The aim of the project is to develop new additives for the lithium electrolytes, forming a stable passivation layer - solid electrolyte interphase (SEI). This layer has a very significant role in lithium-ion cel – protects thermodynamically unstable electrolyte against negative electrode. Its properties plays important roles in the Li-ion batteries, whose key properties, such as cyclability, self-discharge, power density, and efficiency are partly determined by the nature of the SEI. Under the standard conditions, the SEI is leisurely formed by the reduction of organic carbonates (ethylene carbonate, dimethyl carbonate), and is composed of lithium carbonate and, partially, oligomeric dianions. In order to improve stability of the battery work (extend the period of its effective operation), it is necessary to produce a stable SEI with optimal properties such as tightness, high lithium cation conductivity. To accomplish this, the process of SEI formation needs to be controlled instead of the spontaneous creation. It can be done, by addition of compounds with higher reduction potential (easier reducible). By optimizing the chemical structure of such additive, convenient layer, with high lithium and low electron conductivity, can be achieve.

The process of the new additives development will be based on conducted theoretical analysis. Relations between the basic molecular parameters of additive (e.g. LUMO level, dipole moment, chemical hardness) and observed macroscopic properties will be determined. Attempts to calculate the reduction potentials and products of reduction path will allow us to better understand the nature of the processes occurring at the electrode. Based on such knowledge, it will be possible to rationally propose new structures. After synthesis, their electrochemical properties will be tested. The formed layers will be studied by spectroscopic and miscroscopic techniques, to determine composition and morphology of the SEI. The comparison of these approaches (theoretical and experimental) will enable us to draw conclusions to improve created model, and thereby obtain better recommendation of the desired structure changes.

The project is focused on the development of design paths for compounds which in a simple way can undergo an irreversible one-electron reduction. The effects of this work can have indirect influence on our lives in the future, probably dominated by electric devices such as electric cars with highly effective batteries. However, the experience and knowledge that we will gain also will be helpful in other fields of science, where proper comprehension of reduction processes plays an important role.