Quantum entanglement in photoactive prebiotic systems

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Abstract This paper contains the review of quantum entanglement investigations in living systems, and in the quantum mechanically modelled photoactive prebiotic kernel systems. We define our modelled self-assembled supramolecular photoactive centres, composed of one or more sensitizer molecules, precursors of fatty acids and a number of water molecules, as a photoactive prebiotic kernel systems. We propose that life first emerged in the form of such minimal photoactive prebiotic kernel systems and later in the process of evolution these photoactive prebiotic kernel systems would have produced fatty acids and covered themselves with fatty acid envelopes to become the minimal cells of the Fatty Acid World. Specifically, we model self-assembling of photoactive prebiotic systems with observed quantum entanglement phenomena. We address the idea that quantum entanglement was important in the first stages of origins of life and evolution of the biospheres because simultaneously excite two prebiotic kernels in the system by appearance of two additional quantum entangled excited states, leading to faster growth and self-replication of minimal living cells. The quantum mechanically modelled possibility of synthesizing artificial self-reproducing quantum entangled prebiotic kernel systems and minimal cells also impacts the possibility of the most probable path of emergence of protocells on the Earth or elsewhere. We also examine the

quantum entangled logic gates discovered in the modelled systems composed of two prebiotic kernels. Such logic gates may have application in the destruction of cancer cells or becoming building blocks of new forms of artificial cells including magnetically active ones.

Keywords Photosynthetic prebiotic kernel · Quantum self-assembly of prebiotic kernel · Quantum entangled molecular orbitals · Photosynthesis in prebiotic kernels · Quantum entangled photosynthesis · Photosynthetic minimal cell · Electron density transfer · Electron spin density transfer · Quantum entanglement in systems composed of two prebiotic kernels · Molecular quantum entangled logical gates

Introduction

Albert Einstein, Boris Podolsky, and Nathan Rosen described the EPR paradox (Einstein et al. 1935) early in 1935. This was the origin of research into quantum entanglement. Erwin Schrödinger et al. published papers where introduced the term “quantum entanglement” (Schrödinger and Born 1935; Schrödinger and Dirac 1936). Anton Zeilinger also contributed much experimental work toward the discovery of the phenomenon of quantum entanglement. The work of his research group opened up the new fields of quantum teleportation, quantum information, quantum communication and quantum cryptography (Brukner and Zeilinger 2009).

One can also ask whether quantum effects might play a role in processes associated with life because of the biomolecular derivatives in cells are nanoscale systems where quantum effects play a significant role for their function at this scale.

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Discoveries in recent years suggest that nature often uses self-assembly and photosynthesis—the process by which early emerged part of microorganisms which harvest and convert sun radiation energy, carbon dioxide and water into bioorganic derivatives. Our investigated self-assembly of molecules towards supramolecular bioorganic systems mostly depends on the quantum mechanics laws which induce hydrogen and Van der Waals bondings.

Photosynthesis also strictly depends on absorption of quantum portions of light energy. Presence of photosynthesis in nature and in our artificial cells quantum mechanical investigations is one of the most important biochemical reactions on Earth and important in the oldest photo biogenic metamorphosized sedimentary rocks in the world. These oldest fossils of photosynthetic living organisms were found in the Isua Greenstone Belt in Greenland aged 3.7–3.85 billion years (Fedot and Whitehouse 2002; Mojzsis et al. 1996; Nutman et al. 2009; Ohtomo et al. 2013).

Our discovered phenomenon of the quantum entanglement in the prebiotic systems enhance the photosynthesis in the proposed systems because simultaneously excite two prebiotic kernels in the system by appearance of two additional quantum entangled excited states (Tamulis et al. 2012, 2013, 2014; Tamulis and Grigalavicius 2014). We can propose that quantum entanglement enhanced the emergence of photosynthetic prebiotic kernels and accelerated the evolution of photosynthetic life because of additional absorbed light energy, leading to faster growth and self-replication of minimal living cells. The results of quantum entangled photosynthetic enhancement in prebiotic kernels are shortly written in the “[Example of quantum entanglement in vitamin D possessing biological system](#)” section of this article. More detailed description how quantum entanglement enhanced the emergence and accelerated the evolution of photosynthetic prebiotic systems one can find in the “[Phenomenon of in a quantum entanglement photoactive prebiotic kernel](#)” and “[Quantum entanglement in photoactive prebiotic kernel systems](#)” sections of this paper.

We had noticed that in the simulations of photosynthesis within a photosynthetic prebiotic kernel which contained two spatially separated photoactive molecules (sensitizers) [described in the paper (Tamulis and Tamulis 2008)], that for some excited states, quantum entangled charge transfer interactions between the two separated photoactive molecules sometimes took place. The occurrence seemed to be independent of the geometry optimization procedure, i.e., changing the separation distance between these molecules. We originally did not publish the apparent quantum entanglement results then (early 2008) thinking that the result was an occasional aberrant outcome of our quantum calculations.

Existing examples of quantum entanglement in living systems

During last few years several authors have reported that living systems may use quantum coherence and entanglement effects for photosynthesis and also for magnetic orientation during migration in more than 50 species of birds, fishes, insects, etc. (for example Pauls et al. 2013).

Furthermore, Engel et al. (2007) found evidence for quantum coherence in energy transfers in the photosynthetic system of the Fenna–Matthews–Olson bacteriochlorophyll complex of green sulphur bacteria. The apparent quantum coherence effectively yields a ‘wire’ connecting a large peripheral light-harvesting antenna, the chlorosome, to the reaction centre. Collini et al. (2010) presented two-dimensional photon echo spectroscopy measurements on two evolutionarily related light-harvesting proteins isolated from marine cryptophyte algae, which reveal exceptionally long-lasting excitation oscillations with distinct correlations and anti-correlations even at ambient temperature. These observations provide compelling evidence for quantum-coherent sharing of electronic excitation across the 5-nm-wide proteins under biologically relevant conditions, suggesting that distant molecules within the photosynthetic proteins are ‘wired’ together by quantum coherence for more efficient light-harvesting in cryptophyte marine algae.

In accordance with theoretical predictions given in paper (Cai et al. 2010), experimental evidence (Sarovar et al. 2010) suggests that quantum entanglement may exist in a protein structure that is central to photosynthesis in green an oxygenic bacteria.

These research results imply that some aspects of molecular and cellular biological science must be described with quantum physics. For example, a team of scientists at the National University of Singapore suggests that it is quantum entanglement between the electron clouds of nucleic acids in DNA that holds DNA together (Rieper et al. 2011). Rieper et al. modelled the electron clouds of nucleic acids in DNA as a chain of coupled quantum harmonic oscillators with dipole–dipole interactions between nearest neighbours resulting in a van der Waals type bonding. These authors showed that, for realistic parameters, nearest neighbour entanglement is present even at room temperature. These authors found that the strength of the single base von Neumann entropy depends on the neighbouring sites. Thus, we can question the notion of treating single bases as logically independent units. Rieper et al. derived an analytical expression for the binding energy of the coupled chain in terms of entanglement. They showed the connection between entanglement and correlation energy, a quantity commonly used in our quantum

chemistry calculations (Tamulis et al. 2012, 2013, 2014; Tamulis and Grigalavicius 2014).

Upon further reflection and noting that the active components of the artificial living systems synthesized at the Los Alamos National Laboratory (LANL) (Rasmussen et al. 2003) that we were modelling contained on the order of 10^3 atoms, it occurred to us that quantum effects might indeed play a role. Due to this small size, all the active processes (including the self-assembly from component molecules, the absorption of light, and the metabolism) should in principle be investigated using quantum (wave) theory (Tamulis et al. 2006, Tamulis et al. 2008; Tamulis and Tamulis 2007a, b). This encouraged us to perform the systematic search of quantum entanglement phenomenon in the photosynthetic prebiotic kernel systems.

LANL scientists introduced the term “protocell” for the extremely simple, self-reproducing artificial cells that they were attempting to synthesize (Rasmussen et al. 2003). Using quantum mechanical methods, our research group successfully simulated the structure and absorption spectrum associated with the LANL protocell, achieving a difference in wavelength of only 0.2 nm from the most intense experimental absorption line. This was in spite of the fact that due to computing limitations we had to work with a reduced number of fatty acids covering the photosynthetic centre of this protocell (Tamulis et al. 2006, 2008; Tamulis and Tamulis 2007a, b). We concluded that the main quantum mechanical processes of self-assembled photosynthetic supramolecules such as their energy levels/spectra and electron charge hopping primarily depends on the mutual separation of the photosensitizers molecules and the resource molecule on which they are acting and secondarily on the number fatty acid and water molecules. In our earlier publications, we used multiple different terminologies: “artificial living organisms” (Tamulis et al. 2006), “artificial minimal living cells” (Tamulis and Tamulis 2007b), “minimal living cell” (Tamulis and Tamulis 2007a), “self-assembled protocells” (Tamulis et al. 2008), “minimal artificial cell” (Tamulis et al. 2012), “minimal cell” and “minimal protocell” (Tamulis et al. 2013), and other similar names, for what in this paper we refer to “photosynthetic prebiotic kernel”. This is done to establish a consistent terminology and to emphasize that such a supramolecular prebiotic kernel involving quantum entanglement could have played a central role in the start photosynthetic life on Earth. In particular we note that these kernels, while being very small in total atom count, nonetheless possess ability to produce fatty acid molecules associated with building of containers of living organisms. More complex self-replicating protocells covered by fatty acid molecules most probably rapidly emerged due to the quantum entangled photosynthesis because of more absorbed light energy. According to our investigations the

quantum mechanical laws were important in the processes of incorporation of nucleotides in these protocells and evolution towards our defined Fatty Acid World because of possibility to absorb light energy in the yellow and red regions of Sun spectrum (Tamulis and Grigalavicius 2010a, 2011, 2014).

We agree that these definitions might be once again discussed because this is new emerging field of science. However, the name of these supramolecular derivatives is not important. The most important is that we have modelled quantum mechanically the self-assembly of the complex prebiotic kernels systems and quantum entangled photosynthetic phenomena in these simplest minimal cells. We discovered that the emergence of the more complex supramolecular systems possessing nucleotides directly depends on the quantum mechanical laws due to possibility to absorb the yellow and red Sun spectrum energy and due to quantum entangled possibility to absorb more light energy (Tamulis 2008a; Tamulis and Grigalavicius 2010a, b, 2011, 2014; Tamulis et al. 2012, 2013, 2014). Might be that our discovered photosynthetic Fatty Acid World life (Tamulis and Grigalavicius 2010a, 2011) firstly emerged the Isua Greenstone Belt in Greenland which is aged 3.7–3.85 billion years ago, making it among the oldest sedimentary rocks in the world. Examination of the isotopic carbon composition of the apatite therein by geoscientists (Fedot and Whitehouse 2002; Mojzsis et al. 1996; Nutman et al. 2009; Ohtomo et al. 2013) shows that some of it is extraordinarily light, which is indicative of a biogenic origin. Thus these scientists suggest that life already existed on the planet at least 3.7–3.85 billion years ago.

The goals of this review paper are:

1. to discuss the quantum effects including entanglement phenomenon in biological systems in such a way that biologists have an idea that quantum mechanics is omnipresent in living systems (“[Example of quantum entanglement in vitamin D possessing biological system](#)” section);
2. to present various self-assembled photosynthetic structures that we designed, including calculations of their optical properties using time dependent density functional theory (TD-DFT) and a comparison of those results with experimental ones;
3. to summarize the discovered quantum entanglement phenomena in these photosynthetic prebiotic kernel based systems; and
4. to explore the potential use of the discovered quantum entangled logical gates. This could provide a means of controlling photosynthesis in systems composed of photosynthetic prebiotic kernels. The use of quantum entangled logical gates could also provide a basis for future synthesis and spectroscopic measurements.

In the work presented here, quantum entanglement takes the form of a quantum superposition of the active components in artificial living systems. When a quantum calculation of an entangled system is made that causes one photoactive molecule of such a pair to take on a definite value (e.g., electron density transfer or electron spin density transfer), the other member of this entangled pair will be found to have taken the appropriately correlated value (e.g., electron density transfer or electron spin density transfer). Thus, one would expect there to be a correlation between the quantum calculation results performed on entangled pairs; this correlation being maintained even though the entangled pair may have had their separation distances subsequently changed. In our simulations, such changes in separation distance changes took place during geometry optimization procedures, which mimic real-world intermolecular interaction processes. The phenomenon of quantum entanglement was in fact constantly observed during the geometry optimization procedure of the two sensitizers in our photosynthetic prebiotic kernel.

Our quantum entanglement calculations were performed at zero degrees Kelvin and our final structures are partially the result of the initial molecule arrangement selected at the beginning of the optimization procedure (Tamulis et al. 2012, 2013). The starting arrangements were based on our previous quantum mechanical geometry optimizations of single molecules and subsystems. No *ab initio* molecular dynamics calculations were performed to explore the conformational space, since the ultimate results we were interested in were the electronic excitations and charge density gradients associated with them. These in turn will be mostly determined by the proximity of the molecules that are governed by the intermolecular long-range interactions, such as Coulomb and Van der Waals forces. Such interactions can be adequately described by including dispersion correction terms into our optimization. Furthermore, exploring all the possible configurations of these molecules together with explicit solvent molecules using quantum mechanical studies can't be performed at present on systems as large as ours.

We expect that our quantum entanglement calculations results should also be applicable in room temperatures situations based on the work (Cai et al. 2010) where the authors proved that quantum entanglement can be continuously generated and destroyed by non-equilibrium effects in an environment where no static entanglement exists. Therefore we may expect that quantum entanglement can be observed in our photosynthetic kernels or even in the complex biological processes of natural living systems.

All the photosynthetic charge transfers to the precursor of fatty acid molecule (pFA) investigated in our research involve the hopping of photoexcited electrons (including quantum entangled electron density transfer) from the

sensitizer (for example, either a bis(4-diphenylamine-2-phenyl)-squaraine or a 1,4-bis(*N,N*-dimethylamino)naphthalene) to the pFA molecule which results in its cleavage. The new fatty acid produced by this photosynthetic reaction joins the existing the assembly causing it to grow. Repetition of the photosynthetic reaction results in additional growth resulting in a fatty acid micelle or vesicle with an incorporated photosynthetic assembly, i.e., a minimal living cell. The quantum entanglement could have played an important role in the first stages of origins of life and evolution of biospheres because it enhances the photosynthesis, leading to faster growth and self-replication of minimal living cells.

Longer term goals in the use of quantum mechanical simulations might provide a basis for future synthesis and spectroscopic measurements of quantum entangled logic gates which may have application in the destruction of cancer cells or becoming building blocks of new forms of artificial cells including magnetically active ones (Tamulis et al. 2012, 2013, 2014; Tamulis and Tamulis 2008). The solution of basic questions of emergence and evolution of the first living cells or protocells is tightly connected with the rapidly developing field of artificial living technologies in several laboratories around the world. The possibility of synthesizing artificial magnetically active self-reproducing cells also impacts the possibility of the understanding of the emergence of living protocells on the Earth or elsewhere (Tamulis et al. 2014; Tamulis and Grigalavicius 2014).

Example of quantum entanglement in vitamin D possessing biological system

Despite that biological systems are relatively large and wet and existing in relatively large temperatures, some local parts of these systems works exclusively according the quantum physics laws. This concerns the self-assembly (Formation) of supramolecular living systems due to the quantum mechanically conditioned hydrogen bonding and Van der Waals forces. An absorbance of discrete quantum portions light spectrum and the consequencing reorganization of these supramolecules due to the absorbance of light energy is another omnipresent quantum effect in living systems. The quantum portions light energy goes In Formation of living supramolecular derivatives. The origin of word Information is from the Latin verb *informare*, which means to give form. Later the additional quantum portions of light energy goes to Re-Formation of these supramolecules. The quantum physics initiated changes of biological supramolecules leads to Positional Information that causes further to the biological functions of photosynthesis, metabolic reactions, growing, self-replication

and self-reproduction of biological systems possessing cell structure.

We will present for biologists in this section the shortly described bioorganic system where will demonstrate omnipresent quantum effects without detailed explanations. We will give the short statements of our obtained results of quantum mechanical investigations and will formulate the conclusions. That will give for biologists the common view about the omnipresent quantum effects in one certain system. The deep quantum mechanical explanations of used quantum mechanical methods and other our investigated bioorganic systems one will find in the sections: “[Procedures/methodologies that have been used in our laboratory](#)” to “[Phenomenon of quantum entanglement in systems composed of two photoactive prebiotic kernels](#)”.

Life on Earth or elsewhere could have emerged in the form of prebiotic kernels and self-reproducing photoactive fatty acid micelles, which gradually evolved into nucleotide-containing micelles due to the enhanced ability of nucleotide-coupled sensitizer molecules to absorb visible light (Tamulis and Grigalavicius 2011). We had noticed that in the simulations of photosynthesis within a photosynthetic prebiotic kernels which contained photoactive molecules (sensitizers), that nucleotides in minimal protocells or prebiotic kernels of a so-called Fatty Acid World caused wavelength shift and broadening of the absorption pattern potentially gives these molecules an additional valuable role, other than a purely genetic one in the early stages of the development of life (Tamulis and Grigalavicius 2011). We observe similar process when inserting provitamin D molecule in the photoactive prebiotic kernel. The quantum mechanical origin of emergence of provitamin D molecule and enhancement of light harvesting process in the prebiotic kernels are described in this section.

We will shortly describe the results of four quantum physics conditioned effects obtained in the vitamin D possessing biological system:

1. an absorbance of discrete quantum portions light spectrum of provitamin D (ergosterol) molecule;
2. the consequencing reorganization of this provitamin D molecule due to the absorbance of quantum portions of light energy;
3. the self-assembly (formation) of supramolecular provitamin D containing prebiotic kernel systems due to the quantum mechanically conditioned hydrogen bonding and Van der Waals forces;
4. quantum entanglement phenomenon in the provitamin D containing prebiotic kernel systems.

The existence of vitamin D molecules was found in phytoplankton and zooplankton which are dating at least

Fig. 1 Experimental [red (in ethanol)] and calculated [blue (in vacuum) and green (in kernel)] curves of absorbance of provitamin D (ergosterol) are normalized to one at the maximal value. The results of transition dipole moments were calculated by TD-DFT Turbomole PBE0/TZVP method (TURBOMOLE 2009) and later the molar extinction coefficients were calculated with orca_asa program, which is interfaced to ORCA program package. (Color figure online)

750 million years ago (Holick 2003) but it is still not understood the role of this molecule in plankton and most probably these vitamin D molecules which were found in phytoplankton and zooplankton remains from the first emerged livings. Our working hypothesis in this paper is that provitamin D molecule was incorporated in the prebiotic kernel systems and minimal cells for the protection from UV radiation which was very intensive 4 billion years ago.

1. Our quantum mechanical calculations of transition dipole moments of provitamin D (abbreviation ProvD in Fig. 1 molecule in vacuum and inside of kernel of protocell (abbreviation kernel in Fig. 1) were performed by using quantum mechanical time dependent density functional theory (TD-DFT) using Turbomole program package PBE0/TZVP method (TURBOMOLE 2009) and later the molar extinction coefficients were calculated by orca_asa program, which is interfaced to ORCA (Neese 2009) program package. The molar extinction coefficient (ϵ) is a measurement of how strongly a chemical species absorbs light at a given wavelength. It is an intrinsic property of the species. The absorbance (A) of a sample is dependent on the pathlength (ℓ) and the concentration, c , of the species via the Beer–Lambert law, $A = \epsilon \ell c$. The most intense calculated absorbance peaks (see green and blue curves in Fig. 1) correlates with the most intense peak of absorbance in experimental curve of provitamin D in ethanol which possesses three peaks in the UV region. The experimental results were done by Gessner and Newell 2002 and drawn in the Fig. 1 by red curve. Two other calculated peaks (green in Fig. 1) in prebiotic kernel correspond to 1,4-bis(*N,N*-dimethylamino)naphthalene attached covalently to

Fig. 2 VitD180 (in the *right*, there is almost 180 degrees of angle between molecular tails of provitamin D and pFA molecules.) (1) and VitD (in the *left*) (2) ground state RI-BP/SVP optimized structures, images of two systems which contains two photoactive molecules: 1,4-bis(*N,N*-dimethylamino)naphthalene attached covalently to 8-oxo-guanine molecule (in the *bottom*) and separate sensitizer

provitamin D molecule (in the *top*), and pFA (in the *center*), and 47 water molecules after geometry optimization. *Dashed lines* means the hydrogen bonds. Carbon atoms and their associated covalent bonds are shown as *green circles and sticks*, hydrogens—*light gray*, nitrogens—*blue*, oxygens—*red*. (Color figure online)

8-oxo-guanine. Computational and experimental results show that the most intensive are the absorbance peaks in the region 260–300 nm for provitamin D.

1) We can do *first conclusion* that despite this biological system is relatively large and wet and exists in relatively large temperatures, provitamin D (ergosterol) absorbance in the environment of ethanol and in the prebiotic systems proceeds exclusively according the quantum physics laws. Therefore, it is possible to calculate the absorption spectrum using quantum mechanical TD-DFT method in program packages Turbomole and ORCA.

2. We have performed geometry optimization of a photosynthetic prebiotic kernels designated (1) and (2) which contains two different sensitizers: a 1,4-bis(*N,N*-dimethylamino)naphthalene [i.e., $(\text{CH}_3)_2\text{N}-\text{C}_{10}\text{H}_6-\text{N}-(\text{CH}_3)_2$] covalently attached to an 8-oxo-guanine molecule, and an ergosterol (provitamin D) molecule (see Fig. 2). In addition to the sensitizers, the self-assembled photosynthetic prebiotic kernel included a pFA molecule and 47 water molecules. The prebiotic kernel (1) is constructed by such a way that molecular tail of provitamin D molecule is oriented almost 180 degrees to the opposite side of molecular tail of pFA molecule due to reducing of repulsion Coulomb forces between positive electron charges on these molecular tails (see the right side of Fig. 2) The abbreviation of configuration is VitD180. The abbreviation VitD shown in the left side of Fig. 2 means that molecular tail of provitamin D molecule is oriented almost 0 degrees towards the molecular tail of pFA molecule. The geometry optimization procedure showed that these two different

configurations of prebiotic kernels possessing differently oriented the provitamin D molecule are stable.

The geometry optimization of the photoactive prebiotic kernels (1) and (2) were performed by using the DFT RI-BP/SVP method with the Turbomole package. The DFT RI-BP/SVP method performs well enough to describe the process of self-forming of hydrogen bond; the many dashed lines corresponding to the experimental values of hydrogen bonds. This was followed by calculations of the photo-synthetic prebiotic kernels (1) and (2) absorption spectra using the TD DFT PBE0/TZVP method using the Turbomole package. The distances between various molecules in the photoactive prebiotic kernels (1) and (2) after the geometry optimization procedure are shown in Angstroms (Å) in Fig. 2.

As the geometry optimization processes for these supramolecular systems (1) and (2) shows, all of these systems molecules become interconnected by hydrogen bonds. Such bonds are well described by the RI-BP/SVP method used in this paper. Our DFT methods account for electron correlation interactions. If we obtain stable hydrogen bonds—connecting this supramolecular system, it would mean that the systems shown in the Fig. 2 really exists in nature.

We define these supramolecular photoactive centres (1) and (2), composed of a sensitizer molecules (including provitamin D molecule), pFA and a number of water molecules, as a photosynthetic prebiotic kernels.

We propose that such photosynthetic prebiotic kernels could have played a central role on the path to the

Table 1 Results of electronic transition parameters of VitD calculated by PBE0/TZVP//RI-BP/SVP method

Excited states	Individual transitions HOMO-m $\rightarrow$ LUMO + n	Individual transition coefficient	Energy (eV)	Wavelength (nm)	Oscillator strength (arbitrary units)
1	HOMO $\rightarrow$ LUMO	1.00	2.47	501.15	0.0005
2	HOMO-1 $\rightarrow$ LUMO	0.99	2.99	414.18	0.0140
5	HOMO $\rightarrow$ LUMO + 5	0.62	3.73	332.40	0.0390
	HOMO $\rightarrow$ LUMO + 2	0.31			
6	HOMO $\rightarrow$ LUMO + 2	0.62	3.74	331.16	0.0170
	HOMO $\rightarrow$ LUMO + 5	0.24			
12	HOMO-1 $\rightarrow$ LUMO + 2	0.93	4.11	301.47	0.0686

formation of more complex systems that signified the emergence of life. As proposed in our earlier paper (Tamulis and Grigalavicius 2011), these self-assembling photosynthetic prebiotic kernels would have produced fatty acids and covered themselves with fatty acid envelopes allowing them to acquire additional components to become the self-reproducing minimal cells (i.e., minimal protocells) of the Fatty Acid World.

2) We can do *second conclusion* that despite this biological system is relatively large and wet, the self-assembly of provitamin D (ergosterol) molecule containing prebiotic kernels proceeds exclusively according the quantum physics laws and this self-assembly is possible to calculate and visualize by quantum mechanical DFT method in program packages Turbomole and ORCA.

3. We will analyse the prebiotic kernel VitD results of TD-DFT calculations performed by Turbomole PBE0/TZVP//RI-BP/SVP methods that are displaced in the Table 1 and Figs. 3 and 4.

The charge transfer in the 1st excited state is from 1,4-bis(*N,N*-dimethylamino)naphthalene-8-oxo-guanine supermolecule to the pFA molecule (see Table 1; Figs. 3, 4).

The interesting charge transfer in the 2nd excited state shows that electron charge density is transferring from provitamin D (VitD) molecule to the pFA molecule (see Table 1; Figs. 3, 4). This is one of the key issues in our article confirming that provitamin D molecule incorporated in the prebiotic kernel enhance the light harvesting. The HOMO-1 is located on the provitamin D molecule and LUMO is located on the pFA molecule (see Fig. 3) therefore electron density transfer is from the provitamin D molecule to the pFA molecule (see Fig. 4).

Analysis of results displaced in Table 1 concerning the individual transitions of excited states 5 and 6 shows that these states are quantum entangled and gives the additional light harvesting in the UV region due to the incorporation of the provitamin D molecule in the prebiotic kernel. One can see that individual transitions of 5th and 6th excited states in Table 1 are composed of the same HOMO, LUMO + 2 and LUMO + 5 with different coefficients. The HOMO is located on 1,4-bis(*N,N*-dimethylamino)naphthalene-8-oxo-guanine supermolecule. The LUMO + 2 and LUMO + 5

are located on 1,4-bis(*N,N*-dimethylamino)naphthalene-8-oxo-guanine supermolecule and on the provitamin D and pFA molecules (see Fig. 3). The electron charge density transfers in 5th and 6th excited states also are from 1,4-bis(*N,N*-dimethylamino)naphthalene-8-oxo-guanine supermolecule to 1,4-bis(*N,N*-dimethylamino)naphthalene-8-oxo-guanine supermolecule and to the provitamin D and pFA molecules (see Fig. 4). It means that exists quantum superposition of 5th and 6th excited states.

Quantum entanglement occurs when particles such as photons, electrons, molecules as large as buckyballs, and even small bioorganic systems interact physically and then become separated; the type of interaction is such that each resulting member of a pair is properly described by the same quantum mechanical description (state), which is indefinite in terms of important factors such as topological position, momentum, spin, polarization, etc.

Quantum entanglement is a form of quantum superposition. Quantum superposition is a fundamental principle of quantum mechanics that holds that a physical system, such as an electron, exists partly in all its particular, theoretically possible states (or, configuration of its properties) simultaneously; but, when measured or observed, it gives a result corresponding to only one of the possible configurations (as described in interpretation of quantum mechanics).

When a measurement is made and it causes one member of such a pair to take on a definite value (e.g., clockwise spin), the other member of this entangled pair will at any subsequent time (excited state in TD-DFT) be found to have taken the appropriately correlated value (e.g., counterclockwise spin). See results of quantum calculation of spin density transfer as evidences of this statement in the “Definition of photoactive prebiotic kernel systems” to “Phenomenon of quantum entanglement in systems composed of two photoactive prebiotic kernels” sections of this review paper (Tamulis et al. 2012, 2013, 2014). Thus, there is a correlation between the results of measurements performed on entangled pairs, and this correlation is observed even though the entangled pair may have been separated by arbitrarily large distances or changed conformation which do not change the topology of this bioorganic system (Tamulis et al. 2012, 2013, 2014).

Fig. 3 Frontier orbitals of VitD calculated by PBE0/def-TZVP method. Carbon atoms and their associated covalent bonds are shown as *green sticks*, hydrogens—*light gray*, nitrogens—*blue*, oxygens—*red*. *Blue* and *gray* volumes respectively indicate negative and positive parts of the wave function. *Dashed lines* means the hydrogen bonds. (Color figure online)

Fig. 4 Results of electron charge density transfers calculated by PBE0/def-TZVP//RI-BP/def-SV(P) method in certain electronic excited states of VitD. The transferred electron charge density is shown in *light gray* while lost electron density is shown in *blue*. (Color figure online)

Our discovered phenomenon of the quantum entanglement in the provitamin D prebiotic system enhance of photosynthesis in the system because simultaneously excite two prebiotic kernels in the system by appearance of two additional quantum entangled excited states. We can propose that quantum entanglement enhanced the emergence of photosynthetic prebiotic kernels and accelerated the evolution of photosynthetic life because of more absorbed light energy. More detailed description how quantum

entanglement enhanced the emergence and accelerated the evolution of photosynthetic prebiotic systems one can find in the “[Phenomenon of in a quantum entanglement photoactive prebiotic kernel](#)” and [Phenomenon of quantum entanglement in systems composed of two photoactive prebiotic kernels](#) sections of this paper.

For this photosynthetic prebiotic kernel system there are two photo-excitation possibilities: the photoactive supramolecule provitamin D (VitD) molecule—abbreviation

will be A and photoactive supermolecule 1,4-bis(*N,N*-dimethylamino)naphthalene-8-oxo-guanine—B, i.e., containing two different variable inputs and one output (pFA molecule)—abbreviation AB. The system gives a high AB output equal to 1 only in the case if due to quantum entangled state photoelectron is hopping to pFA. Analysis of Table 1 and Figs. 3 and 4 shows that:

if $A = 0$ and $B = 0$, then $AB = 0$;

if $A = 0$ and $B = 1$, then $AB = 0$;

if $A = 1$ and $B = 0$, then $AB = 0$;

if $A = 1$ and $B = 1$, then $AB = 1$.

We state that there are no quantum entangled excitations in 5th and 6th states then the quantum state of all the system is equal to 0. Only in the case if there are quantum entangled excitations in 5th and 6th states then the state of all the system is equal to high value equal to 1. This truth table represents the two variable AND gate in this certain system. More about molecular logic gates one can read in our chapter of handbook (Tamulis et al. 2003a, b).

The 12th excited state initiating the electron charge density transition from provitamin D molecule to the same provitamin D and little to the pFA molecule in the UV region (see Table 1; Figs. 3, 4). The electron charge density redistribution on the provitamin D molecule initiate the reducing of value of electron density on one of covalent bonds in the provitamin D molecule, i.e., reduce the certain covalent bond order. This reducing of covalent bond order initiate the breaking the certain covalent bonds that means the conversion of provitamin D molecule to the previtamin D molecule and later to vitamin D molecule due to the harvesting of UV light. This result coincide with well known experimental results described in paper (Gessner and Newell 2002).

We note that the simultaneous nature of the involvement of two different sensitizers in the energy transfer would also mean that information is being transferred. These entangled 5th and 6th excited states enhance the photosynthetic process in the UV region of the photosynthetic prebiotic kernel containing provitamin D molecule.

3) *Third conclusion*: summarizing the results of time dependent density functional theory method calculated absorption spectrum and images of electron transfer trajectories in prebiotic kernel possessing provitamin D molecule in the different excited states allow to separate quantum entangled photosynthetic transitions which show that provitamin D enhance the photosynthetic process in the UV region. We manifest idea that provitamin D firstly might was included in the protocells as the sensitizer molecule for harvesting of UV radiation 3.7–3.8 billion years ago in the Earth.

4. The 12th excited state initiate the electron charge density transition from provitamin D (ergosterol) molecule to the same provitamin D and little to the pFA molecule in the UV region (see Fig. 4). The electron charge density redistribution on the provitamin D molecule initiate the breaking the certain covalent bonds that means the conversion of provitamin D molecule to the previtamin D molecule and later to the vitamin D molecule due to the harvesting of UV light. This result coincide with experimental results (Gessner and Newell 2002). The Solar radiation spectrum was rich with UV radiation 3.9–3.8 billion years ago in the Earth therefore provitamin D and its metabolites firstly might be included in the protocells as the sensitizer molecule for harvesting of UV radiation. Our discovered quantum mechanical processes of conversion of the provitamin D to previtamin D might be also important for the understanding of the mechanisms of protection from cutaneous melanoma.

4) We can do *fourth conclusion* that despite this biological system is wet and relatively large the absorbance of UV light of provitamin D (ergosterol) molecule and transformation to previtamin D molecule proceeds exclusively according the quantum physics laws and the breaking of covalent bond is possible to calculate and visualize by quantum mechanical TD-DFT method in program package Turbomole.

Quantum entanglement in photoactive prebiotic kernel systems

Procedures/methodologies that have been used in our laboratory

Biological molecules, supermolecules or supramolecules (photosynthetic prebiotic kernels cells) are quantum systems composed of quantum particles: nuclei and surrounding electrons. The electromagnetic interaction of two particles depends upon the interaction of all other quantum particles. Therefore, we are dealing with the complex quantum many-body system.

The quantum mechanical electron correlation interaction density functional theory (DFT) methods (Jensen 1999; Marques et al. 2006) (i.e., high precision quantum mechanical simulations) were used to investigate various self-assembled photoactive bioorganic systems of artificial minimal living cells (Tamulis 2008b, 2011; Tamulis et al. 2006, 2008, 2012, 2013, 2014; Tamulis and Tamulis 2007b). The cell systems studied in these articles are based on peptide nucleic acid (PNA) and consist of up to 400 atoms (not including the associated water solvent shells) and are about 4.5 nm in diameter.

The quantum simulations of single bioorganic molecules possessing closed electronic shells start from an arbitrary

geometry (Cartesian coordinates of the nuclei). Using quantum mechanical semi-empirical and DFT approaches in the GAMESS-US (Schmidt et al. 1993) or TURBOMOLE (TURBOMOLE 2009) or ORCA (Neese 2009) program packages, we obtain the lowest molecular energy that parametrically depends on the coordinates of the nuclei. These coordinates are adjusted using the standard geometry optimization procedure (Neese 2003) to minimize the energy with respect to the nuclear positions. Special care is required to verify that the obtained optimal molecular structure is a global minimum in the phase space of the nuclear ($3n-6$, n being the number of atoms) degrees of freedom.

In order to obtain accurate results in investigating supermolecules, two factors need to be accounted for: (1) the quality of the density functional and (2) the quality of the molecular orbitals (extent of the phase space of the single-electron states).

For geometry optimization of the self-assembly of bio-organic supramolecules in which the separate molecules are associated by hydrogen bonds or Van der Waals forces, the RI-BP (Becke 1993) method was used. RI stands for ‘Resolution of the Identity’ and contributes to the approximation of the above-mentioned Coulomb part (Eichkorn et al. 1995). In addition, the B97d (Grimme 2006) method with Grimme long-range dispersion electron corrections was used. Both of these methods include some electron correlation effects at larger distances that provide relatively good descriptions of the Van der Waals forces and hydrogen bonds. Although the use of GGA functionals typically yield reasonable optimization results, to ensure accurate molecular orbital population during calculations of vertical excitations in large scale systems such as ours, the hybrid PBE0 functional in the TD-DFT kernel was chosen instead. It is known that TD-DFT tends to underestimate charge transfer excitation energies when non-hybrid GGA functionals are used (Treutler and Ahlrichs 1995). Thus, excitations of the two minimal kernel systems were calculated using the PBE0 hybrid functional which has the form $\text{const1}(S + \text{PBE}(X)) + \text{const2} \cdot \text{HF} + \text{PW} + \text{PBE}(C)$, where const1 and const2 are adjustable constants, S refers to the Slater-Dirac exchange energy functional, $\text{PBE}(X)$ and $\text{PBE}(C)$ are the Perdew-Burke-Ernzerhof exchange and correlation energy functional (Perdew et al. 1996). HF denotes the Hartree-Fock exchange and PW is the Perdew-Wang correlation functional (Adamo and Barone 1999). RI-BP and B97d methods were used together with the def-SV(P) (split valence plus polarization) (Weigend and Ahlrichs 2005) and 6-31G(d) (Ditchfield et al. 1971; Schuchardt et al. 2007) basis sets respectively, whereas PBE0 was used together with the def-TZVP basis set (Weigend and Ahlrichs 2005). Only in the case of open electronic shell subsystems we used B97d including Grimme

dispersion electron correction (BP + Disp/RI def) with SV(P) basis set in the Turbomole program package.

The LANL research project used organic neutral radical molecules for quantum information processing (Tamulis et al. 2003b). Neutral radical molecules possess an open shell electronic structure and the DFT approximation maps the associated complex many-body problem onto an effective one-electron problem in which electron-electron repulsion is treated in an average (mean field) way and the simplest antisymmetric wave function is assumed for an N -electron molecule, i.e., a single Slater determinant

$$\Psi = \langle \chi_1(x) \chi_2(x) \dots \chi_N(x) \rangle \quad (1)$$

Here $\chi_i(x)$ are normalized single-particle molecular orbitals (MO) for each respective particle. The exchange of any pair of coordinates or any pair of single-particle MOs has the effect of exchanging two columns or rows respectively, which leads to a change of sign of the determinant, satisfying anti-symmetry. In the case that any coordinates or single-particle wave functions are identical, two columns or rows will be equal, and the determinant will be identically zero. This is a consequence of the antisymmetry requirement, namely the well-known Pauli Principle (Jensen 1999). Following Roothaan’s procedure (Cai et al. 2010), they are expanded as linear combinations of localized atomic basis functions $\phi_k(x)$:

$$\chi_i = \sum \phi_k(x) \cdot C_{ki} \quad (2)$$

In the open shell unrestricted approach, x refers to both coordinate and spin variables:

$$\phi_k(x) = \phi_k(\vec{r})\xi(s) \quad \text{where} \quad \xi(s) = \alpha \text{ or } \xi(s) = \beta \quad (3)$$

(α and β correspond to spin “up” and “down”, respectively). Our research group is also using these quantum-mechanics-based models to investigate the magnetically active logic gates we have proposed for controlling photosynthesis in artificial minimal cells that possess open shell neutral radical molecules (Rinkevicius et al. 2006; Tamuliene et al. 2004; Tamulis 2008b, c; Tamulis et al. 2003a, b, 2004, 2012, 2013, 2014).

Definition of photoactive prebiotic kernel systems

The solution of basic questions of emergence and evolution of the first living cells or protocells is tightly connected with the rapidly developing field of artificial living technologies in several laboratories around the world. The possibility of synthesizing artificial self-reproducing cells also impacts the possibility of the emergence of self-reproducing protocells on the Earth or elsewhere.

In their originally conceived form, LANL’s artificial cells were to consist of a micelle acting as the container, a

light driven metabolism, and a genetic system, whose functions were all very tightly coupled (Cape et al. 2011; DeClue et al. 2009; Edson et al. 2011; Maurer et al. 2009, 2011; Rasmussen et al. 2008). The proposed container was to consist of amphiphilic fatty acid (FA) molecules that self-assembled into a micelle. The hydrophobic interior of the micelle was to provide an alternative thermodynamic environment from the aqueous or methanol exterior and act as a sticking point for the photosensitizer, pFA (food), and the genetic material. Peptide nucleic acid (PNA) was initially chosen as the genetic material as it is far less polar than RNA or DNA. The different nucleotide molecules have different electron donor and electron relay capabilities, and as such, there is also a mechanism for natural selection, with some nucleotides and their orderings being superior to others in their ability to facilitate the metabolism (DeClue et al. 2009; Rasmussen et al. 2008). Practical experimental considerations resulted in changes from the original design. Decanoic acid based self-assembling bilayer vesicles were used as the containers, and DNA as the genetic material (DeClue et al. 2009). In spite of the switch to vesicles, all the active chemistry still occurred in direct association with the bilayer as opposed to within the volume enclosed by it.

The active components of the systems synthesized at LANL and in the Center for Fundamental Living Technology (FLinT) at the University of Southern Denmark (SDU) (Cape et al. 2011; DeClue et al. 2009; Edson et al. 2011; Maurer et al. 2009, 2011; Rasmussen et al. 2008) contain on the order of one thousand atoms. We have investigated various features of these LANL synthesized derivatives starting from self-assembly of component molecules, the absorption of light, and the metabolism using quantum mechanical methods including electron correlation effects (Tamulis et al. 2006, 2008, 2012, 2013, 2014; Tamulis and Tamulis 2007a, b).

The entire artificial cell might be considered to be a molecular electronics or molecular spintronics device that self-assembles according to quantum-based electron interaction potentials and that absorbs light and carries on its metabolism according to quantum electron excitation and tunnelling equations (Rinkevicius et al. 2006; Tamuliene et al. 2004; Tamulis 2008b, c; Tamulis et al. 2003a, b, 2004, 2012, 2013, 2014). Therefore, in this picture, the photo-induced electron charge density or electron spin density transfer in the artificial cell may be viewed as a quantum device-wave trace.

The calculated electron charge tunnelling energy of 2.753 eV (450.3 nm) associated with the eighth excited state of LANL synthesized minimal artificial living cells was investigated by Tamulis et al. (2008) and corresponds to the experimental value of 450.0 nm of the most intense absorption line (Rasmussen et al. 2008). This agreement

implies that the quantum mechanically simulated self-assembled structures of such minimal living cells very closely approximate the realistic ones. This review article uses a collection of quantum mechanical electron correlation tools and applies them to a variety of minimal protocell photosynthetic problems, while also providing a perspective for the synthesis of new forms of living organisms. Nonconventional photosynthetic prebiotic kernel systems which were designed by our research group are presented in this review. Examples of this research include the use of molecular electronics and molecular spintronics logic gates to regulate photosynthesis-like energy transduction systems, as well as to control growth and division of artificial living cells (Tamulis et al. 2014; Tamulis and Grigalavicius 2013; Tamulis and Tamulis 2008).

Longer term goals in the use of quantum mechanical simulations might be to predict the possibility of biochemical experimental synthesis of molecular electronics and spintronics logic elements for information systems based on artificial living organisms, or for the control of nanobiorobots applied in areas such as nanomedicine and cleaning of nuclear, chemical, and microbial pollution.

As a starting point, using DFT PBE/6-31G methods we have performed geometry optimization of a photosynthetic prebiotic kernel designated (**1**) which contains two different sensitizers: a 1,4-bis(*N,N*-dimethylamino)naphthalene [i.e., $(\text{CH}_3)_2\text{N}-\text{C}_{10}\text{H}_6-\text{N}-(\text{CH}_3)_2$] covalently attached to an 8-oxo-guanine molecule, and a bis(4-diphenylamine-2-phenyl)-squinone (SQ) covalently bonded to an 8-oxo-guanine::cytosine supramolecule.

In addition to the sensitizers, the self-assembled photosynthetic prebiotic kernel included a pFA molecule and 50 water molecules. The geometry optimization of the photoactive prebiotic kernel (see Fig. 5a, b) was performed by using the PBELYP/3-21 method with the GAMESS-US package. The DFT PBELYP/3-21 method performs well enough to describe the process of self-forming of hydrogen bond; the many dashed lines corresponding to the experimental values of hydrogen bonds. This was followed by calculations of the photosynthetic prebiotic kernel's absorption spectrum using the TD DFT revPBE method with the 6-31G* basis set using the ORCA (Neese 2003, 2009) package.

The photosynthetic prebiotic kernel visualization have been made more clear in terms of its chemical subunits due to its central importance for the paper. The visualization in Fig. 5b various chemical sub-units are marked by different transparent colours.

Because the appearance of the many hydrogen bonds in the system (**1**) composed of two sensitizers during process of geometry optimization it is difficult visually, we decided to note the formation of the hydrogen bondings which corresponds interactions of two subsystems (**2**) and (**3**) by

Fig. 5 **a** Visualization of a photosynthetic prebiotic kernel (**1**) containing sensitizer molecule squaraine (in the *top*) attached covalently to 8-oxo-guanine:cytosine supramolecule (in the *top-right*) and separate sensitizer molecule 1,4-bis(*N,N*-dimethylamino)naphthalene attached covalently to 8-oxo-guanine (in the *bottom-right*), and pFA (in the *center*), and 50 water molecules after the 836 steps of the geometry optimization. Carbon atoms and their associated covalent bonds are shown as *green spheres and sticks*, nitrogens—*blue*, hydrogens—*gray*, oxygens—*red*. *Dashed lines* means the hydrogen bonds. **b**. Visualization of a photosynthetic prebiotic kernel (**1**) containing sensitizer molecule squaraine (*light red*) attached covalently to 8-oxo-guanine:cytosine supramolecule (*light green*) and separate sensitizer molecule 1,4-bis(*N,N*-dimethylamino)naphthalene (*yellow*) attached covalently to 8-oxo-guanine (*light blue*), and pFA (*light brown*), and 50 water molecules (*light green*) after the 836 steps of the geometry optimization. Carbon atoms and their associated covalent bonds are shown as *green spheres and sticks*, nitrogens—*blue*, hydrogens—*gray*, oxygens—*red*. *Dashed lines* means the hydrogen bonds. (Color figure online)

short high-pitched sound. Each dissociation of proton is marked by longer low-pitched sound. Two pairs of quantum entangled states are marked by two different

permanently playing solfeggio tones: do-re, do-re, and so on. Each dissociation of proton is marked by longer low-pitched sound. Finally, one can hear and account many various sounds in this quantum dynamics self-assembly process of system (**1**).

As the geometry optimization process for this supramolecular system (**1**) shows, all of that system's molecules become interconnected by hydrogen bonds. Such bonds are well described by the PBELYP/3-21 method used in this paper. Our DFT methods account for electron correlation interactions. If we obtain stable hydrogen bonds—connecting this supramolecular system, it would mean that the system shown in the Fig. 5a, b really exists in nature.

We define this supramolecular photoactive center (**1**), composed of a sensitizer molecules, pFA and a number of water molecules, as a photosynthetic prebiotic kernel.

We propose that such photosynthetic prebiotic kernels could have played a central role on the path to the formation of more complex systems that signified the emergence of life. As proposed in our earlier papers (Tamulis and Grigalavicius 2010a, 2011), these self-assembling photosynthetic prebiotic kernels would have produced fatty acids and covered themselves with fatty acid envelopes allowing them to acquire additional components to become the self-reproducing minimal cells of the Fatty Acid World.

The age of the Earth is 4.54 billion years which was confirmed by radiometric age dating of the oldest minerals and meteorite materials; see (Wilde et al. 2001). The oceans may have appeared 4.3 billion years ago in a hot 100 °C reducing environment, and that the pH of about 5.8 rose rapidly towards neutral according to Morse and MacKenzie (Morse and MacKenzie 1988). The study by Maher and Stevenson (Maher and Stevenson 1988) shows that if the deep marine hydrothermal setting provides a suitable site for the origin of life, abiogenesis could have happened as early as 4.0–4.2 billion years ago, whereas if it occurred at the surface of the Earth abiogenesis could only have occurred beginning between 3.7 and 4.0 billion years ago. Between 3.8 and 4.1 billion years ago, changes in the orbits of the gaseous giant planets in the Solar System: Jupiter, Saturn, Uranus, and Neptune may have caused a late heavy bombardment which probably also impacted the time frame for the emergence of life. Evidence from the Moon's surface, might perhaps also provide additional information about this bombardment period and whether it would or would not have delayed the emergence of life on Earth, especially a photosynthetic origin. It might be that our proposed photosynthetic Fatty Acid World life originally emerged 4.2 to 4.0 billion years ago but was periodically destroyed by the bombardment of huge cosmic rocks. Likewise, precursors of chemotrophic Archaeal and Prokaryote single-celled microorganisms might also have evolved in somewhat better protected deep marine

environments. However, they may have been destroyed too if the impacts evaporated the early oceans. The Isua Greenstone Belt in Greenland is aged 3.7–3.85 billion years and contains within it the oldest metamorphosed sedimentary rocks in the world. Indirect evidence from it may be indicative of the earliest appearance of photosynthetic life. Examination of the isotopic carbon composition of the apatite therein by geoscientists (Fedó and Whitehouse 2002; Mojzsis et al. 1996; Nutman et al. 2009; Ohtomo et al. 2013) shows that some of it is extraordinarily light, which is indicative of a biogenic origin. Thus these scientists suggest that life already existed on the planet at least 3.7–3.85 billion years ago.

Nora Noffke and Robert Hazen revealed the well-preserved remnants of a complex ecosystem in a nearly 3.5 billion-year-old sedimentary rock sequence in Australia (Noffke et al. 2013). Exist also some controversial paper of William Schopf of UCLA published a paper in the scientific journal *Nature* arguing that geological formations as old as 3.5 billion years contain fossils resembling cyanobacteria microbes (Schopf et al. 2002). Above mentioned fossilized microbes are micrometers size while our proposed Fatty Acid World minimal cells are approximately one thousand times smaller. We proposed an emergence date of 3.9–3.8 billion years ago for the self-reproducing minimal cells our Fatty Acid World [see Figure 17 of article (Tamulis and Grigalavicius 2010a) illustrating the emergence of fatty acid life].

The quantum mechanical investigation of two different sensitizer molecules: 1,4-bis(*N,N*-dimethylamino)naphthalene— $(\text{CH}_3)_2\text{N}-\text{C}_{10}\text{H}_6-\text{N}-(\text{CH}_3)_2$, and bis(4-diphenylamine-2-phenyl)-squaraine, as well as photosynthetic kernel (1) shown in the Fig. 5a, b were performed on the Linux server cluster of the Institute of Theoretical Physics and Astronomy of Vilnius University (Lithuania).

Phenomenon of quantum entanglement in a photoactive prebiotic kernel

The example discussed here is pertains to the coupled two sensitizer (bis(4-diphenylamine-2-phenyl)-squaraine and 1,4-bis(*N,N*-dimethylamino)naphthalene) photosynthetic prebiotic kernel (1) shown in Fig. 5a, b. Its absorption spectrum was calculated using the final results of the atomic coordinates after the geometry optimization. The details of that spectrum are given in Table 2 and Fig. 6. The spectrum was calculated using the TD DFT revPBE method with the 6-31G* basis set in the ORCA program package. Table 2 only lists those excitations for which electron hopping occurs from the sensitizer supramolecule or supermolecule to the pFA molecule.

The most intense excited state (474.0 nm) of the photoactive minimal kernel (1) is composed of LUMO and

LUMO + 1 individual transitions located on the fatty acid precursor molecule (see Table 2; Fig. 7). This LUMO and LUMO + 1 coupling also allows electron hopping (tunnelling) to the pFA molecules for the most intense absorption excited states.

The difference of electron charge density (certain excited states—ground state) for photosynthetic prebiotic kernel (1) according to the TD DFT calculations and visualized in Figs. 7, 9, and 10, shows the electron charge tunnelling associated with certain excited state transitions. The electron cloud hole is indicated by the dark blue colour while the transferred electron cloud location is designated by the gray colour.

The electron tunnelling transition of the most intense 49th (474.0 nm) excited state of this photosynthetic prebiotic kernel should induce metabolic photo-dissociation of the pFA molecule because the transferred electron cloud is located on the head (the waste piece) of the pFA molecule (see Fig. 7) where it causes this molecule to split due to intense rotation and vibration of the weak chemical bond that joins the waste piece to the fatty acid piece of the pFA molecule.

Quantum entangled states are also involved in some of the photosynthetic reactions. Examples of this include the 27th and 29th states, as well as the 45th and 47th states of Table 2 and shown respectively in Figs. 7, 8, 9, 10 and 11, 12, 13. The phenomenon of quantum entangled states which induce photosynthesis appears only in cases where two photosensitizers are involved and is absent in the case of involvement of only a single sensitizer (Tamulis 2011).

Analysis of the frontier orbitals HOMO-*m* and LUMO + *n* of photosynthetic prebiotic kernel (1) in the 27th (535.4 nm) and 29th (534.2 nm) excited states shows that quantum entanglement exists between the photosynthetic supramolecule SQ-8-oxo-guanine::cytosine and the photosynthetic supermolecule 1,4-bis(*N,N*-dimethylamino)naphthalene-8-oxo-guanine (see Figs. 8, 9, 10). The HOMO-14 and HOMO-15 orbitals are located on the photosynthetic supramolecule and supermolecule with different weights (see Table 2; Fig. 8), while the LUMO orbital is located on the pFA molecule. Thus, electron transition energy might be simultaneously transferred from the photosynthetic supramolecule and supermolecule to the pFA molecule for both the 27th and 29th excited states of this photosynthetic prebiotic kernel. We note that the simultaneous nature of the involvement of two different sensitizers in the energy transfer would also mean that information is being transferred. We have observed during the geometry optimization process of this photosynthetic prebiotic kernel (1) that the quantum entangled states remains not depending on the mutual distances of photosensitizer molecules, i.e., exist invariance of quantum entangled states relative the mutual distance. According to

Table 2 Excitation transitions energies of photosynthetic prebiotic kernel (1) which contains a 1,4-bis(*N,N*-dimethylamino)naphthalene covalently bonded to an 8-oxo-guanine, a SQ molecule covalently bonded to an 8-oxo-guanine::cytosine supermolecule, a pFA molecule, and 50 water molecules

Excited state #	Individual transitions HOMO-m → LUMO + n	Weight of individual transition	Energy (eV)	Wavelength (nm)	Oscillator strength (arbitrary units)
49	HOMO-23 → LUMO + 1	0.0250	2.616	474.0	1.41427
	HOMO-21 → LUMO	0.0163			
	HOMO-20 → LUMO	0.0451			
	HOMO-19 → LUMO + 1	0.1073			
	HOMO-17 → LUMO + 1	0.2716			
	HOMO-16 → LUMO + 1	0.0419			
	HOMO-3 → LUMO + 1	0.0248			
	HOMO → LUMO + 1	0.3698			
27	HOMO-14 → LUMO	0.8423	2.32	535.4	0.00001
	HOMO-15 → LUMO	0.1576			
29	HOMO-14 → LUMO	0.1557	2.32	534.2	0.00165
	HOMO-15 → LUMO	0.8356			
45	HOMO → LUMO + 1	0.1014	2.569	482.5	0.36883
	HOMO-8 → LUMO + 1	0.0130			
	HOMO-16 → LUMO + 1	0.7899			
	HOMO-17 → LUMO + 1	0.0536			
	HOMO-19 → LUMO + 1	0.0114			
47	HOMO → LUMO + 1	0.1149	2.586	479.5	0.43249
	HOMO-8 → LUMO + 1	0.0229			
	HOMO-16 → LUMO + 1	0.1633			
	HOMO-17 → LUMO + 1	0.6391			
	HOMO-19 → LUMO + 1	0.0181			

The energies were calculated using the TD DFT revPBE method with the 6-31G* basis set in the ORCA program package. The weight of the individual excitations are given if larger than 0.01

A. Zeilinger's (Brukner and Zeilinger 2009) quantum information theory this invariance of quantum entangled states relative the mutual distance might be used for quantum information transfer in this certain photosynthetic prebiotic kernel (1) system during two quantum entangled excited states.

Visualization of the quantum entangled electron charge tunnelling associated with the 27th (535.4 nm) excited state is presented in Fig. 9. The transition is mainly from the 1,4-bis(*N,N*-dimethylamino)naphthalene-8-oxo-guanine supermolecule, with a much smaller probability of it being from the SQ-8-oxo-guanine::cytosine supramolecule to the pFA molecule in this system.

Visualization of the quantum entangled electron charge tunnelling associated with the 29th (534.2 nm) excited state is presented in Fig. 10. The transition is mainly from the SQ-8-oxo-guanine::cytosine supramolecule, with a much smaller probability of it instead being from the 1,4-bis(*N,N*-dimethylamino)naphthalene-8-oxo-guanine supermolecule to the pFA molecule in this system.

Analysis of the frontier orbitals HOMO-m and LUMO + n of photoactive kernel (1) associated with the 45th (482.5 nm) and 47th (479.5 nm) excited states shows that quantum entanglement also exists there between the photosynthetic supramolecule SQ-8-oxo-guanine::cytosine

and the photosynthetic supermolecule 1,4-bis(*N,N*-dimethylamino)naphthalene-8-oxo-guanine (see Figs. 11, 12 and 13). The HOMO, HOMO-8, HOMO-16, HOMO-17 and HOMO-19 orbitals are located on the photosynthetic supramolecule and the supermolecule with different weights (see Table 2; Fig. 11), while the LUMO + 1 orbital is located on the pFA molecule. Thus, electron transition energy might be simultaneously transferred from the photosynthetic supramolecule and supermolecule to the pFA molecule for both the 45th and 47th excited states of this photosynthetic prebiotic kernel. We again note that the simultaneous nature of the involvement of two different sensitizers in the energy transfer would also mean that information is being transferred.

Visualization of the quantum entangled electron charge tunnelling associated with the 45th (482.5 nm) excited state is presented in the Fig. 12. The transition is mainly from the SQ-8-oxo-guanine::cytosine supramolecule, with a much smaller probability of instead being from the 1,4-bis(*N,N*-dimethylamino)naphthalene-8-oxo-guanine supermolecule to the pFA molecule of this photosynthetic prebiotic kernel.

Visualization of the quantum entangled electron charge tunnelling associated with the 49th (482.5 nm) excited state is presented in the Fig. 13. The transition is mainly

Fig. 6 The spectrum of self-assembled photosynthetic prebiotic kernel (1). The spectrum was calculated using the TD DFT revPBE method with the 6-31G* basis set

Fig. 7 Visualization of the electron charge tunnelling associated with the 49th (474.0 nm) excited state. The transition is from the *dark blue* to the *light gray* regions, the major part of the transition being between two different regions of the squaraine part of the squaraine-8-oxo-guanine::cytosine supramolecule, but with a minor piece to the pFA molecule (in the center). (Color figure online)

from the SQ-8-oxo-guanine::cytosine supramolecule, with a much smaller probability of instead being from the 1,4-bis(*N,N*-dimethylamino)naphthalene-8-oxo-guanine supermolecule to the pFA molecule of this minimal protocell.

Our discovered phenomenon of the quantum entanglement in the prebiotic kernel system enhance of photosynthesis in the system because simultaneously excite two prebiotic kernels in the system by appearance of two additional quantum entangled excited states. We can

propose that quantum entanglement enhanced the emergence of photosynthetic prebiotic kernels and accelerated the evolution of photosynthetic life because of more absorbed light energy.

For the excited states of this photosynthetic prebiotic kernel system there are two photo-excitation possibilities: the photoactive supramolecule SQ-8-oxo-guanine::cytosine—abbreviation will be A and photoactive supermolecule 1,4-bis(*N,N*-dimethylamino)naphthalene-8-oxo-guanine—B, i.e., containing two different variable inputs and one output (pFA molecule)—abbreviation AB. The system gives a high AB output equal to 1 only in the case if due to quantum entangled state photoelectron is hopping to pFA. Analysis of Table 2 and Figs. 8, 9 and 10 shows that:

if $A = 0$ and $B = 0$, then $AB = 0$;

if $A = 0$ and $B = 1$, then $AB = 0$;

if $A = 1$ and $B = 0$, then $AB = 0$;

if $A = 1$ and $B = 1$, then $AB = 1$.

We state that if there are no quantum entangled excitations then the quantum state of all the system is equal to 0. Only in the case if there are quantum entangled excited (45th and 47th and also 27th and 29th) states then the state of all the system is equal to high value equal to 1. This truth table represents the two variable AND gate in this certain system. More about molecular logic gates one can read in our chapter of handbook (Tamuliene et al. 2004).

In the future, similar processes might be applied for the destruction of tumour cancer cells or to yield building blocks in artificial cells.

All the charge transfers to the pFA molecule investigated in this section involve the hopping of photoexcited electrons (including quantum entangled electron density transfer) from the sensitizer (either a bis(4-diphenylamine-2-phenyl)-squaraine or a 1,4-bis(*N,N*-dimethylamino)naphthalene) to the pFA molecule which results in its cleavage. The new fatty acid produced by this photosynthetic reaction joins the existing the assembly causing it to grow. Repetition of the photosynthetic reaction results in additional growth resulting in a fatty acid micelle or vesicle with an incorporated photosynthetic assembly, i.e., a minimal living cell. The quantum entanglement could have played an important role in the first stages of origins of life and evolution of biospheres because it enhances the photosynthesis due to more absorbed light energy, leading to faster growth and self-replication of minimal living cells.

Phenomenon of quantum entanglement in systems composed of two photoactive prebiotic kernels

Of special interest for applications in the biotechnologies is to investigate phenomena of quantum entanglement in

Fig. 8 HOMO-14 and HOMO-15 (on the *left*) and LUMO (on the *right*) orbitals of the 27th and 29th excited states. Carbon atoms and their associated covalent bonds are shown as *green sticks*,

hydrogens—*light gray*, nitrogens—*blue*, oxygens—*red*. *Blue* and *gray* volumes respectively indicate negative and positive parts of the wave function. (Color figure online)

systems consisting of two prebiotic kernels which are described in detail in the paper by Tamulis et al. (2013). Also relevant is another separate paper concerning magnetically controlled quantum entangled photosynthesis (see the last part of Sect. 4.4 in this paper and Tamulis et al. 2014). This special interest because we have discovered quantum entangled energy and information transfer from one photosynthetic prebiotic kernel to another separate photosynthetic prebiotic kernel. The quantum entangled energy and information transfer is performing using electron density charge transfer in the closed electronic shell subsystems, see (Tamulis et al. 2013) and using electron spin density transfer in the case of open electronic shell subsystems (Tamulis et al. 2014).

The description of geometry optimization of the photosynthetic system composed of two photosynthetic prebiotic kernels is detailed described the paper by (Tamulis et al. 2013). This photosynthetic system (4) composed of two subsystems [(2) and (3)] (see Fig. 14a, b) possesses 534 atoms.

The photosynthetic prebiotic kernel (2) is composed of a sensitizer 1,4-bis(*N,N*-dimethylamino)naphthalene molecule with attached 8-oxo-guanine::cytosine and pFA supramolecule, and water molecules. The 8-oxo-guanine::cytosine supramolecule supplies a replacement electron to the sensitizer after the photoexcited electron has hopped from the sensitizer to the pFA molecule. The photosynthetic prebiotic kernel (3) is composed of a

Fig. 9 Visualization of the quantum entangled electron charge tunnelling associated with the 27th (535.4 nm) excited state. The electron transition is to the pFA molecule (extending from the *bottom-center* to the *center* of the figure), coming mainly from 1,4-bis(*N,N*-dimethylamino)naphthalene-8-oxo-guanine supermolecule (extending from the *bottom-right* to the *right-center*), but with a small contribution coming from the SQ-8-oxo-guanine::cytosine supramolecule which extends from the *bottom-left* to the *top-center* and then to the *right-center* of the figure. Gray indicates regions of increased electron probability while dark blue indicates regions of reduced electron probability. (Color figure online)

Fig. 10 Visualization of the quantum entangled electron charge tunnelling associated with the 29th (534.2 nm) excited state of photosynthetic prebiotic kernel (1). The electron transition is to the pFA molecule (extending from the *bottom center* to the *center* of the figure) and comes mainly from the top center region of the SQ-8-oxo-guanine::cytosine supramolecule that itself extends from the *bottom left* to the *top center* and on to the *right center* of the figure. A very small contribution (too small to be seen in the figure) comes from the 1,4-bis(*N,N*-dimethylamino)naphthalene-8-oxo-guanine supermolecule (extending from the *bottom right* to the *right center*). Gray indicates regions of increased electron probability while dark blue indicates regions of reduced electron probability. (Color figure online)

sensitizer bis(4-diphenylamine-2-phenyl)-squaraine molecule attached covalently to 8-oxo-guanine::cytosine supramolecule, and pFA and water molecules, as was already mentioned in the section above.

The initial distance between the edging molecules in subsystems (2) and (3) was done equal to 8.4 Å, i.e., a few times larger in comparison with the experimental Van der Waals distances between organic molecules (see Fig. 14a) because we decided to observe the movie of self assembly of two subsystems. The geometry optimization of system (4) was performed by using the DFT method B97d and the 6-31G(d) basis set in the G09RevB.01 program package. The process of geometry optimization reduced the distance between the (2) and (3) subsystems (compare Fig. 14a, b) due to Van der Waals interactions between these subsystems.

Because the appearance of the many hydrogen bonds in the system (4) composed of two photosynthetic prebiotic kernel during process of geometry optimization it is difficult visually, we decided to note the formation of the hydrogen bondings which corresponds interactions of two subsystems (2) and (3) by short high-pitched sound. Each dissociation of proton is marked by longer low-pitched sound. Two pairs of quantum entangled states are marked by two different permanently playing solfeggio tones: do-re, do-re, and so on. Each dissociation of proton is marked

by longer low-pitched sound. Finally, one can hear and account many various sounds in this quantum dynamics self-assembly process of two subsystems (2) and (3) into the system (4).

The main issues of investigations of photosynthetic system (4) composed of two subsystems [(2) and (3)]:

1) Analysis by our methods in the different excited states allows us to separate quantum-entangled photosynthetic transitions between neighbouring prebiotic kernel models. This means that a quantum-entangled phenomenon of energy and information transfer exists in these model units, which might correspond to prebiotic self-reproducing organisms which existed in the photosynthetic prebiotic kernel stages of the emergence and evolution of life. The possibility of synthesizing artificial self-reproducing quantum entangled cells also impacts the possibility of the emergence of such a kind self-reproducing protocells on the Earth or elsewhere.

Our discovered phenomenon of the quantum entanglement in the two prebiotic kernel system enhance of photosynthesis in the system because simultaneously excite two prebiotic kernels in the system by appearance of two additional quantum entangled excited states. We can propose that quantum entanglement enhanced the emergence

Fig. 11 HOMO-m (in the *left*) and LUMO + 1 (in the *right*) orbitals of 45th and 47th excited states of photosynthetic prebiotic kernel. *Blue* and *gray* volumes respectively indicate negative and positive parts of the wave function. (Color figure online)

Fig. 12 Visualization of the quantum entangled electron charge tunnelling associated with the 45th (482.5 nm) excited state. The transition to the pFA molecule (in the *center*) is mainly from the squaraine part of the SQ-8-oxo-guanine supermolecule (*top-right*), with a minor contribution coming from the 1,4-bis(*N,N*-dimethylamino)naphthalene-8-oxo-guanine supermolecule (*right-bottom* molecule)

Fig. 13 Visualization of the quantum entangled electron charge tunnelling associated with the 47th (479.5 nm) excited state. The transition to the pFA molecule (in the *center*) is mainly from SQ-8-oxo-guanine::cytosine supramolecule (in the *upper-right*), with a minor contribution coming from the 1,4-bis(*N,N*-dimethylamino)naphthalene-8-oxo-guanine supermolecule (extending up from the *right-bottom*)

of photosynthetic prebiotic kernels and accelerated the evolution of photosynthetic life because of more absorbed light energy.

2) A two variable, quantum entangled AND logic gate was modelled in the system described, which consists of

Fig. 14 **a** Image of system (4) composed of two photosynthetic prebiotic kernels (2) (in the *right-bottom*) and (3) (in the *left-top*) before geometry optimization. Carbon atoms and their associated covalent bonds are shown as *green sticks*, hydrogens—*light gray*, nitrogens—*blue*, oxygens—*red*. *Dashed lines* show the hydrogen bonds. **b** Image of system (4) composed of two photosynthetic prebiotic kernels (2) and (3) after geometry optimization. Carbon atoms and their associated covalent bonds are shown as *green sticks*, hydrogens—*light gray*, nitrogens—*blue*, oxygens—*red*. *Dashed lines* show the hydrogen bonds. (Color figure online)

two input photoactive sensitizer molecules containing two different variable inputs and one output. In future, this process might be applied to nanomedicine.

The quantum mechanical self-assembly of two separate magnetically active and photoactive supramolecular open electronic shell subsystems (5) and (6) in the system (7) with different possessing neutral radical molecules was investigated by means of density functional theory methods (see Fig. 15a and Tamulis et al. 2014). Only few not connected by hydrogen bonds water molecules are in

Fig. 15 **a** Image of system (7) composed of two magnetically active photosynthetic prebiotic kernels: (5) possessing neutral radical 5-(4-(1-hydroxyethyl)phenyl)pentanoic acid molecule (in the top) and (6) possessing neutral radical 5-(2,8-dimethyl-1,3-dioxo-2,3-dihydro-1H-phenalen-5-yl)pentanoic acid molecule (in the bottom) before geometry optimization. Carbon atoms and their associated covalent bonds are shown as green sticks, hydrogens—light gray, oxygens—red. Dashed lines show the hydrogen bonds. **b** Image of system (7) composed of two photosynthetic minimal protocells (5) and (6) after geometry optimization. (Color figure online)

between two photosynthetic prebiotic kernels (5) and (6) in the system (7) (see Fig. 15a).

The initial distance between the edging molecules of (5) and (6) subsystems was done equal to 7.6 Å, i.e., few times large in comparison with than experimental Van der Waals distances between organic molecules (see Fig. 15a) because we decided to observe the movie of self assembly of two subsystems. The geometry optimization of system (7) was performed by using the DFT method RI-BP with Grimme dispersion electron correction and SV(P) basis set in the Turbomole program package.

The process of geometry optimization reduced the distance between the (5) and (6) subsystems (compare Fig. 15a, b) due to Van der Waals interactions between these subsystems. All water molecules are connected by hydrogen bonds in between two photosynthetic prebiotic kernels (5) and (6) in the system (7) (see Fig. 15b) after geometry optimization procedure.

Absorption spectra as well as electron spin density transfer trajectories associated with the different excited states were calculated using time-dependent density functional theory method PBE0 using TZVP basis set in Turbomole program package. The results allow separation of the quantum entangled photosynthetic spin density transitions within the same photosynthetic prebiotic kernel [(5) or (6)] and with the neighbouring photosynthetic prebiotic kernel in the system (7). Analysis of frontier orbitals HOMO-*m* and LUMO + *n* of the system (7) in the excited states 13th shows that there also exists quantum entanglement between two photosynthetic minimal protocells (5) and (6). This means that electron spin density transition energy (and information) might be transferred at the same time (during excited state 13th) from the two different photosynthetic prebiotic kernels (5) and (6) in the system (7).

We have found a two variable, quantum entangled AND logic gate in the system (7), consisting of two input photoactive neutral radical molecules and one output (pFA molecule).

Longer term goals in the use of quantum mechanical simulations might include: be (a) to predict the possibility of biochemical experimental synthesis of molecular electronics and spintronics logic elements for information systems based on artificial self-reproducing organisms (Tamulis et al. 2012, 2013, 2014; Tamulis and Tamulis 2008), (b) to control nanobiorobots applied in areas such as nanomedicine and cleaning of nuclear, chemical, and microbial pollution. The solution of basic questions of emergence and evolution of the first self-reproducing cells or protocells is tightly connected with the rapidly developing field of artificial self-reproducing technologies in several laboratories around the world. The possibility of synthesizing artificial magnetically active self-reproducing cells also impacts the possibility of the emergence of self-reproducing protocells on the Earth or elsewhere.

The quantum mechanical investigations of two types of neutral radical molecules: 5-(4-(1-hydroxyethyl)phenyl)pentanoic acid molecule 5-(2,8-dimethyl-1,3-dioxo-2,3-dihydro-1H-phenalen-5-yl)pentanoic acid molecule and separate photoactive prebiotic kernels: (2), (3) and (5), (6) possessing neutral radical molecules have been performed on the Linux servers cluster of our research group. Dr. Jonas Baltrusaitis has performed quantum chemical calculations of the systems of prebiotic kernels (4) and (7)

using the 2000 node supercomputer of the University of Iowa.

Summary

- (A) More and more research results anticipate that molecular and cellular biology science can be described with quantum entanglement phenomenon. For example, an analytical expression was derived for the binding energy of the DNA coupled chain in terms of entanglement and show the connection between entanglement and correlation energy, a quantity commonly used in our quantum chemistry calculations (Tamulis et al. 2012, 2013, 2014). The paper contains the review of quantum entanglement investigations in living or self-reproducing systems.
- (B) The review of synthesis of artificial cells and quantum mechanical modelling of self-assembling of photoactive supramolecular systems with observed quantum entanglement phenomenon is presented. It is possible to make the following statements concerning our investigated self-assembled photosynthetic prebiotic kernel with two different photosynthetic centres and model systems composed of two photosynthetic prebiotic kernels:
1. The pairs of quantum entanglement excited states of a photosynthetic prebiotic kernels (1), (2) and (3), or (5) and (6) are composed of the HOMO- m states located on the sensitizer supramolecule and the sensitizer supermolecule and the LUMO + n on a fatty acid precursor molecule. This coupling promotes electron hopping (tunnelling) from these photoactive derivatives to the pFA molecules in the excited states.
 2. The results allow separation of the quantum entangled photosynthetic electron density or electron spin density transitions within the same photoactive prebiotic kernel [(1), (2), (3) or (5), (6)] and with the neighbouring photosynthetic prebiotic kernels in (4) or (7) possessing photoactive close shell molecules or photoactive open electronic shell neutral radical molecules. This means that electron density or electron spin density transition energy (and information) might be transferred at the same time from the two different photosynthetic prebiotic kernels in the system.
 3. Analysis by our methods in the different excited states allows us to separate quantum-entangled photosynthetic transitions between neighbouring prebiotic kernel models. This means that a

quantum-entangled phenomenon of energy and information transfer exists in these model units, which might correspond to prebiotic self-reproducing organisms which existed in the photosynthetic prebiotic kernel stages of the emergence and evolution of life. The possibility of synthesizing artificial self-reproducing quantum entangled cells also impacts the possibility of the emergence of such a kind self-reproducing protocells on the Earth or elsewhere. Our discovered phenomenon of the quantum entanglement in the prebiotic kernel systems enhance of photosynthesis in the system because simultaneously excite two prebiotic kernels in the system by appearance of two additional quantum entangled excited states. We can propose that quantum entanglement enhanced the emergence of photosynthetic prebiotic kernels and accelerated the evolution of photosynthetic life because of more absorbed light energy, leading to faster growth and self-replication of minimal living cells.

4. Different two variable, quantum entangled AND logic gates were discovered in these photosynthetic prebiotic kernel systems (1), (4) and (7) described, which consist of two input photoactive sensitizer derivatives containing two different variable inputs and one output. It is proposed that a similar process might be applied for the destruction of tumour cancer cells or to yield building blocks in artificial cells and in magnetically active artificial cells.

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