THEORETICAL MODELING

Phenomenon of Quantum Entanglement in a System Composed of Two Minimal Protocells

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Abstract The quantum mechanical self-assembly of two separate photoactive supramolecular systems with different photosynthetic centers was investigated by means of density functional theory methods. Quantum entangled energy transitions from one subsystem to the other and the assembly of logically controlled artificial minimal protocells were modeled. The systems studied were based on different photoactive sensitizer molecules covalently bonded to a noncanonical oxo-guanine::cytosine supramolecule with the precursor of a fatty acid (pFA) molecule attached via Van der Waals forces, all surrounded by water molecules. The electron correlation interactions responsible for the weak hydrogen and Van der Waals chemical bonds increased due to the addition of polar water solvent molecules. The distances between the separated sensitizer, nucleotide, pFA, and water molecules are comparable to Van der Waals and hydrogen bonding radii. As a result, the overall system becomes compressed, resulting in photo-excited electron tunneling from the sensitizer (bis(4-diphenylamine-2-phenyl)-squarine or 1,4-bis(N,Ndimethylamino)naphthalene) to the pFA molecules. Absorption spectra as well as electron transfer trajectories associated with the different excited states were calculated using time dependent density functional theory methods. The results allow separation of the quantum entangled photosynthetic transitions within the same minimal protocell and with the neighboring minimal protocell. The transferred electron is used to cleave a "waste" organic molecule resulting in the formation of the desired product. A two variable, quantum entangled AND logic gate was proposed, consisting of two input photoactive sensitizer molecules and one output (pFA molecule). It is proposed that a similar process might be applied for the destruction of tumor cancer cells or to yield building blocks in artificial cells.

Keywords Quantum self-assembly · Photosynthetic centers · Minimal protocell · Minimal cell · Electron entangled molecular orbitals · Electron transfer · Quantum entangled photosynthesis · Molecular quantum entangled logical gate

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