1. PHD PROJECT DESCRIPTION (4000 characters max., including the aims and work plan, all in English)

Project title: Synthesis and studies on physicochemical properties and bioactivity of composite materials formed by polymer/oxo-titanium(IV) clusters and polymer/titania nanoparticles

1.1. Project goals: The aim of the project is to develop a method, which allows on the controlled synthesis of selected multinuclear titanium(IV) oxo-complexes with a strictly defined $\{Ti_a\text{-}(\mu_i\text{-}O)_b\}$ core structure, and their application for the manufacture of polymeric/inorganic composite materials. The essence of the proposed studies is to determine the conditions for the Ti(IV) oxo-complexes synthesis, with particular emphasis on their structural conversion processes control. The isolated microcrystals of oxo-complexes, will be used to obtain polymer/inorganic composites, e.g. coatings and fibrous materials, of the defined properties, especially optical, photocatalytic and biological ones. For this reason, the project assumes the structural characterization of synthesized compounds and studies on their physicochemical, optical, mechanical properties, as well as on their biological activity.

1.2. Outline: The photocatalytic activity of materials based of TiO_2 is utilized in water splitting, purification of air and water, reduction of environmental pollutants and in antimicrobial applications [1-5]. Recently, much attention has been devoted to the use of titanium oxo-clusters (TOCs) as compounds exhibiting similar properties to TiO_2, but being characterized by the discrete molecular structure [6-10]. The use of selected oxo-complexes for the production of polymer/TOCs composite systems, which ensure them the antimicrobial properties, is the issue that we want to PhD student solve during the implementation of the proposed project. Stable mononuclear complexes with the citric acid (-cit) of the general formula $[Ti(H_xcit)_3]^{n-}$ (x = 0-2 and n = 2-8) [11,12] and the octanuclear oxo-complex $[Ti_8O_{10}(cit)_4]$ are the examples, which show pronounced bioactivity, including anti-cancer one against various cancer cells. [13]. An analysis of literature data indicates a significant importance of TOCs in the synthesis of inorganic-polymer composite materials, which are produced through the introduction of metal oxo-clusters into the polymer matrix [14]. The possible interactions between inorganic and organic components may result in an improvement of the composite mechanical properties and its bioactivity. The unique properties of oxo-clusters can give completely new

properties to the composite material in comparison to the base polymer [14-26]. Therefore, the studies on the synthesis of TOCs possessing titanium-oxide core of the desirable architecture, size, and physicochemical properties, are important from the viewpoint of bioactive inorganic-organic composite materials formation. We intent to PhD student carry out proposed studies in order to understand the relationship between the structure of multinuclear titanium(IV) oxo-complexes (TOCs) and their biological activity. Analysis of the literature data has shown that so far no research systematic findings on this topic.

1.3. Work plan: The proposed project assumes synthesis of selected oxo-complexes, for which the oxo-titanium core structures have been determined during the earlier works. The use of appropriate carboxylic acids, containing functional groups with potential bioactive properties will be most important issue at the stage of oxo-complexes synthesis. The structural and physicochemical studies of isolated complexes are ~~an~~ important part of these investigations. Research on the production of composite materials created by introducing Ti(IV) oxo-complexes into the polymer matrix will be of key importance for the project. Work on this part of the project will be carried out at the Faculty of Chemistry of the Nicolaus Copernicus University and in the cooperation with the Center of Polymer and Carbon Materials of the Polish Academy of Sciences in Zabrze. The doctoral student's broad approach to the issue of composite material, i.e. research on coating materials, moldings of various shapes, filaments that can be used in 3D technologies, as well as nanofibers, will be important. The evaluation of antimicrobial properties of the fabricated materials will be based on studies on their ability to reduce the formation of aggregates/biofilms of reference microbial strains, with the specific physiological characteristics, which are relevant to clinical microbiology. As the part of this task, it is planned to PhD student carry out of tests including: (a) biostatic/biocidal properties of both oxo-complexes and composite systems produced, (b) survival time of selected pathogenic bacteria and fungi in the presence of modified biological materials, (c) adhesion of selected microorganisms to different surfaces of obtained biomaterials, (d) the ability of these microorganisms to create on the tested surfaces a single- or bi-species biofilm. The assessment of the impact of the titanium-oxygen skeleton structure on the biological activity of the isolated oxo-complexes, will be important.