

Abstract Submitted  
for the MAR09 Meeting of  
The American Physical Society

**Electronic Structure Analysis for Proteins on the FMO Method**

TOMOKI KOBORI, SHINJI TSUNEYUKI, KEITARO SODEYAMA, University of Tokyo, KAZUTO AKAGI, Tohoku University, KIYOYUKI TERAOKURA, JAIST, HIDETOSHI FUKUYAMA, Tokyo University of Science — The enormity and complexity of proteins have rendered their electronic structure calculation very costly. Although recently established Fragment Molecular Orbital (FMO) method enables us to calculate total energy of a huge protein precisely based on quantum mechanics, the method does not refer to one-electron orbitals and one-electron energy spectrum. In this paper we propose a method of analyzing electronic structure of a protein based on first principles calculation with reasonable accuracy and CPU cost. We construct one-electron Hamiltonian of proteins by assembling the output of the FMO method: fragment orbitals are determined by fragment monomer calculation, while interaction and overlap between fragment orbitals in different fragments are obtained from dimer calculation. After one-electron Hamiltonian matrix of the whole system is fabricated with the fragment orbital basis, one-electron energy spectrum is obtained by its diagonalization. If the matrix dimension is too large, unimportant orbitals are eliminated from the matrix so that the diagonalization of the Hamiltonian becomes feasible. The method is applicable to both the Hartree-Fock method and the density functional theory. In this paper, validity of the method is verified by some test calculations of small peptides.

Tomoki Kobori  
University of Tokyo

Date submitted: 19 Nov 2008

Electronic form version 1.4