Quantum information artificial living organisms or quantum nanobiorobots

for nanomedicine and cleaning of nuclear, chemical and microbial pollutions

(project)

Arvydas Tamulis and Vykintas Tamulis

Vilnius University Institute of Theoretical Physics and Astronomy, Vilnius, Lithuania

E-mail: tamulis@itpa.lt

WEBsite: http://www.itpa.lt/~tamulis/

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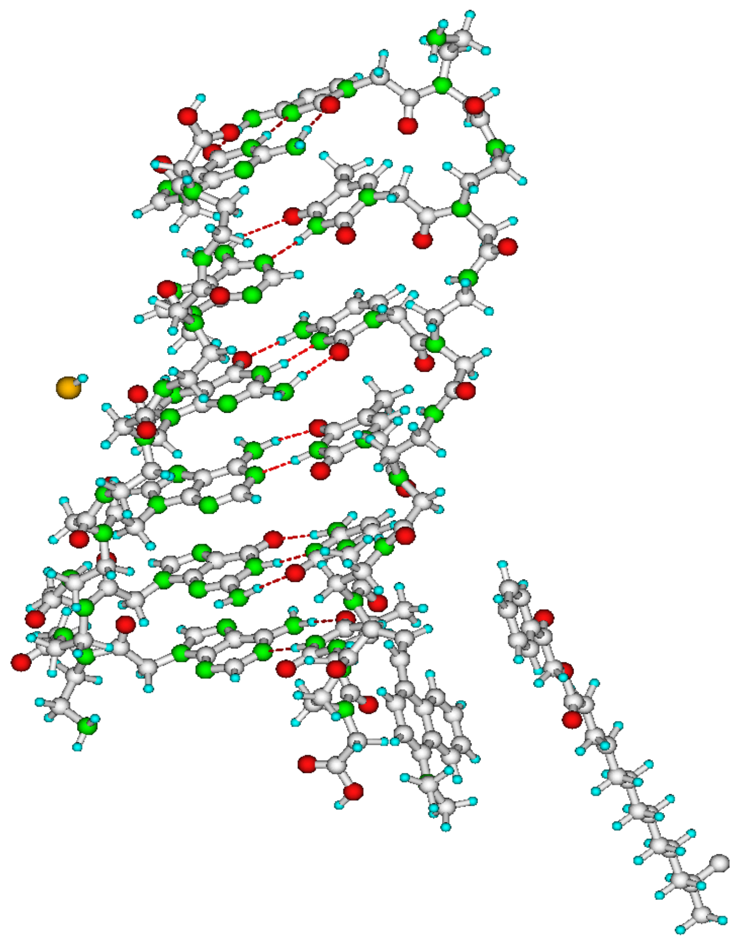
We have started from quantum mechanical investigations of artificial minimal cell proposed in the paper [1]:

[1] S. Rasmussen, L. Chen, M. Nilsson, and S. Abe, *Artificial Life*, vol 9, 267-316, 2003.

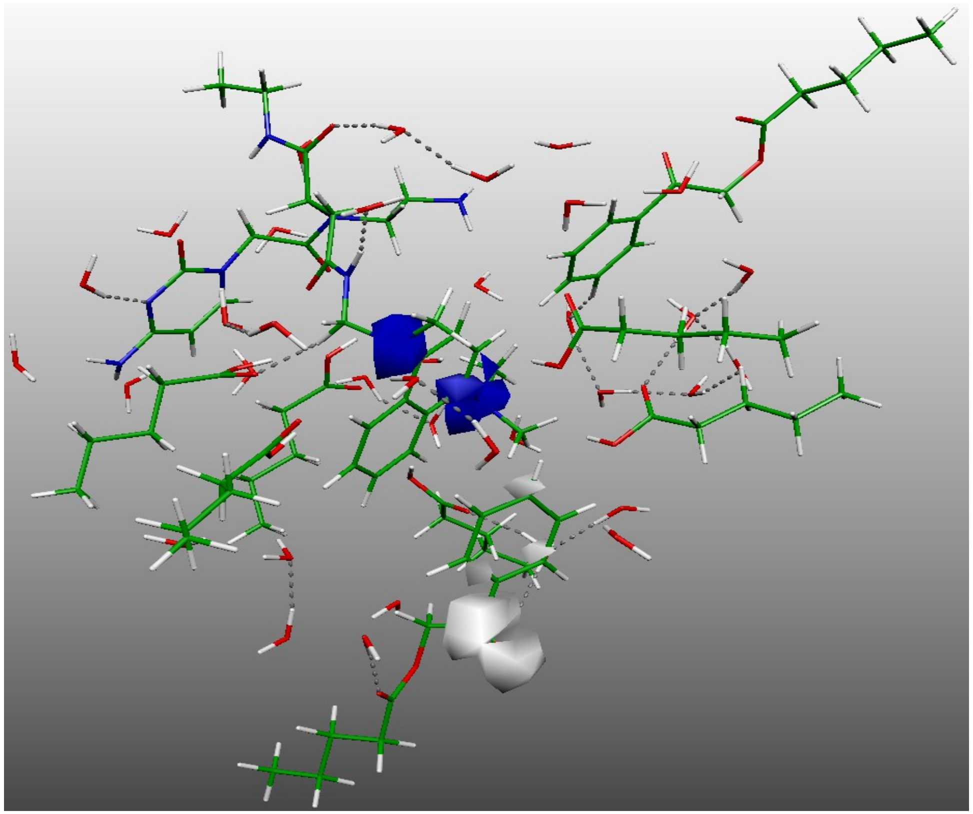
Some of the main parts of one of the artificial protoorganism proposed in [1] include a PNA double helix molecule which is covalently bonded to the 1,4-bis(N,N-dimethyl-amino)naphthalene sensitizer molecule shown at bottom center, a precursor of fatty acid (pFA) molecule (bottom right), an SH anion molecule (center left). Carbon atoms are shown as grey spheres, hydrogens are blue, oxygens – red, nitrogens – green, sulfur – gold. Quantum self-assembly was done by electron correlation quantum mechanical (QM) GAMESS-US package methods on LANL Altix 3000 [2].

[2] A. Tamulis, V. Tamulis A. Graja. Quantum mechanical modeling of self-assembly and photoinduced electron transfer in PNA based artificial living organism, *Journal of Nanoscience and Nanotechnology*, **6, 965-973 (2006)**.



Visualization of the QM electron charge tunnelling in the self-assembled artificial minimal cell associated with the most intensive excited state is given in the figure below. The electron cloud hole is indicated by the blue color while the transferred electron cloud location is visualized by the grey colour. The QM time dependent (TD) DFT PBEPBE/6-31G model calculation indicated that the most intense electron charge transition from the 1,4-bis(N,N-dimethylamino)naphthalene sensitizer molecule to the pFA molecule (in bottom) is equal to 440.0 nm [3]. Small shift to blue in comparison with the experimental value of 450 nm is possible to understand as being due to the greater number of water and FA molecules found in the real system.

[3] A. Tamulis,V. Tamulis, "Measure of Complexity and Photoinduced Electron Tunneling in Photosynthetic Systems of PNA Based Self-Assembled Protocells", book of abstracts of Third Annual meeting COST Action P10 "Physics of Risk" & Workshop on "Complex System Science", Vilnius Lihuania, 13-16 May 2006, p. 59-60.



We have performed search for suitable stable neutral radical molecules for molecular quantum computers in Los Alamos National Laboratory project: "Quantum Computing in Self-Assembled Arrays of Radical Molecules".

A. Tamulis, V. I. Tsifrinovich, S. Tretiak, G. P. Berman, D. L. Allara, "Neutral Radical Molecules ordered in Self-Assembled Monolayer Systems for Quantum Information Processing", arXiv.org e-Print archive, Quantum Physics, http://arxiv.org/list/quant-ph/0307?100, quant-ph/0307136 [abs, pdf], July, 2003.

J. Tamuliene, A. Tamulis, J. Kulys "Electronic Structure of Dodecyl Syringate Radical Suitable for ESR Molecular Quantum Computers", ***Nonlinear Analysis: Modeling and Control*****, Vol. 9, No 2, p.p. 185-196 (2004).**

Issues of this research:
Our results indicated that stable neutral radical molecules should be used to create a macroscopic ensemble of quantum entangled 3-spin groups, as a first step in quantum information processing.
The spins of such a group could be connected by spin dipole-dipole interaction. Application of a nonuniform external magnetic field should allow selective excitation of every spin inside the group.

Our research presented in the previous slides might be as basis for creation of the new project:

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The main objectives of this project are:

1) To develop the molecular electronic and spintronic logical nanodevices;
2) To implement logically controlling molecular logical nanodevices for self-assembly and photochemistry (growth and self-replication) in the artificial living quantum information organisms;
3) To construct quantum computing molecular artificial living systems nanostructures organized to complex quantum information systems;
4) To develop reprogrammable quantum nanobiorobots.

Potential applications:

Reprogrammable artificial living quantum information organisms and quantum nanobiorobots will be prepared for nanomedicine and cleaning of nuclear, chemical and microbial pollutions in the case of terrorist attacks.

We are looking around for the partners, mainly experimentalists who may support the realisation of this project.