

## PHD PROJECT DESCRIPTION

(4000 characters max., including the aims and work plan to be published online)

**Project title:** Surface modification of titanium dioxide nanotubes with selected transition metal complexes for the design of functional biomaterials with antibacterial and therapeutic properties

### 1.1. Project goals

The main objective of the project is to design and comprehensively characterize TiO<sub>2</sub> nanotubes (TNTs) modified with selected transition metal complexes (TMCs) or metal nanoparticles derived from these complexes, and to evaluate their potential as functional biomaterials.

### 1.2. Outline

Nanostructured TiO<sub>2</sub>, particularly in the form of nanotube arrays, has emerged as a promising material for biomedicine, including implantology and controlled drug delivery systems. Due to their high surface area, chemical stability, and excellent biocompatibility, TNTs enable efficient surface functionalization and immobilization of biologically active compounds.

It enables the preparation of implant surfaces with enhanced antibacterial properties while maintaining high biocompatibility and promoting tissue integration. In this context, transition metals such as Ag, Cu, Pt, and Au, and their complexes, are of particular interest due to their diverse biological activities (antibacterial activity, cytotoxicity).

In the literature, modification of TNTs with TMCs or their decomposition products is only slightly reported. This project aims to address this gap.

Among the expected results are:

- Development of novel nanostructured biomaterials with tunable biological properties,
- Identification of relationships between metal or its complex and antibacterial/biological activity,
- Determination of optimal material configurations for biomedical applications (e.g., implants, drug delivery systems),
- Publication of results in peer-reviewed scientific journals with high impact factors.

The proposed research aligns with current trends in the development of advanced functional biomaterials. The results may contribute to the design of next-generation implant surfaces with improved resistance to bacterial infections and enhanced therapeutic functionality. The project has both fundamental scientific value and potential practical applications in medicine and materials science.

### 1.3. Work plan

The project will be carried out in the following stages:

**1. Synthesis of TNTs** by electrochemical anodization of titanium alloys, such as Ti6Al4V, under controlled process conditions (voltage, time, electrolyte).

**2. TNTs surface modification** using, e.g., the drop casting method or covalent bonding of the complexes to TNT surfaces after their preliminary functionalization with bridging ligands (e.g., mercaptoorganosilanes). Formation of metal nanoparticles will be achieved through chemical reduction or thermal treatment of the complexes, or electrochemical deposition.

**3. TNT-based material characterization** before and after their modifications in terms of their morphology (SEM, TEM, AFM), chemical composition (EDX, XPS), material properties (wettability, nanoindentation), and structure (XRD, Raman).

**4. Biological evaluation** will be conducted during antibacterial assays, cytotoxicity tests, and the correlation of the materials' physicochemical properties with their biological activity.

**5. Kinetic studies** on the release rate of metal ions/complexes from the obtained nanomaterials will be carried out under physiological conditions (e.g., in PBS) using, e.g., ICP-OES.

### 1.4. Literature (max. 7 listed as a suggestion for a PhD candidate preliminary study)

- N.K. Awad, *et al.*, *Mat. Sci. Eng. C* **76** (2017) 1401.
- Y. Cheng, *et al.*, *J. Mater. Chem. B* **6(13)** (2018) 1862.
- Y. Sun, *et al.*, *Front. Bioeng. Biotechnol.* **10** (2022) 1074083.
- Y. Fu, A. Mo, *Nanoscale Res. Lett.* **13(1)** (2018) 187.
- J. Lincho, *et al.*, *J. Environ. Chem. Eng.* **12(3)** (2024) 112990.
- A. Topolski, *Polyhedron* **230** (2023) 116218.
- M. Grodzicka, A. Topolski, *ChemPlusChem* **91(4)** (2026) e202500716.

### 1.5. Required initial knowledge and skills of the PhD candidate

The PhD candidate, in addition to general knowledge in inorganic chemistry and mathematics, must be familiar with methods for surface characterization and kinetic measurements, especially in relation to substitution in TMCs. In addition, the PhD candidate should possess basic skills in using software for data analysis (e.g., spreadsheets and statistical software).

### 1.6. Expected development of the PhD candidate's knowledge and skills

The project's realization will help the PhD candidate deepen their knowledge of surface chemistry and modern methods for nanomaterial surface modification. The candidate will improve their organizational skills and their focus on a problem-solving approach.