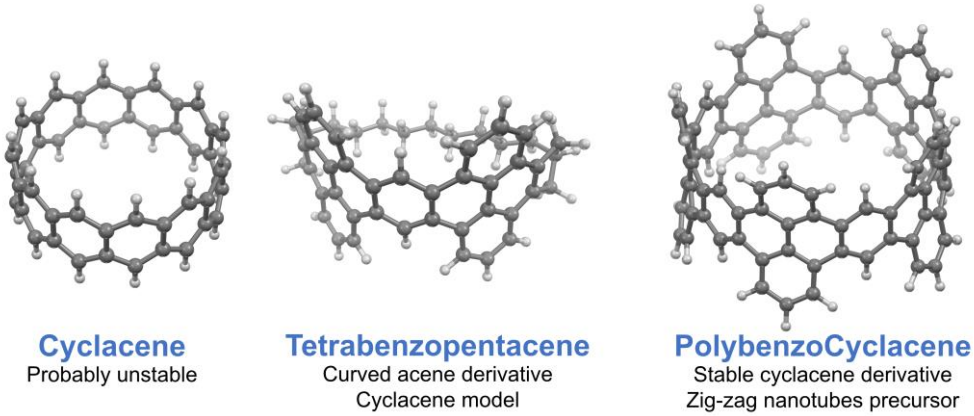
Recent progress in organic synthesis has allowed the synthesis of desirable chemical compounds, whose preparation seemed practically impossible not so long ago. A good example are the so-called carbon nanorings and nanobelts; nanometer-size rings composed solely of carbon and hydrogen atoms that have been successfully synthesized only in the last decade. Structurally, carbon nanorings and nanobelts are single segments of carbon nanotubes and thus have been proposed as precursors for the bottom-up synthesis of high-quality uniform nanotubes, which would be of great importance for the development of new technologies such as organic electronics.

Unfortunately, only nanorings and nanobelts being precursors of armchair or chiral nanotubes have been synthesized so-far. Despite numerous attempts, the precursors of zig-zag carbon nanotubes – cyclacenes – remain elusive. This is due to the fact that cyclacenes, cyclic analogues of acenes, according to theoretical predictions should be extremely unstable. Their synthesis is further hampered by the lack of appropriate synthetic methods that would be able to convert the corresponding strain-free cyclic precursors into a highly strained cyclacene system.

The main goal of this project is to develop efficient strain-building reactions enabling the synthesis of stable derivatives of cyclacene. These studies will be carried out using curved analogues of acenes as simplified, small molecule models of the corresponding cyclacenes. In order to stabilize the curved systems of acene and cyclacene, additional fused benzene rings will be introduced into the target structures. The potential synthetic pathways towards these targets will be preselected based on the results of the theoretical modeling of various reactions using the Density Functional Theory. The most promising reactions will then be utilized in the synthesis of alkyl-bridged curved acene derivatives. If successful, the accumulated knowledge and the developed methodology will be applied in the synthesis of a table derivatives of cyclacene.



Both types of target products, curved acenes and cyclacenes, are extremely interesting compounds that should exhibit exceptional photophysical, electrochemical and supramolecular properties. For this reason, the properties of the obtained derivatives will be thoroughly examined and compared with their planar counterparts.

The implementation of this project will lead to the development of a methodology for the synthesis of strained aromatic and macrocyclic systems. It will also significantly expand the knowledge about the properties of curved polycyclic aromatic hydrocarbons. Preparation of stable cyclacene derivatives will be an important step towards the bottom-up synthesis of zig-zag carbon nanotubes. This achievement will be of great significance for the development of modern nanotechnologies.