The progress of the science in the last decades allowed the fabrication of materials films with thicknesses of nanometers. Such films in (opto)electronic devices (i.e. transistors, solar cells, gas sensors or biosensors) are often combined into multi-layered structures of materials with different properties. The effectiveness of a device is determined by properties of component layers. The key issue are processes occurring on the surface and interface between materials or between a material and atmosphere. The most important for electronic devices effectiveness are electronic, chemical and morphological properties of materials. Thus, the prediction of those properties and physicochemical processes occurring at the interfaces are crucial for design of structures to be applied.

In the era of high computational power, new possibilities have been opened in materials science. The properties of materials can be predicted before the preparation of physical samples. Application of quantum chemistry modelling of studied materials can be used in the pre-selection of the most promising structures, limiting the experimental measurements to a narrow group of structures with optimal properties. Therefore, the cost and the time needed to characterize new structures are reduced and effectiveness of the research is improved.

The hybrid structures defined as structures consisting of at least two components from different groups of materials have attracted a lot of attention lately. The most common combination is crystal-like inorganic layer connected with organic molecular layers. Such structures combine the advantages of both kinds of materials.

The attractive group of materials that can be applied as an organic part of the structure are metallo-phthalocyanines (MPcs). The most common materials for inorganic layers are metal oxides. The metal oxide that recently has been gaining attention is aluminum oxide. It has been studied and applied for almost a century. However, with an increasing interest in nanoscale materials, aluminum oxide nanostructures became one of the most popular material with applications in molecular separation, catalysis, energy generation and storage, (opto)electronics, sensors and biosensors. The latest trends in the materials science are focused on sustaining the high quality of devices, but in the same time reducing the cost of production. In the same time, one of the most important challenges for scientists is to utilize the recyclable materials and find possible ways for materials recovery. From this point of view, the importance of aluminum and aluminum oxide investigation should not be underestimated. These materials can be applied as a cheaper alternatives for other metals and metal oxides as electrodes, gate materials in metal-semiconductor field effect transistors or substrates for gas sensors. Even though there are number of computational and experimental studies of aluminum oxide surfaces, the aluminum oxide/organic (i. e. MPcs) interfaces are not well characterized. However, there are several papers demonstrating potential applications of such interfaces in solar cells or transistors. The investigation of MPcs influence on aluminum oxide properties besides the electronic devices, can be also utilized for aluminum recovery. There are recent studies demonstrating the possibility of MPcs application as aluminum corrosion inhibitors. Thus, the aim of this project is to apply new methodology based on theoretical modelling prior experimental characterization for understanding the processes on the surfaces and interfaces in the structures based on aluminum oxides and metallo-phthalocyanines (MPcs).

Potential results of the project can open the possibility to gain both – economical and environmental benefits in the production of effective devices based on recyclable aluminum and its oxide. The further broad impact of the project on materials science, apart from the characterization of the interface between particular oxide and MPcs, will be providing a methodological hint for design of similar systems.