

## **Project 2.2. C-H Activation for Industrial Renewal” (CHAIR)**

**Supervisor:** prof. Daniel T. Gryko

**Institute:** Institute of Organic Chemistry, Polish Academy of Sciences

**Unit:** Institute of Organic Chemistry, Polish Academy of Sciences

**WWW:** <https://www.icho.edu.pl/>, [https://ww2.icho.edu.pl/DTG\\_group/](https://ww2.icho.edu.pl/DTG_group/)

### **Background:**

Polycyclic aromatic hydrocarbons (PAHs) are important molecules with expanding applications as optoelectronic materials, commonly obtained via cross-couplings of prefunctionalized building blocks. Accordingly, C-H functionalization could offer unprecedented tools for the synthesis of hardly studied, appealing PAHs such as perylene and corannulene incorporating heteroatoms or corannulene featuring axial chirality. Indeed, the presence of axially chiral motifs on PAHs could drastically impact their physical properties providing them yet unexplored properties.

### **Aim:**

Synthesis of perylene and corannulene analogs with incorporated heteroatoms will be targeted via direct arylation, radical-anions coupling and Scholl reaction. PhD-student will perform in-depth optimizations to determine the steric/electronic factors governing these reactions. In parallel, physicochemical characterization of the new materials will allow subsequent rational design of advanced PAHs. PhD-student will further explore different strategies to build up perylene & corannulenes analogs via C-H arylation focusing mainly on intramolecular transformations (design of simple-linked precursors); synthetic routes such as radical-anion coupling, nucleophile-electrophile addition and Scholl reaction will be explored; 2) elucidate electronic requirements for dehydrogenative fusion; 3) investigate the optical properties of synthesized PAHs.

### **Requirements:**

MSc in chemistry, specialization – organic chemistry. Good knowledge of English.

Additional requirement: the candidate can not be citizen of Poland or if he/she is a citizen of Poland the person has to prove that last 3 years before the end of recitation spent continuously abroad.