Topologically coupled stable diradicals with tunable singlet-triplet energy gaps for molecular materials

The proposed research project deals with an unusual class of organic compounds – stable diradicals of type **A** and **B** and polyradicals, which exhibit tunable magnetic properties. The centerpiece of the molecular design of these compounds are two heterocycles **I** (Figure 1), which are connected either directly (**A**) or through a π linker (**B**) determining their magnetic ground state. The first phase of the project, to be accomplished in this proposal, focuses on understanding of chemistry and properties of these di- and poly-radicals. In the next phase, selected diradicals will be appropriately substituted to self-organize into columns providing unidimensional conduits for charge transport and for propagation of magnetic interactions. Such materials are sought after for modern technologies.

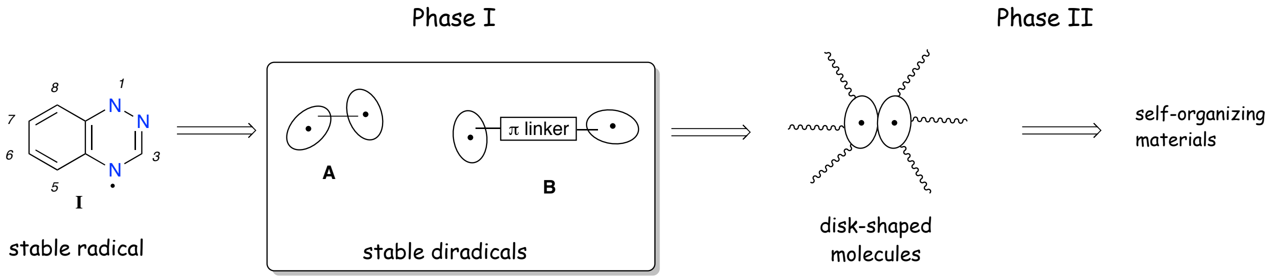

Figure 1. Diradicals **A** and **B** formed by connecting two molecules of the 1,4-dihydrobenzo[*e*][1,2,4]triazin-4-yl (**I**) either directly (**A**) or through a π linker (**B**). Their substitution with appropriate groups leads to self-organizing materials, including liquid crystals. The dot represents an unpaired electron.

Magnetism, typically associated with certain metals and minerals, is one of the most fundamental natural phenomena, and is indispensible for modern technologies ranging from a simple compass to information storage and processing devices. It originates from properties of an unpaired electron and its cooperative interactions with other electrons. In organic compounds Nature prefers pairing of electrons and those with unpaired electron - organic radicals - typically are highly reactive. There is only a very small group of stable organic compounds with unpaired electrons – stable organic radicals - and their magnetic properties are truly fascinating with a vast potential for technological applications. In this project we connect two exceptionally stable radicals **I** in such a way as to induce controlled magnetic interactions between the electron spins. The most interesting scenario is when the two electrons exhibit strong cooperative interactions giving rise to a ferromagnetic coupling.

Organic compounds proposed in this project, besides being truly fascinating and defying Nature, belong to a larger group of high-spin organic materials, which are being considered as key components of the next generation of information storage and processing devices built from individual molecules. Therefore, the proposed molecules will be investigated with a broad range of physical method and with help of scientists from other research areas.

In the context of the proposed studies, new synthetic methods will be developed, unknown organic compounds and diradicals will be obtained and properties, such as spectroscopic and magnetic, of the prepared materials will be investigated. The planned synthesis of a significant number of compounds will result in establishing of molecular structure – properties relationships, which will allow rational design of new structures, such as those self-organizing mentioned above, with desired behavior.

The proposed program is focused on education and training of young researchers and the creation of modern interdisciplinary workforce for scientific and technological challenges of the 21st Century.