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Fragment molecular orbital method: analytical energy gradients

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Abstract

The fragment molecular orbital (FMO) method, which aimed to calculate large molecules such as proteins, was proposed in a previous work. The method divides a molecule into small fragments and performs MO calculations on the fragments and the fragment pairs to obtain the total energy of molecule. The method with the analytical energy gradient at the HF level of theory has been incorporated into the GAUSSIAN 94 (G94) package. Geometry optimization calculations using the energy gradients were successfully performed on a model peptide, methyl-capped glycine trimer.

1. Introduction

Recently, we proposed the fragment molecular orbital (FMO) method for calculating large molecules and molecular clusters. [1–3] The method divides a molecule into fragments and MOs of fragments and fragment pairs are calculated to obtain the total energy and properties of the molecule. The method avoids the MO calculation of whole molecule and is expected to reduce computational time drastically for large molecules. Another advantage of the method is its ease in utilizing parallel processing, since the fragments and the fragment pairs can be calculated independently.

The method has been incorporated into the ABINIT ab initio MO package [4] (ABINIT-MP) and the GAUSSIAN 94 (G94) package [5] (FragG94). Both programs are parallelized for the FMO calculations. The ABINIT-MP program is parallelized using message-passing interface (MPI) [1] and runs on a supercomputer equipped many processors [3]. The largest calculation performed so far is the single point energy calculation of estrogen receptor (a protein with 240 amino acid residues; 4000 atoms) at the HF/STO-3G level [6]. It took 7.8 h on HITACHI SR8000 using 256

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[1] MPI: A Message-Passing Interface Standard, MPI forum, 1995.

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