



We are planning to investigate synthesis of certain new polycyclic aromatic compounds that possess properties such as curved geometry and paramagnetism. The efforts towards target molecules will be driven by the advancement of synthetic methodology. We will seek improved understanding of a key chemical reaction responsible for assembling the structural core of the envisaged targets. By adjusting the catalyst used in this process, as well as other conditions, we are planning to conduct this reaction with a level of control over the distribution of isomeric products, selectively obtaining the ones that are useful for further transformations. The scope of this method will also be expanded to include certain unprecedented types of substrates.

Some of the target molecules possess an open-shell character: they contain unpaired electrons, which imparts a range of unusual properties. Depending on the character of interaction between these electrons, these compounds can act as molecular magnets, and are of interest for prospective applications in spintronics. These materials also tend to absorb light in the near-infrared range and to reversibly lose or accept electrons, adopting a range of ionic forms. On this basis further potential applications in organic electronics and as functional dyes have been envisaged.

Another category of our synthetic targets is the negatively curved polyaromatic structures. A unique property of such molecules is the intrinsically decreased ability to interact with one another and form aggregates. This quality results in a relative ease of solubilization. In particular, this greatly facilitates dissolution in water through the introduction of hydrophilic groups. It is hypothesized that curved, non-aggregating polyaromatic surfaces dispersed in water may be used for binding of various biologically important molecules, such as nucleosides, thyroid hormones, steroid hormones, neurotransmitters, and DNA-intercalating drugs. We are planning to prepare water-solubilized negatively curved polyaromatic compounds and conduct molecular recognition experiments to determine their potential as molecular sensors.