now been popular in the field of computational biochemistry and pharmachemistry, where proteins with a few hundred amino acid residues can be routinely computed within Kitaura's original two-body expansion (FMO2) of fragments. In Ref. [2], we developed the four-body extension (FMO4) in which the contribution from up to fragment tetramers are included. FMO4 provides better accuracy than does FMO2, and furthermore it makes the treatment of 3-dimensional cluster models of solids (with proper band-gap) tractable. The applicability of FMO4 to solids is promising to attack various important problems in the nano-biotechnology as an emerging field (e.g. fabrication of safer implants or protein-based chemical sensors). In this context, we [3] recently reported the FMO4 calculations to investigate the interaction between a designed peptide, with sequence of Arg1-Lys2-Leu3-Pro4-Asp5-Ala6 [4], and the silica surface modeled by a large cluster model including 257 silicon atoms (under an explicitly hydrated condition). The electron correlation effect was taken into account at the second-order perturbation (MP2) level with the Cholesky decomposition technique for acceleration. The importance of three charged residues (Arg1, Lys2 and Asp4) in the peptide-silica interaction was found, where the contributions from not only the electrostatic attraction but also the charge-transfer were addressed. The poster will resume the details of calculations and results in Ref. [3].Additionally, some preliminary data about ionic solids such as apatite and alkali halide will be presented as well.

[1] *The Fragment Molecular Orbital Method: Practical Applications to Large Molecular Systems*, edited by D. G. Fedorov, K. Kitaura (2009, Boca Raton, CRC press).
[2] "Development of the four-body corrected fragment molecular orbital (FMO4) method", T Nakano, Y. Mochizuki, K. Yamashita, C. Watanabe, K. Fukuzawa, K. Segawa, Y. Okiyama, T. Tsukamoto, S. Tanaka, Chem. Phys. Lett., 523 (2012) 128-133.
[3] "Modeling of peptide - silica interaction based on four-body corrected fragment molecular orbital (FMO4) calculations", Y. Okiyama, T. Tsukamoto, C. Watanabe, K. Fukuzawa, S. Tanaka, Y. Mochizuki, Chem. Phys. Lett., 566 (2013) 25-31.
[4] "A Hexapeptide Motif that Electrostatically Binds to the Surface of Titanium", K. Sano, K. Shiba, J. Amer. Chem. Soc. 125 (2003) 14234-24235.