Spin injection to large polycyclic aromatic hydrocarbons - construction of stable ring-fused [1,2,4]triazinyl radicals

The increasing demand for modern technologies is conducive to the dynamic development of the electronics industry, thus driving the global economy. The expected limitations of current technologies open the door to the search for new solutions in the field of organic molecular electronics. More and more often, for designing of materials for organic electronics, stable organic radicals are used, which, apart from favorable electronic properties, give materials magnetic properties. In such systems, the unpaired electron spin plays the role of a magnetic factor - desired in spintronics (information processing) and provides access to multiple stable redox states (anion, radical, cation) desired *e.g.* in organic batteries. Moreover, paramagnetic organic materials have also found application in semiconductor materials, spin valves, photovoltaics and OLEDs. All these systems rely to a greater or lesser degree on molecular order on the surface or in the volume. Therefore, further progress related to the construction of properly functionalized radicals and the study of their self-organization is one of the greatest interests and challenges of modern materials science.

This proposal addresses these challenges and deals with construction of molecular materials, which permit extensive studies and address the current needs of modern science. Therefore, we propose to develop a unique class of large paramagnetic aromatic hydrocarbons (LPAHs) containing π-delocalized 1,4-dihydro[1,2,4]triazin-4-yl radical (Figure 1), and investigate their electronic and magnetic properties in the context of fundamental science and applications related to information storage and processing.

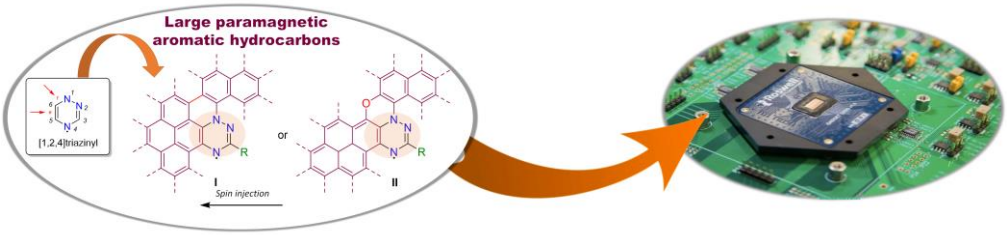

Figure 1. General structures of large paramagnetic polycyclic aromatic hydrocarbons **I** and **II** with the 1,4-dihydro[1,2,4]triazin-4-yl fragment as a paramagnetic structural motif.

The obtained materials will be characterized using a wide range of physical-organic tools that include UV-Vis and EPR spectroscopy, electrochemical and magnetic studies. Consequently, accomplishing of the project goals will make a significant contribution to further progress in developing of technologies based on organic functional materials.

The presented project is the first stage of a broader research program, which the PI intends to establish at the University of Łódź, and which is aimed at investigation of organic paramagnetic materials in the broad context of molecular electronics in modern technologies especially for data processing and manipulation. This research program provides excellent opportunities for young chemists to broader insight into structure-properties relationship.