Quantum Entangled Photosynthesis and OR Logic Gates Controlling Minimal Artificial Cell

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Abstract: Density functional theory methods were used to investigate self-assembled photoactive bioorganic system of interest for logically controlled artificial minimal cell. The cell system studied is based on cytosine and noncanonical oxo-guanine nucleobases and consisted of up to 366 atoms and are up to 2.5 nm in diameter. The electron correlation interactions responsible for the weak hydrogen and Van der Waals chemical bonds increase due to the addition of a polar water solvent molecules. The distances between the separated sensitizer, nucleobase, fatty acid precursor, and water molecules are comparable to Van der Waals and hydrogen bonding radii. As a result the associated electron correlation interactions compress the overall system resulting in an even smaller gap between the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) electron energy levels and photoexcited electron tunneling occurs from the sensitizer (bis(4-diphenylamine-2-phenyl)-squarine and 1,4-bis(N,N-dimethylamino)naphthalene) to the precursor fatty acid, or to the cytosine molecules. Analysis of time dependent density functional theory method calculated absorption spectrum and images of electron transfer trajectories in the different excited states allow to separate quantum entangled photosynthetic transitions or destruction of 8-oxo-guanine::cytosine supramolecule. Two variable quantum OR logic gate consists of three subsystems: two photoactive sensitizer molecules and 8-oxo-guanine::cytosine supramolecule (or pFA) molecule, *i. e*. containing two different variable inputs and two different outputs.

KEYWORDS: quantum self-assembly of photosynthetic centers; visualization of photoexcited electron tunneling from sensitizers to precursor fatty acid molecules; molecular logical gates controlling photosynthesis and self-reproduction; quantum entangled photosynthesis