Fragment Molecular Orbital Method Program ABINIT-MP: Application to Proteins

Tatsuya Nakano[*1], Tsuguchika Kaminuma[*1], Masami Uebayasi[*2] and Toshiyuki Sato[*3],

[*1]National Institute of Health Sciences, [*2]National Institute of Bioscience and Human-Technology, [*3]Fuji Research Institute Corporation, University of Tsukuba,

Recently we have proposed the fragment molecular orbital method for calculating large molecules such as proteins. The method, with some modifications for a practical convenience, was applied to some small proteins. The calculated total energies were well compared with those from the conventional ab initio MO method; the errors were within about 2 kcal/mol. It indicates that the fragment MO method is sufficiently accurate and useful to study electronic properties of large molecules.