Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Development of electronic structure calculation for biomolecules based on fragment molecular orbital method with three-body term
TOMOKI KOBORI, graduate student, SHINJI TSUNEYUKI, Professor, KEITARO SODEYAMA, Post doctoral researcher — Recently established fragment molecular orbital (FMO) method enables us to calculate total energy of large molecules very precisely with less computational cost than conventional molecular orbital methods. The method firstly divides a biomolecule into N fragments. Secondly calculations of all fragments and fragment pairs are performed, and finally total energy can be obtained with those of fragments. We recently developed a method of calculating electronic structure of the whole system based on FMO. In this method, called FMO-LCMO, one-electron Hamiltonian of the whole system is constructed by assembling fragment Hamiltonians described by fragment molecular orbitals, with which one-electron energy spectrum and wave functions of the whole system are obtained easily[1]. In this presentation we propose a new scheme of FMO-LCMO based on the three-body FMO method, in which fragment trimers are taken into account in the total energy calculation. It will be demonstrated that the accuracy of the energy spectrum and wave functions of large molecules is drastically improved by considering fragment-fragment interaction through Hamiltonians of fragment trimers [1]

Chem.Phys.Lett. 476,104-108(2009)

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Date submitted: 20 Nov 2009 Electronic form version 1.4