

DESCRIPTION FOR THE GENERAL PUBLIC

(state the objective of the project, describe the research to be carried out, and present reasons for choosing the research topic)

The origins of life on Earth are still shrouded in mist of mystery, even though there are many credible hypotheses. This project may shed light on some aspects of the so-called RNA world hypothesis. According to it, the first living organisms were based on the proto-RNA molecules, that played a role of both modern informational polymers and enzymes. Such macromolecules would be capable of self replication—a hallmark of life. It is worth noting that currently the laboratory synthesis of RNA and DNA chains without relying on the enzymatic catalysis, and consequently the living organisms, is extremely difficult. That is why we are still not sure how it was possible to occur spontaneously on the early Earth.

It seems that the first traces of early life that flourished in the oceans date back to at least 3.7 billion years ago. At that time the amount of ultraviolet (UV) radiation reaching the Earth's surface was many times higher than at present, due to the lack of the ozone layer and higher activity of the young Sun in this spectral range. The first living organisms capable of metabolism and replication were probably based on π -electronic macromolecules susceptible to UV radiation induced damage, that reached these molecules unattenuated through cellular structures present in contemporary living organisms. Thus, UV radiation was probably not only an efficient energy source, driving the early stages of abiogenesis, but also an important selective factor.

This project is an extension and continuation of our previous theoretical studies on photochemistry of hypothetical synthetic routes to RNA nucleotides and photostability of important intermediate species. It will be carried out in collaboration with the experimental teams. *Ab initio* calculations provide a number of relevant insights into the mechanisms of UV radiation induced processes, that cannot be derived solely from spectroscopic studies. Quantum chemical simulations support the interpretation of experimental results and allow for determination of the molecular mechanisms of these processes.

We plan to study the mechanisms of selected photochemical processes, that could have lead to abiotic synthesis of nucleic acid bases, nucleotides and amino acids, as well as simple sugars and amphiphiles—all the necessary building blocks of life. We hope that our results could bring us a bit closer to answering perhaps the most momentous and fascinating question of modern science. The question of our origins.