Reg. No: 2019/35/N/ST4/02594; Principal Investigator: mgr in . Tomasz Franciszek Sokolnicki

The aim of this project is focused on the synthesis of new silane coupling agents (SiCAs) based on the modification of cyclic siloxanes, silazanes, eugenol and other terpenes, as well as malonic acid derivatives. The idea is to build a new class of SiCAs by the application of non-expensive reagents and simple chemical transformations, like substitution on an alkyl or acyl carbon atom and functionalization of unsaturated carbon-carbon bonds in hydrosilylation reaction using various transition metal catalysts (Ir, Pt, Rh, Ru). Only such approach, which concerns the application of straightforward and productive methods, based on the non-expensive substrates may give the chance for the implementation of the new SiCAs in industry. The presence of various groups in the structure of reagents prone to functionalization makes the project challenging in the area of processes stereo-, regioselectivity and their productivity.

An important task of the planned research is the synthesis of coupling compounds with various numbers of functional groups compatible with the organic (polymer) and inorganic (silica) matrix. There is a real chance, by the application of the new, synthesized within this project, SiCAs, to reduce the amount of coupling agent in the final composite composition, and in a controlled manner affect the cross-linking density of the material, as well as the mechanical and physico-chemical properties.

The obtained SiCAs will be applied as modifiers of various types of silica (colloidal, fumed and precipitated) used as fillers in the polymer industry. The properties of silane-coated silica will be determined.

The silane coupling agents (SiCA) are organosilicon compounds having the ability to combine materials with different structures and properties. The special properties of these compounds result from possessing two different groups responsible for interacting with these materials. One of these functions is the silicon atom, with easily hydrolyzable alkoxy groups capable of further condensation with hydroxyl groups on the polar surface of the inorganic material. The other is the organic moiety with the affinity to a hydrophobic polymer chain. Silane coupling agents have found numerous applications in the preparation of various types of materials: coatings, sealants and also rubber composites. The interest in the synthesis and application of these compounds is constantly growing, which can be measured by the number of published scientific reports (6572 publications and 41 155 patents, Scopus and Google Patents database, respectively, 09.12.2019). The literature focused mostly on the synthesis of difunctional silanes. The project will develop a new class of silanes with the different numbers of functional groups with the affinity to inorganic and organic matrixes. It is a novel approach, which is also synthetically demanding due to the presence of various functional groups in the structures of reagents.

This project fulfills the frontier research criteria, especially those concerning catalytic processes and material chemistry aspects (obtaining desired products with high yield and selectivity), which is a challenging synthetic task.

Due to the lack of literature reports on the synthesis of SiCAs based on the cyclic siloxanes, silazanes, malonic acid derivatives and terpenes to undertake the research in this subject seems to be fully justified and the development of synthetic procedures constituted a scientific novelty. Simple, efficient and selective protocols for the synthesis of these compounds, as well as their further application as coupling agents in silica is an important issue since the SiCAs global market in 2018 was valued on 523.1 mln USD.