Quantum Chemistry for Photo Biology and Giant Molecular System

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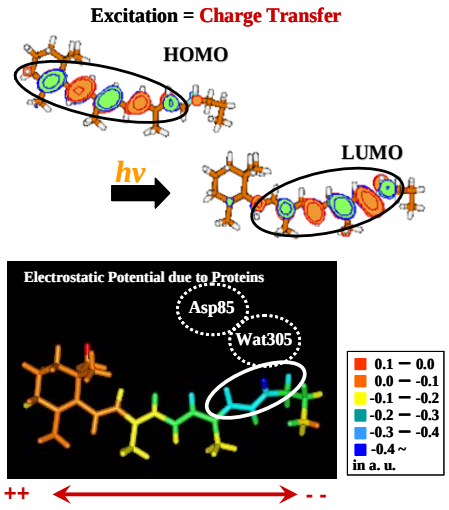
Photo-electronic processes in biochemical and giant-molecular systems are of much interest and importance as key steps in biology and molecular engineering. Quantum chemistry offers basic methodologies for clarifying the principles behind the phenomena. For studying complex phenomena, the methodology must be reliable enough, since otherwise, it is impossible to draw meaningful conclusions from the calculations.

The SAC/SAC-CI method[1] is a useful and reliable established method for studying ground, excited, ionized and electron attached states of molecules: singlet-to-septet ground and excited states of one and two-electron processes with energy gradients. Its program code is widely distributed through Gaussian03[2] and a detailed explanation of the theory, wide applicability, program accounts, how-to-use-it, and references were given in the SAC-CI home page of our laboratory[1].

In this talk, we present some applications of our SAC/SAC-CI methodology combined with the MM method to photo-biological processes like those in photosynthetic reaction centers,[3] retinal proteins,[4] and firefly luciferase,[5] etc. Figure shows a mechanism of color-tuning in retinal proteins.[4] It was shown that the reliability of the theory was crucial for clarifying the electronic origins of the processes.



We then show an extension of this method to giant molecular systems.[6] For investigating giant systems, size-extensivity in energy and size-intensivity of properties must be satisfied. We show that these properties are certainly satisfied by our method. We apply the giant SAC/SAC-CI method to the calculations of potential energy curves of the ground and excited states of some molecular crystals.

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