Lithium ion battery technologies are currently the fastest growing area associated with the storage and conversion energy for mobile devices, hybrid and electric vehicles, as well as for storage of energy from renewable sources and smart grids. There has also been renewed interest in technology of Na-ion batteries, due to the widespread availability and low cost of sodium. Li-ion (Na-ion) batteries make use of capability of transition metal compounds M_aX_b (M-a transition metal; X = O, S, polyanion PO_4) with a layer structure or skeleton to reversibly incorporate one or more moles of lithium or sodium per mole of M_aX_b into their structure at room temperature without fundamental changes in crystallographic structure. The reaction of intercalation of lithium (sodium) into transition metal compounds M_aX_b is of ionic-electronic nature and undergoes according to the equation: $xLi^+ + xe^- + M_aX_b \leftrightarrow Li_xM_aX_b$. In this reaction, the energy of deep level *d* electrons is used, which having a value of several eV / atom provide an opportunity for accumulating a few hundred Wh / kg. Fig. 1 schematically illustrates the operating mechanism of commercial $Li_xC_6/Li^+/Li_{1-x}CoO_2$ battery.

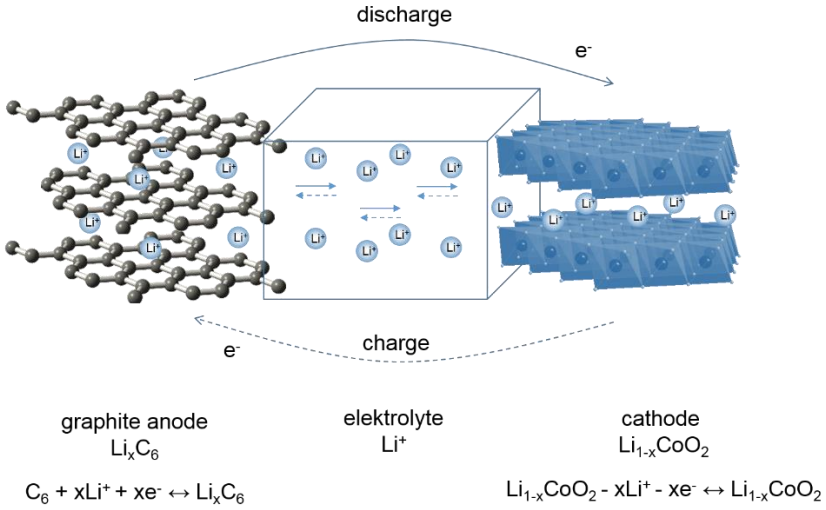

Fig. 1. Operating mechanism of $Li_xC_6/Li^+/Li_{1-x}CoO_2$ cell.

Studies show that the cathode limits the most important functional parameters of Li-ion and Na-ion batteries, such as energy and power density. The current density obtained from a cell is determined by the electronic-ionic conductivity of a cathode material, while the number of charge / discharge cycles significantly depends on reactions occurring at the electrode material/electrolyte interphase. The safety of the battery is connected with the thermal and chemical stability of the electrode materials and electrolyte.

Control over processes in Li-ion and Na-ion batteries requires an interdisciplinary approach in the fields of physics, chemistry and solid state electrochemistry, materials science, electronic structure modeling, modeling of structural and chemical stability of the cathode materials and the use of advanced research techniques.

The project presents a new approach to the design of functional properties of layered transition metal oxides for Na-ion batteries, based on the correlation between the electronic structure and electrochemical properties of cathode materials (the nature of the discharge curve, capacity, current density, structural and electrochemical stability which also strongly depend on electronic structure). This approach may prove to be a breakthrough in the development of safe materials for high performance Na-ion batteries. Confirmation of the formulated hypothesis requires a comprehensive large-scale interdisciplinary research involving physics, chemistry and solid state electrochemistry, as well as computer modeling. In order to demonstrate the correlation between the parameters of the electronic structure of cathode material and electrochemical properties (cell parameters) precise tests of cathode materials will be carried out, namely structural studies, studies of transport, optical and magnetic properties, measurements of electron specific heat, Moessbauer spectroscopy, NEXAFS and calculations of the electronic structure for both starting cathode materials (after synthesis) as well as a function of sodium intercalation degree, in characteristic points of the discharge curve. For above mentioned measurements following series of layered transition metal oxides were selected: $Na_xCo_{1-z}Mn_zO_{2-y}$, $Na_xCo_{1-z}Fe_zO_{2-y}$, $Na_xFe_{1-z}Mn_zO_2$, $Na_xCo_{1/3}Ni_{1/3}Mn_{1/3}O_{2-y}$, $Na_xFe_{1-z-d}Ni_zMn_dO_{2-y}$ and $Na_xNi_{1/3}Mn_{2/3-w}Ti_wO_{2-y}$ $0<x\leq1$, $0\leq z\leq1$, $0.1\leq d\leq0.9$, $0\leq w\leq{}^2/_3$.