DESCRIPTION FOR THE GENERAL PUBLIC

The development of natural resources (i.e. crude oil, natural gas, etc.) on the energy market and forecasts for energy needs make it necessary to seek new alternative sources of energy and materials for its storage. Currently, a very prospective solution is to store energy using lithium-ion batteries, which are among the most popular batteries in generally available portable electronic devices. Since the introduction of conventionally performed electrode (anode) of graphite, the potential impact of carbon nanotubes (CNT) on the technology of lithium batteries started to be estimated. Because of the higher electrical conductivity and an increased surface area, the new electrode materials based on chemically modified multi-walled carbon nanotubes (MWCNT), whose obtainment is the objective of the present project, may replace the commercially used graphite in anodes and thus improve battery capacity. MWCNT have a lot more defects (structural, interstitial sites, gaps) than SWCNT, which has a significant impact on the physicochemical properties of nanotubes. A larger number of defects results in better diffusion of lithium into the structure of the MWCNT and thus increases the capacity of the battery.

Native carbon nanotubes are chemically inactive and the presence of carbon atoms of sp^2 hybridization in hexagonal structure prevents formation of chemical bonds with the surrounding molecules. To solve these problems, many methods are used to modify the surface of the CNT. Connection of functional groups to the CNT can have a huge impact on their properties, such as, dispersion in organic solvents or polymer matrices. Surface modification of CNT by introducing heteroatoms to structure changes the chemical properties - increased reactivity, change conductivity, and many others.

Preliminary studies of Applicants and of the National Science Center projects, which have been realized so far, show an extraordinarily positive effect of the addition of salt organophosphate containing selenium or sulphur atoms to the multiwall carbon nanotubes in the process of charge-discharge of the cell, increasing its capacity and service life.

The scientific aim of the project is to obtain the component of the lithium-ion cell based on multi-walled carbon nanotubes (MWCNTs) functionalized with phosphoroselenoates. The nucleophilic substitution of phosphoroselenoates anions is possible due to the electrophilic nature of carbon atoms in halogenated carbon nanotubes.

The research program proposed by us, concerning synthesis, qualitative and phase composition, crystal structure and electrochemical properties, should allow for selection of the most optimal $(RO)_2P(O)Se^-M^+$ systems and for functionalization of multi-walled carbon nanotubes with them for practical use.

A complete physico-chemical analysis of the obtained phosphoroselenoates (by use of NMR spectroscopy and elemental analysis) and systems of nanotubes will be performed by means of thermal analysis DSC/TG, the analysis employing scanning electron microscopy SEM with EDS analyzer, transmission electron microscopy TEM, X-ray diffraction analysis XRD, X-ray photoelectron spectroscopy XPS and FTIR spectroscopy, Raman. A full analysis of electrochemical processes (cyclic voltammetry, chronopotentiometry, corrosion potential, electrochemical impedance spectroscopy) will be carried out. The implementation of the proposed project will lead to the enlargement of knowledge on materials built from carbon structures functionalized by salts containing heteroatom and their use as potential electrode materials for the production of new types of lithium-ion batteries.