## Reg. No: 2016/23/N/ST8/00274; Principal Investigator: mgr in . Katarzyna Silarska

The design of various electrochemical devices for energy conversion, such as fuel cells requires the development of a new class of materials with the desired properties such as high electrical conductivity, significant chemical resistance and durability under operating conditions. This is not possible without the research of a fundamental nature, which determines the correlations between the chemical composition, atomic-scale or micro level structure and the basic properties and potential application. In the group of studied and optimized materials for applications in electrochemistry are mainly ceramic protonic conductors with number of unique properties which suggests the possibility of further modifications. Proton conductors are mainly compounds of the perovskite structure with general formula ABO<sub>3</sub>, where in position A is a bivalent cation from the group of alkaline earth (e. g. Ba<sup>2+</sup>, Sr<sup>2+</sup>, Ca<sup>2+</sup>), while in the position B is usually ion Ce<sup>4+</sup> or Zr<sup>4+</sup>. The name of this group of compounds derived from the mineral perovskite CaTiO<sub>3</sub> (calcium titanate), discovered in 1838 in the Ural Mountains by Gustav Rose and is named after Russian mineralogist L. A. Perovski. The compounds of the perovskite structure are usually doped in B sublattice by introducing into the structure the element with lower valency than the native, which results in the formation of oxygen vacancies. In atmospheres containing hydrogen the formation of protonic defects occurs in this type of materials.

Research on the materials from the perovskite ABO<sub>3</sub> type group (including A = Ba, Sr; B = Ce, Zr) are primarily aimed at increasing the proton conductivity of these materials and improving their chemical resistance, particularly in atmospheres containing CO<sub>2</sub>. So far, the proposed methods of modifying comprised mainly introducing of acceptor dopants from the lanthanides group and yttrium, the formation of solid solutions with BaTiO<sub>3</sub> and BaZrO<sub>3</sub> or modification of the microstructure through the choice and optimization of synthesis method. Another direction of optimization is to improve the electrical conductivity and chemical resistance by creating a composite materials such as  $BaCe_{0.9}Y_{0.1}O_3$ -Ba<sub>3</sub>(PO<sub>4</sub>)<sub>2</sub> and  $BaCe_{0.9}Y_{0.1}O_3$ -BaWO<sub>4</sub>. Results showed the possibility of creation the materials with improved functional properties like electrical conductivity and chemical resistance in the presence of CO<sub>2</sub>.

The aim of the planned research in the framework of this project is to identify the opportunities of effective modification of selected properties of materials based on barium cerate (BaCeO<sub>3</sub>) with glassy phase with required composition and quantity, which soften at elevated temperatures and becomes a "liquid" phase. It is assumed that such modification of the material will improve the electrical properties and chemical resistance in atmospheres containing  $CO_2$  and will affect other properties of the materials.