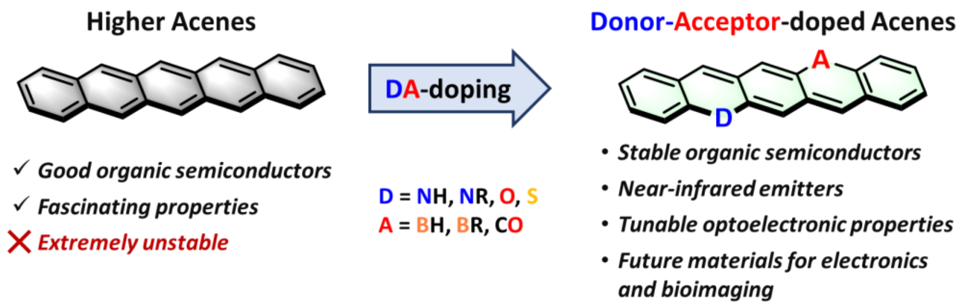
Donor-acceptor-doped acenes and cyclacenes

The growing awareness of global environmental problems has pushed scientists to look for new and greener alternatives to many technologies related to energy production, conversion, and storage. In addition, replacements for traditional electronics based on silicon and heavy or rare-earth metals are sought, as their life cycles generate a high level of pollution or have substantial carbon footprints. To find solutions to these problems, scientists have turned their attention to π-conjugated organic molecules, compounds containing systems of alternate single and double bonds. Acenes are an especially interesting group of π-conjugated aromatic compounds owing to their unique photophysical properties and excellent semiconductivity, which make them promising candidates for applications in organic electronics, such as in organic field-effect transistors (OFETs) and organic light-emitting diodes (OLEDs). Furthermore, acenes participate in important energy conversion processes, namely triplet-triplet annihilation upconversion and singlet fission, which are predicted to improve the efficiencies of future photovoltaic cells. However, higher acenes are characterized by high reactivity and suffer from extreme instability, which prevents their use in real-life applications at the current stage. To fully unleash the potential of these molecules, an efficient stabilization method of the acene system is necessary.

In this project, we propose a novel method to stabilize higher acenes and their cyclic relatives, cyclacenes, by doping them with donor and acceptor moieties at carefully selected positions in such a way that the resulting compounds would retain the key structural and electronic advantages of the parent systems and yet exhibit high stability both in solution and in the solid state. In addition to good stability, the new donor-acceptor-doped analogues should also be highly advantageous in terms of their optoelectronic properties, which are beneficial from the applicational perspective: narrow bandgap, absorption/emission in the near-infrared region, and tuneable singlet-triplet energy gap.



The project consists of several related tasks. Research will start from the synthesis of simple donor-acceptor-doped pentacene analogues as a proof of concept for our new acene stabilization method. The gathered experience will be utilized in more challenging syntheses of doped analogues of higher acenes containing one or more donor-acceptor pairs. The subsequent preparation of donor-acceptor-doped cyclacene, a macrocyclic version of acene, will be the crowning achievement of this project and a breakthrough on its own. The synthetic work will be supported by feedback from quantum chemical calculations and experimental characterization of the obtained targets, which will help to optimize the molecular design in order to achieve the most valuable physical features and optoelectronic properties.

The successful implementation of this project will lead to the development of novel π-conjugated materials that will be interesting from the point of view of applications in materials science, that is, in organic electronics, where they can serve as semiconductors in field-effect transistors or photoactive materials in organic photovoltaics. In addition, near-infrared fluorescence may render them promising fluorophores for bioimaging and sensing. Their synthesis and isolation will help to understand the structure-property relationships of extended π-conjugated systems and facilitate future work on the design of new organic semiconductors and fluorescent dyes. Furthermore, stable donor-acceptor-doped cyclacenes may be of interest because of their potential supramolecular sensing capabilities.