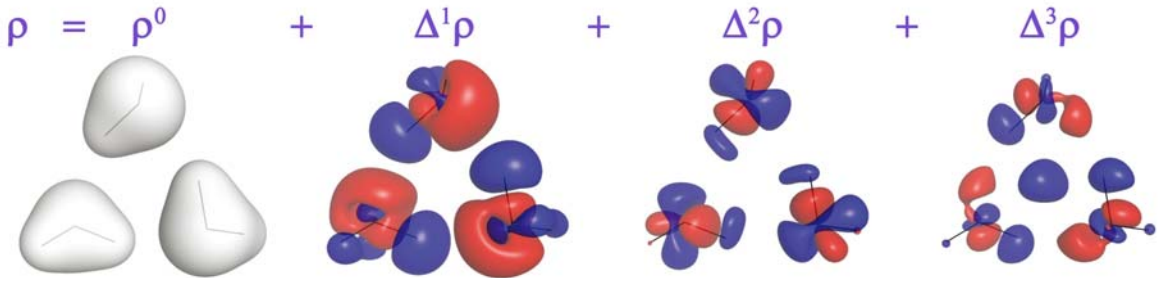
Properties of proteins and nano materials calculated with the fragment molecular orbital method

Dmitri G. Fedorov
CD-FMat, AIST, Tsukuba, Japan

By fragmenting large molecular systems into pieces called fragments and computing the properties of fragments and interactions between them, one can perform quantum-mechanical calculations very efficiently and also obtain very rich insight into their properties. The two types of systems in the title are only two important examples, and other systems can be treated as well.

The fragment molecular orbital method (FMO) is based a series expansion of properties such as energy or electron density ρ. In the series, the starting point is the electronic state of isolated fragments, to which the polarization, charge transfer and other physically well-defined contributions are added.

By enhancing the series expansion with a decomposition analysis, it is possible to evaluate the **polarization**, **electrostatic interaction**, **charge transfer (CT)**, **exchange-repulsion**, **dispersion**, **solvent screening** and other properties. As an example, the total electron density ρ of a cyclic water trimer can be decomposed as



isolated **polarization** **pairwise charge transfer** **CT coupling**

The interaction energies between fragments provide useful insight into molecular recognition of drug ligand molecules by amino acid residues in proteins. FMO can also be used to compute electronic excited states, IR and Raman spectra, and other properties. Geometry optimizations and MD simulations of large molecular systems can be performed. For nano materials, density of states can be computed from a series expansion of the Fock matrix.

The FMO program is distributed free of charge inside GAMESS package. Several GUIs are also available (Facio, FU and others).

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