

This research project is devoted to the synthesis of functionalized nanographenes, which belong to ultramodern nanomaterials used in photovoltaics, organic electronics, medicine – the list of applications for this class of materials is very long. The terms "graphene" and "nano", that appeared in the previous sentence, are on lips of everyone interested in the latest achievements of science and technology. These days the above-mentioned terms are declined in all grammatical cases, they occur in the context of many of the latest technologies, without which it would be difficult to imagine our civilization. Graphene is a flat, ultrathin structure made of carbon atoms joined together as in a honeycomb, while "nano" determines the size of matter particles, e.g. pieces of graphene (< 100 nm). "Functionalized" means having structural elements, e.g. hydrocarbon chains, chromophores – giving the entire structure the required features (e.g. ability to emit light of a specific color, solubility). The aim of the project is to create new possibilities in the synthesis of functionalized nanographenes, including those heteroatom-doped (e.g. nitrogen, sulfur), using the APEX and bottom-up strategies, that means using structures from simple ones to very complex ones. Its key tool, which is a decisive factor to ensure innovativeness, is a totally novel, so far unknown, domino-type reaction between perylene or its derivatives and 1,4-diaryl-1,3-diynes. The mentioned "domino" consists of Diels-Alder diyne cycloaddition into perylene (or its derivatives) bay region followed by cycloisomerization. The domino products will undergo further transformations, e.g. cycloaddition to the second bay region, cyclodehydrocondensation, and others. Finally, the obtained functionalized nanographenes will be characterized with strictly planned and controlled structure, which will possess expected properties. The properties will be crucial for their attractiveness for organic electronics and photovoltaics. The domain of photovoltaics is the conversion of solar energy into electricity (solar cells), while organic electronics deals with construction of "organic diodes" – systems emitting light under the influence of electricity. Photovoltaics and organic electronics are modern fields of knowledge and technology. We all come in contact with them in our everyday life using, for example, smartphones, tablets and various types of renewable energy sources. In order for these numerous devices and technologies associated with them to serve us and constantly develop, it is necessary to progress in the field of production of new materials (e.g. conductive polymers, light emitting materials, nanographenes) with expected properties, and thus the progress in organic synthesis. Constant technological advancement requires conducting basic scientific research, aimed at, among others, designing and obtaining new materials and their precursors (chemical compounds), and comprehensive examination of the properties of newly manufactured semi-products and products. This kind of research is interdisciplinary, combining elements of chemistry (organic chemistry, catalysis, organic synthesis, computational chemistry), materials science and physics. Due to the presence of structural elements from perylene in the nanographenes and other appropriate structural motifs, it will be possible to control their properties (or even adapt them to certain expectations), for example, conduction and the ability to emit light with the expected color. The project implementation also includes a phase called chemistry in silico (chemistry in silicon that is theoretical calculation) – thanks to the results of calculations it will be possible to rationally plan the structures for synthesis and to plan the conditions for conducting the reaction. Obtained chemical compounds, potential nanomaterials emitting light or converting them into electricity and potential "building blocks" for the synthesis of "artificial metals" will then be comprehensively tested in terms of their physicochemical properties (useful for future applications). Importantly, it is also planned to test the attractiveness of the compounds obtained in technologies – e.g. OLED, solar cells and prototype devices will be constructed. Thanks to the analysis of synthesis results, theoretical calculations, comprehensive property research and pre-application tests, knowledge about structure-reactivity-expected properties relations will be obtained. The results of the project will be helpful to specialists in the field of chemistry and chemical technology, materials technology and organic electronics who want to perform advanced application tests (to create and examine ready-made devices). The authors of this interdisciplinary project represent research groups from various areas of chemistry, physics and materials chemistry. The implementation of the project will contribute to the development of cooperation between them and the personal scientific development of each of the project participants. Above all, however, knowledge about the synthesis, properties and application possibilities of functionalized nanographenes will be broadened – a group of modern molecular materials that is known, developed and comprehensively used in modern science, in particular chemistry, and modern technologies, including organic electronics.