Recent development of the fragment molecular orbital method

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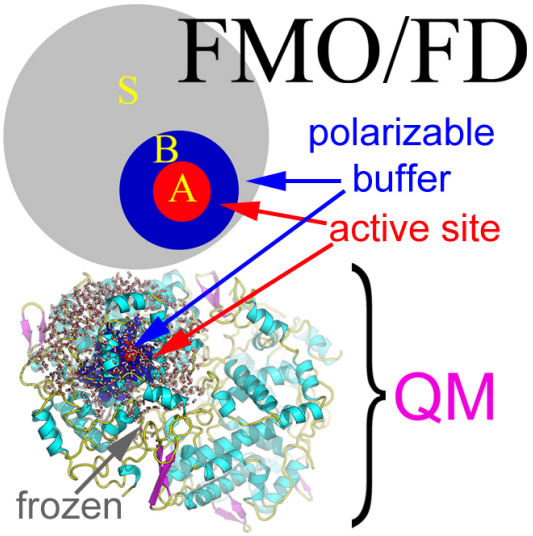
The fragment molecular orbital (FMO) method [1] enables large scale quantum-mechanical calculations of systems containing thousands of atoms, using conventional methods such as RHF, DFT or MP2. In FMO, the system is divided into fragments, and the total properties are computed from those of fragments and their pairs. Recent progress in the method development will be reviewed, including the fast geometry optimisation method FMO/FD [2], followed by a summary of recent applications [3]. More information about FMO including freely distributed software can be found in [4].



In FMO with frozen domain (FD), only the essential part of the system, polarizable buffer B including the active site A, is recomputed at each point in a geometry optimisation. The rest of the system, domain F, is computed only at the initial geometry. The complex of prostaglandin H(2) synthase-1 and ibuprofen, containing 19471 atoms at the B3LYP-D/6-31G* level for domain A and RHF/STO-3G for F was optimised in 32 h on 6 dual CPU quad-core 2.83 GHz Xeon nodes using GAMESS.

References

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[2] D. G. Fedorov, Y. Alexeev, K. Kitaura. Geometry optimization of the active site of a large system with the fragment molecular orbital method. J. Phys. Chem. Lett. 2 (2011) 282-288.

[3] T. Sawada, D. G. Fedorov, K. Kitaura. Role of the key mutation in the selective binding of avian and human influenza hemagglutinin to sialosides revealed by quantum-mechanical calculations. J. Am. Chem. Soc. 132 (2010) 16862-16872.

[4] http://staff.aist.go.jp/d.g.fedorov/