Quantum Modelling of Processes in Artificial Living Organisms and Elements of Molecular Computers

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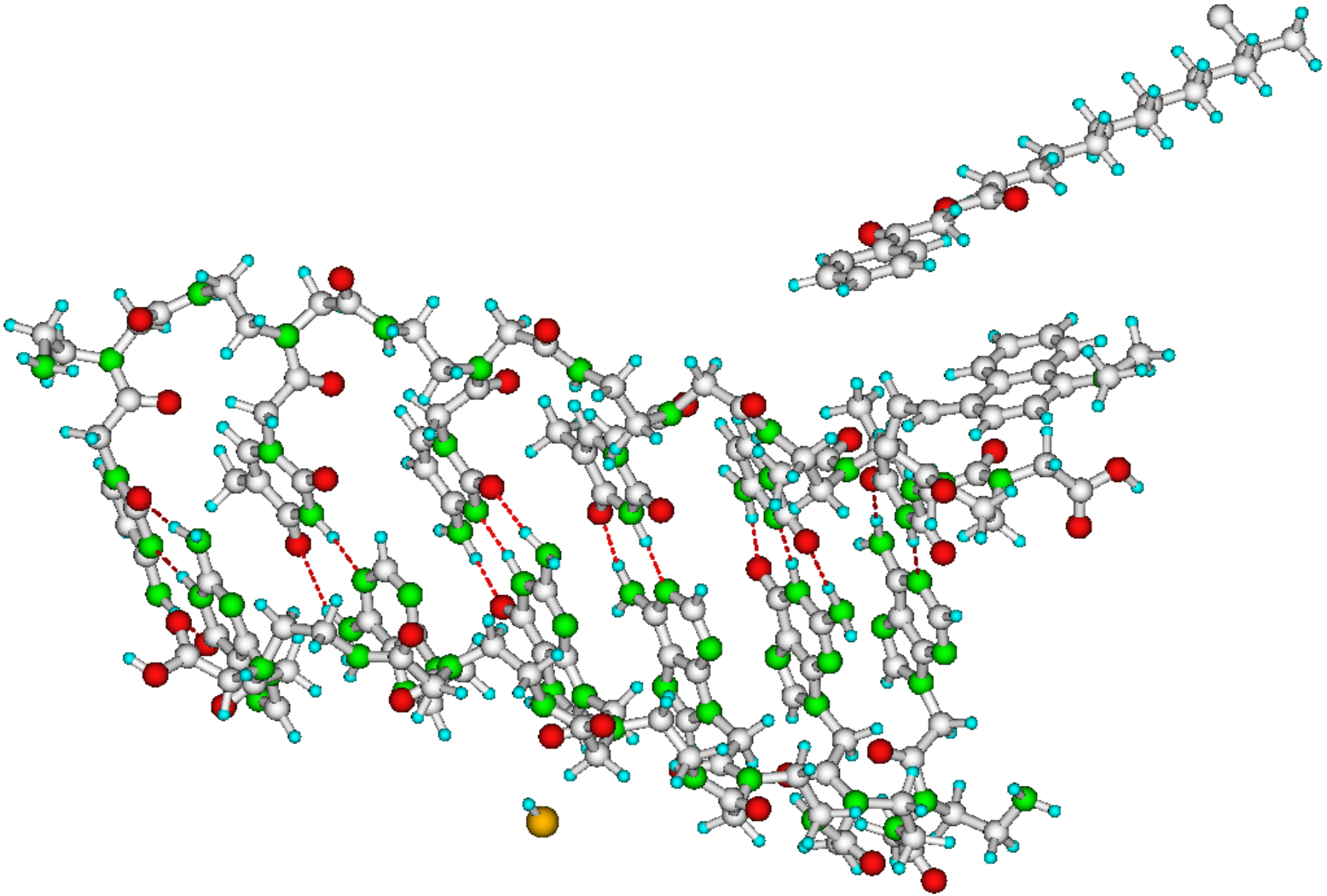
1. ***Quantum Modelling of Artificial Photosynthetic Systems Based on Assemblies of Modified Peptide Nucleic Acids (PNA) and Lipid Molecules.***

This research we are performing in the framework of EU FP6 granted consortium: 'Programmable Artificial Cell Evolution (PACE)'.

We need Baltic Grid sources because we are doing now exact quantum mechanical simulations of self-assembly and electron migration processes in peptide nucleic acids surrounded by lipid molecules in the excited states using Time Dependent Density Functional Theory.

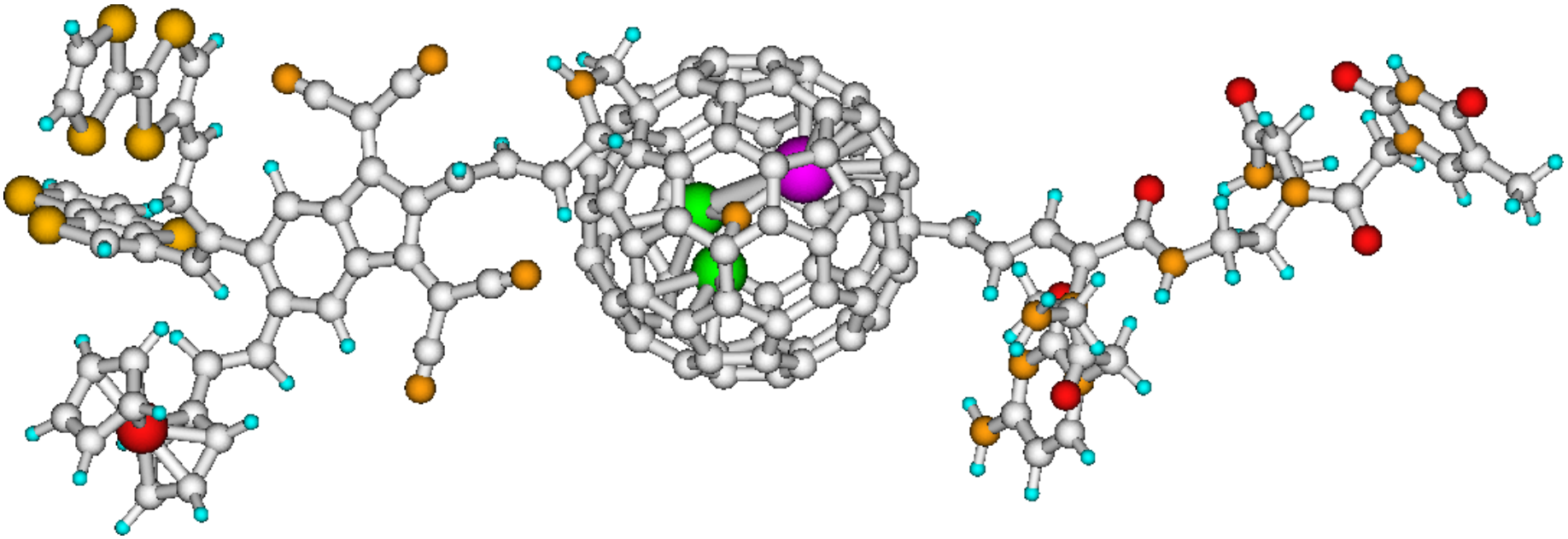
The main components of artificial living organism see in the next slide.



2. Quantum Modelling of Elements of Molecular Computers

This research we are performing in the framework of NorFA granted consortium: 'Quantum Modelling of Molecular Materials'

Quantum mechanical modelling of electron and spin transfer in logically controlled artificial photosynthetic systems (see figure bellow) needs Baltic Grid sources.



CONCLUSION

Quantum mechanical modelling using parallel programmes running on Baltic Grid PC clusters should allow to predict the geometry, electronic and spintronic structure in ground state of biological supermolecules and supramolecules consisting from arround 10,000 atoms, and spectra, electron charge and spin transfer in excited states for biological molecules consisting from arround 1,000 atoms.