## Reg. No: 2020/37/B/ST5/03451; Principal Investigator: prof. dr hab. Andrzej Janusz Kotarba

The dynamic development of implantology stimulates a significant increase in the demand for new biomaterials. The implants, in addition to the specific mechanical properties, must exhibit both high biocompatibility and resistance to bacterial infections. This is a challenge for modern materials science. In this context, one of the most frequently studied classes of biomaterials are carbon-based materials such as graphene flakes, nanotubes, fibers, diamond-like carbon coatings. The research proposed in the project focuses on the surface functionalization of carbon materials, in line with these challenges.

The main goal of the project is to develop the functionalized carbon materials with particular attention to optimizing their surface properties for biomedical applications. The materials will be surface-modified with the use of low-temperature plasma in order to obtain surface functional groups. Their type and surface coverage can be precisely controlled by adjusting plasma treatment parameters (type and partial pressure of the feed gas, power, time of exposure). The excited molecules of various gases (O<sub>2</sub>, N<sub>2</sub>, NH<sub>3</sub>, SF<sub>6</sub>, H<sub>2</sub>) allow to introduce different functional groups (-OH, -CHO, -COOH, -NH<sub>2</sub>, -NO<sub>2</sub>, -F) onto the surface. The studies (including our own) show that the presence of such specific surface adsorption centers plays a crucial role in the interaction with physiological fluids, cells, and bacteria. As a consequence, it is directly correlated with the quality of the implant-organism interface. Thus, a versatile method allowing the introduction of a specific type and controlled concentration of functional groups is of great importance.

Presently, carbon surfaces with various properties are obtained through classical chemical methods which are multi-stage and labor-intensive. Plasma surface modification opens completely new possibilities for fine-tuning of the biomaterials surface properties for specific applications. It is worth noting that effective surface modification using plasma is obtained within minutes.

The research proposed in the project is a typical example of interdisciplinary research. The work packages in the project include preparatory work (surfaces of carbon materials with introduced functional groups), in-depth physicochemical characteristics with particular reference to the surface (spectroscopic and microscopic methods) and evaluation of the influence of functional groups on biological properties (cellular and microbiological tests). Moreover, theoretical calculations are also planned, consisting in quantum-mechanical modeling of carbon surfaces with various functional groups. Modern computational methods allow obtaining molecular models of isolated and interacting functional groups introduced to surfaces. The results of calculations (location of atoms on the surface, the geometry of chemical bonds, distribution of electron density, change of surface potential, Fermi level) are a great help in the interpretation and analysis of experimental results. The coupling between the experimental and theoretical approaches will allow understanding the nature of chemical interactions at the interface of the carbon implant - biological material. Such interactions determine implant acceptance and minimize the risk of post-operative infection.

In a wider perspective, the proposed project will not only provide new comprehensive knowledge in the field of biomaterials surface chemistry but also practical premises for the design of implants. Determination of the factors influencing the undesired bacterial adhesion and the desired adhesion of eukaryotic cells will contribute to the design of novel implant materials with key functions (increased biocompatibility, lower probability of infection).