Development and Applications of the Fragment Molecular Orbital Method

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Abstract

The fragment molecular orbital method (FMO)[1] is a powerful tool to handle very large systems quantum-mechanically. This is accomplished by dividing a molecule into fragments (monomers) and then performing individual monomer and dimer calculations in the Coulomb field due to other fragments. Systems as large as consisting of 20,000 atoms were computed by the method.

1. Dmitri G. Fedorov, Kazuo Kitaura, *J. Phys. Chem. A, 111,* 6904-6914 (2007).

2. Tsutomu Ikegami, et al., *Proc. of the ACM/IEEE SC|05 Conference*, p.10 (2005).