Lithium batteries are currently the fastest growing technology of energy storage. Nowadays it is intended mostly for mobile devices and transportation, but in the future it is expected to spread on energy back-up for production lines, energy storage in renewable energy systems and smart grids. The important issue related to application of Li-ion batteries in cars is related to their safety. Much higher energy density of the batteries for electric or hybrid cars, as compared to the case of portable electronics, forces very strict safety standards, which have to be met. This leads to a constant search for a more stable cathode materials, demonstrating superior structural, thermal stability and compatibility with organic electrolytes.

Operation of Li-ion batteries is based on reversible lithium intercalation into transition metals compounds M_aX_b, (M – transition metal; X=O,S) with layered or skeleton structures. Intercalation occurs at room temperature and does not bring any principal changes to the crystal structure. Intercalation of lithium into host structure involves both ions and electrons and can be written as:

$$xLi^+ + xe^- + M_aX_b \leftrightarrow Li_xM_aX_b$$

In this process, the energy of deep energy levels of the *d*-type electrons in transition metal compounds, which have a value of several eV/atom, offers the possibility of energy storage in the order of several hundreds of Wh/kg, which enables manufacturing of energy storage devices with high volumetric and gravimetric energy density. Extended studies point out that it is the cathode which limits principal parameters of lithium batteries, such as density of energy and power, while graphite anode restricts only the charging rate of the cell. Current density of the cell is determined by ionic-electronic transport properties of cathode material, whereas number of charge/discharge cycles significantly depends on the processes occurring at the interfaces of electrode material/electrolyte. Safety in use of the cell depends on the thermal and chemical stability of the electrode materials and electrolyte.

Currently, in commercial Li-ion batteries, in addition to $LiCoO_2$, also $LiNi_{1-y}Co_yO_2$ and $LiMn_2O_4$-based materials are used as oxide cathodes. However, they exhibit significant limitations: low cyclic reversibility of charge/discharge processes, voltage decay on cycling, related to inadequate structural and electrochemical stability. Control over the processes occurring in the Li-ion batteries requires an interdisciplinary approach and the use of sophisticated techniques. Cooperation in the field of physics, chemistry and electrochemistry of solids, broadly defined materials science and modelling of materials, including electronic structure calculations, modelling of structural and chemical stability of electrode materials is indispensable.

The objective of the project is achievement of extended knowledge of the factors influencing electrochemical performance and structural and electrochemical stability of layered transition metal oxide cathodes for lithium batteries. Determination of the correlation between crystal and electronic structure, valence of transition metals, transport properties and electrochemical properties of the cathode materials enable control of these properties, allowing for the design of the safe cathode materials with desired properties. The project presents a new approach to design functional properties of layered transition metal oxide cathode materials for Li-ion batteries, based on the correlation between the crystal and electronic structure of the cathode material and its electrochemical properties (discharge curve character (OCV), capacity, current density and structural and electrochemical stability). Such approach enables achieving quality breakthrough in the understanding of mechanism of instability of these oxide materials and allows to develop enhanced and safe materials for Li-ion battery technology.

In order to develop criterion of structural and electrochemical stability of oxide cathode materials for lithium batteries necessary is extended research: structural and electrochemical studies, analysis of oxidation state of transition metal ions, transport properties, electronic paramagnetic resonance investigations, experimental investigations of electronic structure – NEXAFS and electronic specific heat along with DFT (KKR-CPA) electronic structure calculations. All these will allow for determination of important relation between crystal structure, electronic structure and electrochemical stability of cathode material and their influence on efficiency and reversibility of lithium intercalation process, which has a direct effect on functional parameters of Li-ion batteries.