

Project name: IRN AP1487188 "Development of technology for obtaining an efficient cathode material for creating competitive sodium-ion batteries"

Relevance: The rapidly growing demand in the world for lithium ion batteries (LIB) is associated with the use of LIB in mobile electronic devices, hybrid and electric vehicles, as well as in alternative energy systems. But the limited reserves of lithium on earth, its high cost and growing demand require the creation of chemical current sources (CPS) based on other cheap and common metals, for example, sodium for creating sodium-ion batteries (SIB). The relevance of developing a technology for obtaining efficient cathode materials for NIA, due to the fact that they are key components of HIT, which mainly determine the final energy density and cost of the battery. But the cathode materials in LIBs generate lower energy densities compared to LIBs, since ions Na^+ has a large ionic radius and redox potential. Therefore, it is necessary to develop a technology for obtaining more efficient sodium-containing cathode materials for SIB.

Purpose: to develop a technology for obtaining an efficient cathode material, including a nanomaterial capable of increasing the capacitive, specific energy parameters of existing sodium-ion batteries (SIB) to the level of lithium-ion batteries (LIA).

Expected and achieved results:

1. A conceptual model of a competitive NRA will be created by increasing the efficiency of the cathode material.
2. Technologies will be developed for obtaining efficient cathode materials for NIA by methods of mechanical and solid phase synthesis.
3. Technologies will be developed for obtaining efficient cathode materials for NIA by methods of exposure to optical, microwave and laser radiation.
4. A technology for obtaining efficient composite cathode materials for SIB will be developed.
5. A technology for nanostructuring cathode materials will be developed to obtain homogeneous-mixed nanomaterials with specified particle sizes for SIB.
6. The structures and electrophysical parameters of the synthesized samples will be investigated.
7. The electrochemical parameters and characteristics of cathode materials in the composition of SIB will be investigated.
8. A physicochemical analysis of the synthesized samples will be carried out in order to identify criteria for the search for effective cathode materials for SIB.
9. Cathodes based on synthesized materials and a laboratory model of SIB will be made. Test tests of cathodes as part of SIB will be carried out, including life tests.

Based on the results obtained in the project, at least 3 (three) articles or reviews will be published in peer-reviewed scientific journals, indexed in the Science Citation Index Expanded Web of Science database or having a Cite Score percentile in the Scopus database of at least 50 (fifty), and also at least 1 (one) article or review in a peer-reviewed foreign or domestic publication recommended by COXON.

The results of the work will be reported at international conferences. On this topic, it is planned to file a patent with the Kazakh or Eurasian patent bureau and publish a book or chapter of a book in foreign or Kazakh publishing houses.

Study group members:

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Information for potential users:

Of practical interest are cathode materials capable of generating a specific energy capacity of 145–200 mAh/g in the voltage range from 2.3 to 4.5 V as part of SIB. There are currently no such sodium-containing cathode materials. Therefore, it is necessary to increase the efficiency of cathode materials for NIA. We plan to create a SIB model based on the developed cathode materials with a specific energy consumption of at least ~ 145 mAh/g in a wide voltage range. The creation of effective sodium-containing cathode materials will help reduce the cost of SIB.

The technology for producing efficient cathode materials for SIB is planned to be protected by a patent. Having a patent can facilitate the launch of production facilities for the production of competitive SIB in large cities of the Republic of Kazakhstan, where there are production facilities for the production of lead-acid batteries.

Additional Information:

To evaluate the efficiency of using sodium and lithium materials in metal-ion batteries (MIB) as a cathode material, the main parameters of these two types of MIA were compared in [1] (Table 1).

Table 1. Main characteristics of Na and Li cathode materials in MIB

| Parameters | Cathode - sodium (Na) | Cathode - lithium (Li) |
|-------------------|---------------------------------|---------------------------------|
| Cost | 0.07–0.37 евро кг ⁻¹ | 4.11–4.49 евро кг ⁻¹ |
| Energy intensity | 1.16 Ач/г ⁻¹ | 3.86 Ач/г ⁻¹ |
| Operating voltage | – 2.7 В | – 3.0 В |
| Ionic radius | 0.98 Å | 0.69 Å |
| Melting point | 370.7 K | 823.5 K |

It follows from the tabular data that if the energy intensity in NIA is increased to LIB, then the cost of SIB will be significantly lower than LIB. Therefore, SIBs may be more competitive than LIBs.

Literature

1. Thackeray M.M., Wolverton C., Isaacs E.D. Electrical energy storage for transportation – approaching the limits of, and going beyond, lithium-ion batteries. *Energy & Environ. Sci.* – 2012. – Vol. 5, №7. – P. 7854-7863.

2022 Report for Project AP1487188

During the reporting period in 2022, under the project AP1487188 "Development of a technology for obtaining an effective cathode material for the creation of competitive sodium-ion batteries", the following research tasks were completed:

1. A conceptual model of a competitive SIB has been created by increasing the efficiency of the cathode material. The creation of a conceptual model of a competitive SIB is necessary, because using it, you can visually understand the structure of the modeled subject area and the relationships between its elements. Such a model structures the research process, makes it possible to link theory and empirical data, guides the collection of data and their subsequent interpretation.

2. Technologies have been developed for obtaining efficient cathode materials for SIB by the methods of mechanical and solid phase synthesis. $\text{Na}_3\text{Fe}_2(\text{PO}_4)_3$ and $\text{Na}_2\text{FePO}_4\text{F}$ polycrystals were obtained by solid-phase and mechano-synthesis. The structural and electrochemical properties of the synthesized samples were studied.

Based on the results of the research conducted, 2 theses of reports were published at international conferences:

1. Nogai A.S., Uskenbaev D.E., Nogai A.A. Influence of thermodynamic factors on the production of $\text{Na}_3\text{Fe}_2(\text{PO}_4)_3$ and $\text{Na}_2\text{FePO}_4\text{F}$ polycrystals by solid-phase synthesis. *Proceedings of the International Conference: "Seifullin Readings 18(2) - Science of the 21st century, the era of transformation"*, V.1, S. 264-266, KATU. S. Seifullina, Astana, 2022

2. Nogai A.S., Uskenbaev D.E., Nogai A.A. On the question of the relationship between the structure and conductive properties of $\text{Na}_2\text{FePO}_4\text{F}$ polycrystals obtained by various synthesis methods. *Proceedings of the International Conference: "Global Science and Innovation 2022: Central Asia"* No. 3(17). Astana, September 2022, Series "Technical Sciences" Vol. 3, P. 34 – 35.

Article in a journal included in the Scopus base with a percentile of 0.2.

3. Nogai A.S., Nogai A.A., Stefanovich S.Yu., Uskenbaev D.E. Electrochemical properties of $\text{Na}_3\text{Fe}_2(\text{PO}_4)_3$ cathode materials produced by various synthesis methods and evaluation of the possibility of their use in sodium-ion batteries. // *Eurasian Journal of Physics and Functional Materials*. 2022, 6(3), P. 223-233. DOI: 10.32523/ejpfm.2022060307.