

The dynamics of development of the battery industry in the world is unparalleled. A gigantic growth of the lithium batteries market is expected – a 1000% increase in the field of electric cars, a huge growth also in the field of stationary energy storage. Huge considerable demand in Li-ion batteries results from the fact that they have the highest gravimetric and volumetric energy density in comparison with other commercially available electrochemical batteries. The batteries with high capacity can play a significant role in the future economy based on renewable energy sources. Production of electricity from renewable energy sources in solar or wind power plants is strong dependent on changing weather conditions. This results in unstable energy parameters and creates problems with connection to networks, frequency fluctuations and quality of current.

The world's limited lithium resources no longer appear to be sufficient for the rapidly growing lithium battery market. Therefore, there is a swift search for alternative technologies to store electricity, such as reversible electrochemical Na-batteries. Sodium batteries are not a completely new alternative. Research carried out parallel with lithium cells, however due to the fact that in the 1990s lithium was relatively cheap and lithium materials showed better electrochemical parameters – there was a rapid development of lithium materials, which led to commercialization of lithium-ion batteries. Currently, there is a rapid return to research on sodium batteries, due to abundant sodium resources and its low prices. Na-ion batteries are predestinated to large scale energy storage, especially from renewable energy sources. The attention is also drawn to the significant reduction of cobalt content in material electrodes, which has become a critical element.

Recently Prussian blue  $\text{Fe}_4[\text{Fe}(\text{CN})_6]_3 \cdot n\text{H}_2\text{O}$  and its analogues (PBAs) are considered as the most promising cathode materials for high energy Na-ion batteries due to their low price, availability of substrates and a production process with low energy consumption and not polluting the environment. However, PBAs suffer by insufficient cycle life, so its further development in enhancement battery parameters requires intensive interdisciplinary studies.

PBAs exhibit a stable crystal structure with big number of large interstitial positions for  $\text{Na}^+$  ions connected by wide channels, which constitute fast diffusion paths for sodium ions, what allow for the reversible deintercalation/intercalation of 2 moles of  $\text{Na}^+$  ions per  $\text{Na}_2\text{Fe}[\text{Fe}(\text{CN})_6]$  formula unit and give high theoretical capacity of 170 mAh/g, significantly exceeding the capacity of transition metal oxides, sulfates and phosphates.

The conditions of liquid chemistry type synthesis commonly used for fabrication of PBAs favour the formation of various types of defects, majority of which spoil its electrochemical properties. Crystal water formed under crystal growth occurs as coordination water and as interstitial water occupying the positions of  $\text{Na}^+$  ions. Both types of crystal water block the rapid diffusion paths for sodium ions and reduce battery performance. PBAs have another serious drawback – very low electronic conductivity. We assume that a partial substitution of Fe by another 3d metal ions can improve transport properties of PBAs. We plan also the fabrication of the carbonaceous (carbon nanotubes, graphene, reduced graphene oxide) composites with PBAs in order to improved macroscopic electronic conductivity of the cathode material and enhance electrochemical performance of the Na-ion batteries based on PBAs.

Due to the decisive role of the PBAs cathode material in Na-ion batteries we will focus on the comprehensive large scale interdisciplinary research involving chemical composition, crystal structure, electronic structure, effects of nanoscale, valence of transition metal ions, transport properties, chemical stability and electrochemical tests of the batteries. Great emphasis will be placed on developing and optimization of synthesis method to obtain PBAs with the lowest possible number of defect.

The *NaBat* project will present a synergistically approach based on the defect engineering, electronic structure engineering and microstructure engineering in the development of PBAs cathode material for high energy density Na-ion batteries based on low cost and earth abundant elements.

Regardless of the important application aspect of the project, its implementation will make a significant contribution to the existing state of knowledge in the field of determining the relationship between the nature of chemical bonds, crystal and electronic structure, defects structure, the oxidation state of transition metal ions, transport properties, 3D microstructure and reactivity of solids, what is still open problem in material engineering.