

## **Project 2.5 Synthesis of curved derivatives of acenes - towards bottom-up synthesis of zig-zag carbon nanotubes**

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### **Background:**

The PhD candidate will be responsible for the synthesis of the building blocks and macrocyclic strain-free precursors, as well as their conversion into the derivatives of curved acenes. The acquired knowledge and experience will be used in attempts to synthesize the stable derivatives of cyclacene – precursors for the bottom-up synthesis of zig-zag carbon nanotubes.

### **Aim:**

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 pathways 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.

### **Requirements:**

- A PhD student should hold a Master degree in chemistry and have experience in working in an organic chemistry laboratory,
- he or she should also have broad knowledge in the modern synthetic methodology as well as be familiar with spectroscopic techniques used to characterize the organic compounds (NMR and MS)
- an additional advantage will be the experience in the synthesis of polycyclic aromatic compounds or dyes and the knowledge of quantum chemical calculation methods (DFT).