

***Ab initio* fragment molecular orbital method and its application to large bio-molecules**

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Abstract. We are developing an approximate *ab initio* MO method, the fragment MO (FMO) method, for the calculation of the structures and properties of large molecules and molecular clusters. In this method, a molecule is divided into small fragments and *ab initio* MO calculations on the fragments and the fragment pairs are performed to obtain the total energy and properties of the molecule. The FMO method has been shown to accurately reproduce the total energy and the structures of molecules obtained from conventional *ab initio* MO calculations. The advantage of the method is its ease in utilizing parallel processing, since fragments and fragment pairs are calculated independently. Using this method, the binding energy between lysozyme (a protein with about 2,000 atoms) and tri-[N-acetyl-gulcosamin] (an inhibitor) was calculated at the HF/6-31G level. An analysis of interaction between each amino acid residue and the ligand revealed that several residues play an important role in the binding of the ligand.