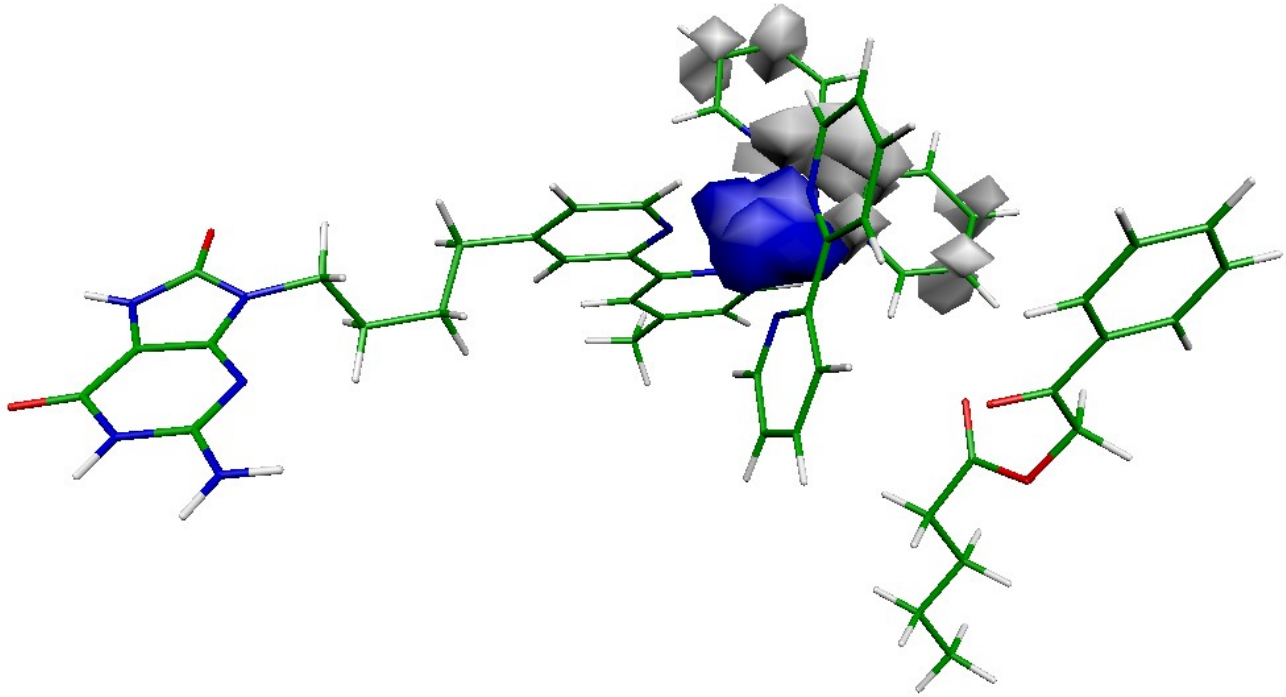

Figure 1. Visualization of calculated quantum mechanical process of photosynthesis of artificial protocell synthesized in USA LANL [1]. During fifth excited state the single electron is hopping (tunneling) from Ru atom of photosynthetic center (dark blue cloud of electron hole) to the one of ligands (grey cloud of electron). Carbon atoms and their associated covalent bonds are shown as green spheres and sticks, hydrogens are in light grey, oxygens – red, nitrogens – blue.

[1] A. Tamulis, V. Tamulis, H. Ziock, S. Rasmussen, "Influence of Water and Fatty Acid Molecules on Quantum Photoinduced Electron Tunnelling in Photosynthetic Systems of PNA Based Self-Assembled Protocells", printing process in *"Multi-scale Simulation Methods for Materials", eds. R. Ross and S. Mohanty, John Wiley & Sons, Inc., New Jersey,* 2006.

This research was performed by using TD DFT B3LYP/Dgauss ORCA software installed in our new dual processor Opteron servers Linux cluster in Theoretical Molecular Electronics and Spintronics research group of Vilnius University Institute of Theoretical Physics and Astronomy (fee Figure 2 below).

My question is: how to calculate quantum mechanically the further electron migration from ligand to the precursor of fatty acid molecule (right side of Figure 1) ?

Maybe it is necessary to reoptimize the geometry in the fifth excited state by G03/HF/CIS or TURBOMOLE and then to do the single point calculation by TD DFT B3LYP/Dgauss/ORCA and automatically we should get electron charge transfer from ligand to precursor of fatty acid molecule? Any suggestions?

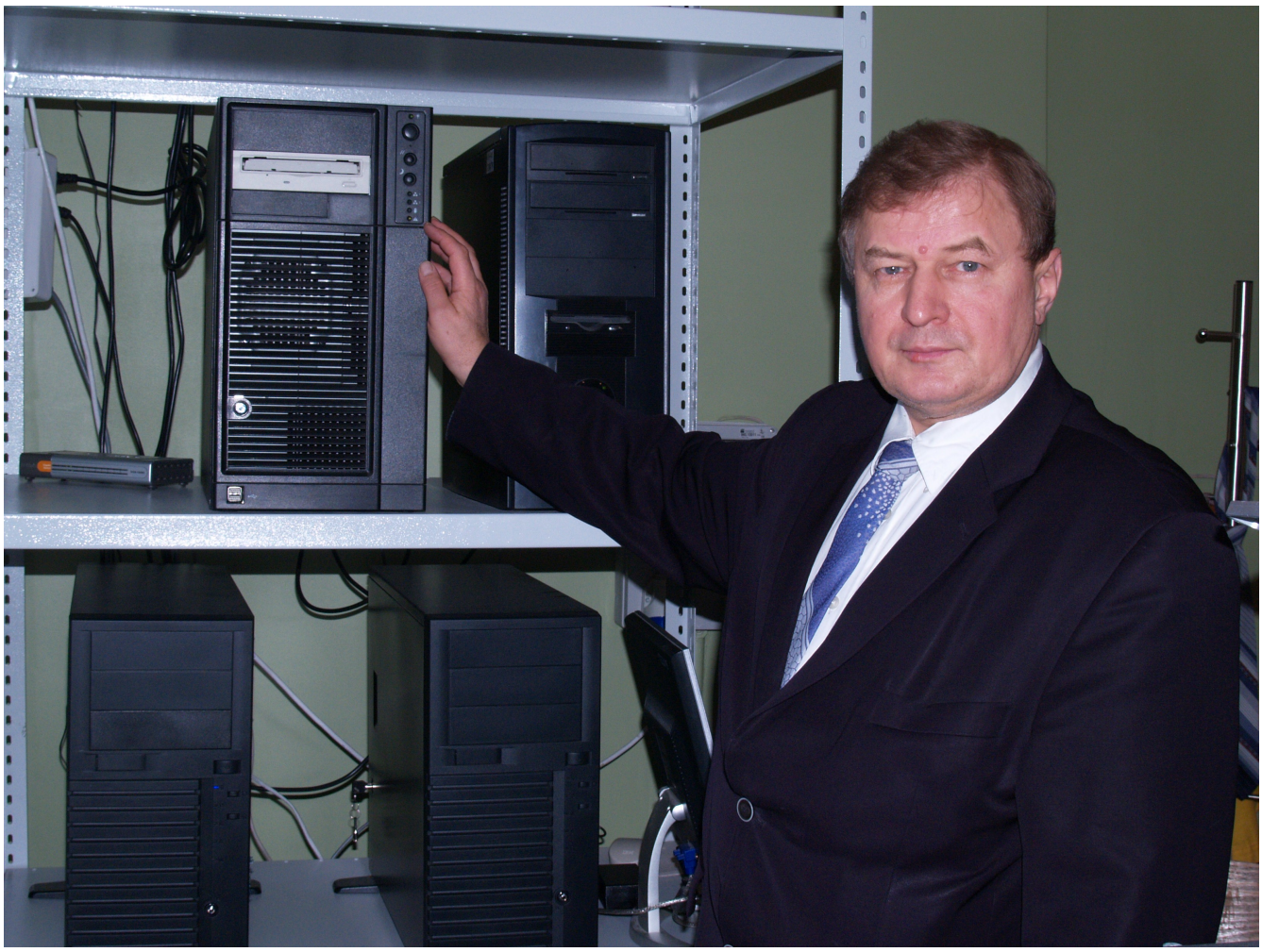

Figure 2. New dual processor Opteron servers Linux cluster in Theoretical Molecular Electronics and Spintronics research group (http://www.itpa.lt/~tamulis/) of Vilnius University Institute of Theoretical Physics and Astronomy purchased on the grants of EU FP6 "Programmable Artificial Cell Evolution" www.protocell.org/PACE and Lithuanian State Science and Studies Foundation.