FMO-MO 法による大規模分子軌道計算
－A Large Scale Molecular Orbital Calculation Using Fragment Molecular Orbital Method－

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We have been developing the computational tool to obtain the molecular orbitals for large molecules such as proteins and molecular clusters without excessive calculation costs. In our method, the entire Fock matrix is generated by the technique based on the fragment molecular orbital method [1], which is applicable to large systems and suitable for the parallel processing. To solve the large scale generalized eigenproblem, we use Sakurai-Sugiura method [2]. Because this method solves several number of linear equation which has a large granularity and master-worker type of execution, the method is sufficient for parallel processing on the computers of the distributed memory parallel architecture. And the method is favorable to calculate only a small number of eigenvalues and corresponding eigenvectors of the large scale matrix. Our method has high parallelization efficiency and the communication cost is negligible to the total calculation costs. Thus, this is one of the right applications for using the Grid technology.

HOMO and LUMO of Lysozyme are depicted in Figure. Reaction centers of Lysozyme are clearly shown in the Figure.

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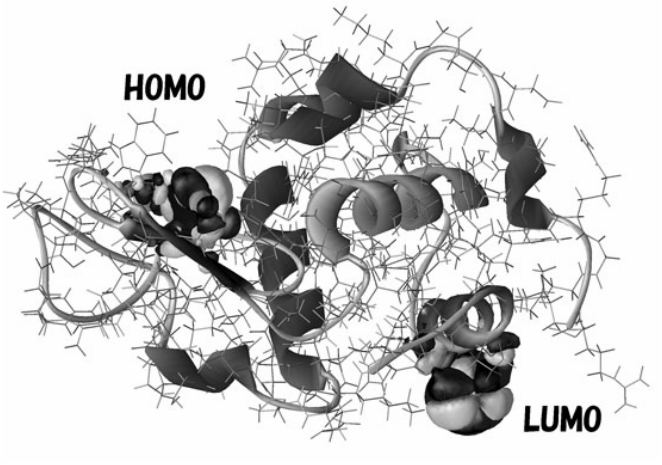

Figure. HOMO and LUMO of Lysozyme.

【References】

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[2] T. Sakurai and H. Sugiura, J. Comput. Appl. Math., 2003, **159** 119.