

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

Project title: Innovative solutions for the introduction of heteroatoms to porous carbon matrixes

1.1. Project goals

- ✓ The project aims to develop a method of obtaining porous carbon matrixes enriched with single heteroatoms, especially nitrogen (N), sulfur (S), phosphor (P), oxygen (O) or boron (B) and innovative solutions with the dual form of these heteroatoms.
- ✓ To explore the relation between the chemical structure of carbon materials (morphology, presence of heteroatoms, surface modification) and their electrochemical activity for potential application in Zn-air batteries, fuel cells, supercapacitors and photovoltaic cells (DSSCs).
- ✓ To upgrade the knowledge and skills in the area of “green” energy harvesting devices design.
- ✓ To upgrade social competences as team working and cooperation spirit.

The Research and Modeling Group for New Materials Research Synthesis (head: Professor Jerzy P. Lukaszewicz) researches wet and electrochemical exfoliation of graphene. These studies are combined with three-dimensional structuring by hard-templating of exfoliated graphene flakes.

1.2. Outline

The oil-free and laser-free method of obtaining 3D structures based on graphene using aqueous suspensions of commonly available graphite is new on a global scale and has no equivalent in the scientific and patent literature. The essence of the method is to use the phenomenon of spontaneous aggregation of separated graphene flakes previously obtained by wet exfoliation of commercial graphite/graphene powder. Aggregation occurs under conditions of thermal shock that occurs when the graphene suspension is in contact with a hot substrate. Then there is rapid evaporation of the dispersing liquid and self-organisation of graphene petals into three-dimensional structures resembling flowers. The proposed method uses widely available reagents (commercial graphite/graphene powder, water, surfactants) and is environmentally friendly. This project aims to develop, investigate and characterize novel, stable and cost-efficient electrodes for Zn-air batteries, fuel cells, supercapacitors and photovoltaic cells (DSSCs). The knowledge and experience in materials chemistry and electrochemistry, as well as access to highly specialised equipment (TEM, Raman spectrometer, Potentiostat/Galvanostat), is required for the successful realisation of the planned studies.

1.3. Work plan

The following research stages will be included in the research to obtain the doctoral degree:

- 1) Formation of carbon mixtures from hard and soft templates and so-called binders.
- 2) Alternative synthesis pathway exploiting so called “oil-free and laser-free” procedure
- 3) Carbonization in a different range of temperature 500-1200°C of investigated carbon material / template / binder mixtures obtained by soft and hard templating.

- 4) Enrichment of carbon materials with heteroatoms: nitrogen, sulfur, transition metals and innovative solutions with the dual form of these heteroatoms using novel irradiation method.
- 5) Physico-chemical characterization of obtained carbon matrixes by instrumental methods: nitrogen adsorption (porous structure and surface area), elemental analysis (chemical composition), XPS spectroscopy (chemical structure of the surface), X-ray (crystal structure), Raman spectroscopy (identification of graphene agglomeration degree), SEM/HRTEM microscopy (identification of spatial structure).
- 6) Research on selected applications of obtained porous carbon matrixes: electrode material for Zn-air batteries, fuel cells, supercapacitors and photovoltaic cells (DSSCs).

1.4. Literature

- 1) P. Kamedulski, W. Zielinski, P. Nowak, J.P. Lukaszewicz, A. Ilnicka, 3D hierarchical porous hybrid nanostructure of carbon nanotubes and N-doped activated carbon, *Scientific Reports* 10 (1), 1-11, **2020**.
- 2) P. Kamedulski, S. Truszkowski, J.P. Lukaszewicz, Highly Effective Methods of Obtaining N-doped Graphene by Gamma Irradiation, *Materials* 13 (21), 4975, **2020**.
- 3) P. Kamedulski, J.P. Lukaszewicz, L. Witczak, P. Szroeder, P. Ziolkowski, The Importance of Structural Factors for the Electrochemical Performance of Graphene/Carbon Nanotube/Melamine Powders towards the Catalytic Activity of Oxygen Reduction Reaction, *Materials* 14 (9), 2448, **2021**.
- 4) X. Luo, Y. Chen, Y. Mo, A review of charge storage in porous carbon-based supercapacitors, *New Carbon Materials* 36 (1), 49-68, **2021**.

1.5. Required initial knowledge and skills of the PhD candidate

- 1) Basic knowledge on photovoltaic devices and their design
- 2) Orientation in contemporary and future trends in the area of "green" energy harvesting methods
- 3) Analytical thinking
- 4) Eager to learn
- 5) Ability to work in the laboratory (plan and perform synthesis, spectral measurements, electrochemical tests)
- 6) Understanding of materials synthesis and chemistry
- 7) Thinking oriented on innovation and application
- 8) Knowledge of carbon material science
- 9) Knowledge about basic methods to characterize obtained compounds
- 10) Eager to work hard

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

- 1) Project management: the ability to plan and organize the project as well as delegating and negotiating tasks among project members.
- 2) Perseverance: the driver and determination to continue and finish a PhD student project.
- 3) Supervising and coaching: the ability to transfer knowledge and inspire others.
- 4) Communication skills in English at conferences and in writing publications.
- 5) Writing grant proposals.
- 6) Research data collection, analysis and conversion to research papers.