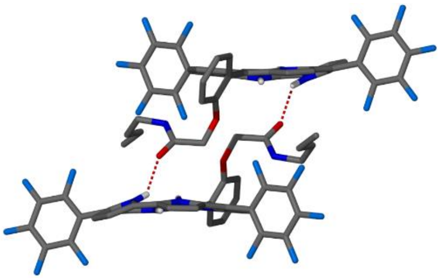
Synthesis, self-assembly and long-range electron transfer in amide-functionalized self-assembled corroles

There is no doubt that life depends on interactions between the molecules (i.e. on supramolecular chemistry). Vast majority of compounds present in cells, undergo either self-organization process (proteins, DNA) or supramolecular interactions with other compounds (that happens e.g. in enzymes). In such large and complex molecules, electron transfer is an important process. It influences the functions of biomolecules and its fluctuations can cause far-reaching consequences, typically negative ones. Proteins are complicated organic compounds and quite often in order to replace them, chemists use synthetic molecules with somewhat simpler structure but at the same time possessing key elements such as multiple amide bonds and prosthetic groups.

In this project we will design, synthetize and study such organic compounds containing both amide bonds (being basic backbone of proteins) and corroles, which are structurally relative to porphyrins. Porphyrins are 'pigments of life' since they are responsible for red color of blood (reversible oxygen binding) and green color of plants (photosynthesis). The novel type of hydrogen bonds between macrocyclic core and amide groups will induce the formation of various unprecedented oligomers and possibly supramolecular polymer.



Consequently, in this project we will realize the following research tasks: organic synthesis, studies of self-assembly of organic molecules and photophysical studies of these molecules at various conditions. The last part of research will be conducted in California Institute of Technology (US). First part of investigation will be focused on bis(amido-corroles) – compounds containing two hydrogen bonds. Subsequently, we will move towards dyes containing also perylene-bisimide scaffold (as an electron-acceptor) and additional hydrogen bonds derived from amino acids residues. In both cases crystallographic methods will allow to establish structure in the solid state and nuclear magnetic resonance method will enable to perform analogous studies in the solutions. Photophysical measurements will require both steady-state and time-resolved methods.

It is expected that these molecules will interact forming larger supramolecular entities. Hydrogen bonds formation (hence optical properties) will be dependent on concentration as well as on the type of solvent, and therefore it will be amenable for manipulations.

The results of this project will not only allow to establish relationship between the structure of these bis(amido-corroles) as well as bis(amido-corroles)-perylene-bisimides, and two competitive mechanisms of electron-transfer: *via* tunneling and *via* hopping. In broader perspective, results of our project should broaden our knowledge about function of proteins in the cells. They will be also useful in design of more efficient systems for photo-driven water splitting based on solar energy.