Nonbenzenoid polycyclic aromatic hydrocarbons as molecular models of defected graphene

PI: Bartłomiej Pigulski, Faculty of Chemistry, University of Wrocław

Conjugated all-carbon systems are materials of the future and graphene is the most important member of this family. However, one-layer benzenoid (containing only hexagons) graphene is just a starting point. Structural modifications of graphene provide endless possibilities to create materials with new and useful properties. Such modifications can be, for example, odd-membered ring defects, few layers of graphene instead of only one or more than one modification at the same time (Figure 1).

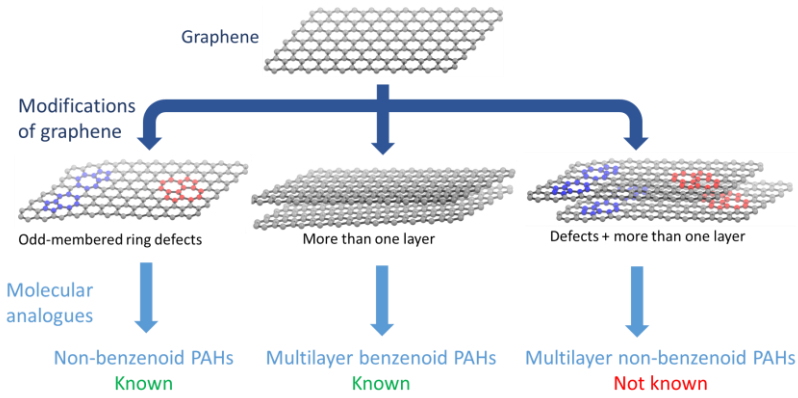

Figure 1. Tuning of the properties of graphene: odd-membered ring defects, few-layer graphene, defected few-layer graphene.

However, **the implications of different types of topological defects on the physicochemical properties of graphene remain poorly understood.** That is why recently their molecular analogues are very hot and intensively explored topic in organic chemistry. Such molecular analogues with precisely defined structure are called polycyclic aromatic hydrocarbons (PAHs) or nanographenes. PAHs containing odd-membered ring defects or benzenoid nanographenes forming multiple layers are known but so far **multilayer supramolecular complexes of PAHs with odd-membered defects are not known**.

The goal of this project is to **fill that gap in research on odd-membered nanographenes**. PAHs containing azulene defects (Figure 1, blue defects) were selected due to their additional huge potential in organic electronics. The first stage of this project is **the development of novel synthetic pathways** leading to azulene-embedded polycyclic aromatic hydrocarbons (PAHs). Additionally target molecules will exhibit unusual properties as **near-infrared absorption** despite rather small size of π-conjugated skeleton. The target molecules were **carefully designed in terms of their topology** and finally it will allow to form their **multilayer supramolecular complexes** in solution and in the solid state. This type of supramolecular structures is a way to further **tune optical properties** of non-benzenoid PAHs and is a model and will be **the first example of defected multilayer nanographene**.

The deep understanding of the influence of defects on properties of bulk graphene is crucial from the point of view of its applications and will contribute to the rational design of organic materials.