Biomolecular calculations based on electron-correlated fragment molecular orbital methods

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This talk will review recent developments in the ab initio fragment molecular orbital (FMO) method and its applications to bio-macromolecules, especially focusing on the roles of electron correlations.

Kitaura et al. [1] have proposed an ab initio FMO method by which large molecules such as proteins and nucleic acids can be easily treated with chemical accuracy. In the ab initio FMO method, a molecule or a molecular cluster is divided into fragments, and the MO calculations on the fragments (monomers) and the fragment pairs (dimers) are performed to obtain the total energy that is expressed as a summation of the fragment energies and inter-fragment interaction energies (IFIEs) [2]. Recently, the FMO methodology has been developed so as to include the descriptions of various properties other than energies and the electron correlation effects on the bases of MP2 [3], DFT [4], CI [5] and QMC [6] methods.

The ABINIT-MP and BioStation Viewer programs have been used for the applications of FMO method [7]. For instance, the FMO method was applied to the problem of transcriptional regulation, including the interactions of nuclear receptor, ligand molecule, transcription factor and DNA [8-10]. Detailed interactions between biomolecules and the roles of each amino acid residue were revealed through analyses of IFIEs, charge distribution and orbital configuration [11]. Electrostatic and van der Waals dispersion interactions were found to be equally important in molecular recognition. It was thus found that the inclusion of electron correlation was essential to obtain appropriate pictures for biomolecular interactions. Other applications such as the photo-excitation process in fluorescent protein [12] will also be illustrated.

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