

Electricity storage and conversion of chemical energy into electricity are currently one of the leading research fields. Dynamic development of technologies based on reversible lithium-ion batteries is associated with the ever-growing demand for new energy sources, which are necessary for mobile devices, electric and hybrid cars, renewable energy storage and improving flexibility of large power units and intelligent "smart grids". Such considerable interest in Li-ion technologies results from the fact that they possess the highest gravimetric and volumetric energy density in comparison with other, commercial electrochemical batteries.

However, due to the shrinking resources of lithium and its location (politically unstable areas, e.g. Argentina, Bolivia or Chile), it can be noticed a growing interest in Na-ion technology, where the availability and low price of sodium is a significant advantage. Na-ion batteries, as an alternative to Li-ion, plays an important role especially in large-scale applications, in which gravimetric and volumetric energy density is not the most important criterion, as in the case of portable electronics or electric cars.

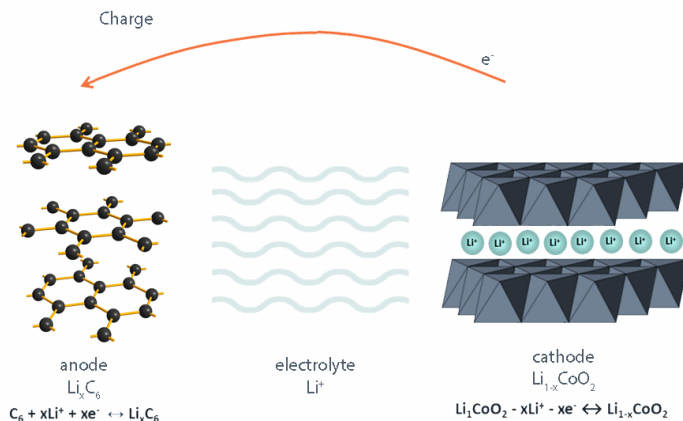


Fig. 1 Operation of the $\text{Li}_x\text{C}_6|\text{Li}^+|\text{Li}_{1-x}\text{CoO}_2$ commercial battery.

The operation of Na-ion batteries (analogous to Li-ion batteries) is based on the sodium intercalation/deintercalation processes, which uses ability of the transition metals M_aX_b compounds ($\text{M}=\text{3d}$ metal; $\text{X} = \text{O}, \text{S}$, polyanion PO_4) with a layered or 3d structures for reversible insertion into their structure one or more moles of sodium per mole of M_aX_b at room temperature without substantial changes in the crystallographic structure. Fig. 1 schematically shows the mechanism of the operation of commercial type $\text{Li}_x\text{C}_6/\text{Li}^+/\text{Li}_{1-x}\text{CoO}_2$ battery.

In this project, the author intends to use the developing by her method - electronic structure engineering - to study a new generation of cathode materials for sodium-ion batteries based on layered high-entropy oxides (HEO). Initial research of the author showed that it is possible to obtain layered high-entropy Na_xMO_2 oxides containing 4 or 5 cations in the same atomic proportions in the sublattice of the transition metal, which exhibit interesting physicochemical and electrochemical properties.

Based on the author's experience in materials for sodium-ion batteries and literature data, the aim of the research project is to determine the mechanism and processes occurring during operation of Na-ion cells with a cathode based on layered high-entropy oxides. The author of the project proposes the investigation of the two groups of HEOs:

- $\text{Na}_x\text{Mn}_{1/5}\text{Fe}_{1/5}\text{Co}_{1/5}\text{Ni}_{1/5}\text{M}_{1/5}\text{O}_2$, where $\text{M} = \text{Cu}, \text{Mg}, \text{Zn}, \text{Al}, \text{Ti}, \text{V}, \text{Zr}, \text{Nb}$
- and
- $\text{Na}_x\text{Mn}_{1/6}\text{Fe}_{1/6}\text{Co}_{1/6}\text{Ni}_{1/6}\text{Cu}_{1/6}\text{M}_{1/6}\text{O}_2$, where $\text{M} = \text{Mg}, \text{Zn}, \text{Al}, \text{Ti}, \text{V}, \text{Zr}, \text{Nb}$.

The project will include determining the correlation between the crystal and electronic structure, the oxidation state of the transition metals, transport and electrochemical properties of the cathode materials, which will allow control over these properties and allow the design of safe, functional cathode materials for sodium-ion batteries. The controlling of the processes occurring in Na-ion cells, due to its complexity, requires an interdisciplinary approach in the field of solid state physics, chemistry and electrochemistry, material engineering, modeling of the electronic structure, structural and chemical stability of materials and the use of advanced solid state physics research techniques.