

## Brief information about the project

Name of the project	AP09058322 «Synthesis and investigation of a composite based on a metal-organic framework (MOF) for its application as an anode material in sodium-ion batteries»
Relevance	Certainly, the topic of sodium sources is relevant for Kazakhstan, and despite the absence of their production in the republic, its development is necessary. This creates favorable conditions for launching domestic production of sodium-ion batteries (SIBs). Additionally, it is important to note that with further development, the market in Kazakhstan may witness the emergence of innovative materials based on MOF, the prospects of which extend beyond just battery production.
Purpose	Develop a synthesis method for a MOF composite as an anode material with high electrical conductivity, capacity, and durability for its subsequent application in Na-ion batteries.
Objectives	<ol style="list-style-type: none"><li>1. Synthesis of a stable metal-organic framework (MOF) compound via hydrothermal method. Based on literature data, MOF-Zn(EDTA) was chosen due to its high specific capacity (243.2 mAh/g), presence of interlayer space allowing for easy intercalation-deintercalation of sodium ions, as well as the affordability and availability of starting reagents.</li><li>2. Synthesis of MOF composite and fabrication of anode material based on it. Silver nanopowder was selected as a modifying agent primarily for validating the mechanism of action of the highly conductive additive, while copper nanopowder was chosen as an affordable and suitable material meeting the required properties.</li><li>3. Investigation of structural and electrochemical characteristics of the anode material based on the MOF composite. This stage is closely related to the previous one, as it involves analyzing the impact of the structural organization of the multi-component material on its electrochemical properties. It aims to identify the dependence of electrochemical characteristics (specific capacities, charge-discharge rates, material stability during prolonged cycling) on the composition, structure, and conditions of obtaining the anode mass.</li><li>4. Study of the kinetics of intercalation processes in the anode material based on the MOF composite. The final stage of the work involves establishing theoretical principles of charge transfer in the hierarchically organized MOF-based anode material.</li></ol>
Expected and achieved results	- A metal-organic compound $Zn_2(EDTA)(H_2O)$ was synthesized via the hydrothermal method with process optimization achieved through control of temperature, pH, and synthesis duration.

	<p>- Synthesis of a new structure with a composition of Zn<sub>2</sub>EDTA was realized during the investigation of the Zn<sub>2</sub>(EDTA)(H<sub>2</sub>O) compound. It was demonstrated that precise pH control plays a crucial role in phase formation of this compound.</p> <p>- The potential of Zn<sub>2</sub>(EDTA)(H<sub>2</sub>O) and Zn<sub>2</sub>EDTA MOF compounds as anode materials for sodium-ion batteries based on aqueous electrolytes was explored. Oxidation-reduction processes related to zinc deposition and hydrogen evolution were identified through cyclic voltammetry, limiting their use as anodes for water-based batteries.</p>
<p>Research team members with their identifiers (Scopus Author ID, Researcher ID, ORCID, if available) and links to relevant profiles</p>	<ol style="list-style-type: none"> <li>1) Ivan Trusov, ResearcherID: H4522-2018, ORCID: 0000-0002-6534-1389, Scopus Author ID:57200513467</li> <li>2) Starodubtseva Alena, ORCHID: 0000-0003-4344-2039; Scopus Author ID: 57988905100</li> <li>3) Lepikhin Maxim, Scopus Author ID: 56436632000.</li> <li>4) Kan Tatyana, Scopus Author ID-57359426400, ResearcherID-LF-3477-2024, ORCHID-0000-0002-1222-2060</li> <li>5) Zhigalenok Yaroslav, Scopus Author ID-57862139800, ResearcherID-GSC-9737-2022, ORCHID-0000-0003-1452-1248</li> <li>6) Vladislav Dubrovsky</li> <li>7) Malik Seilbek</li> </ol>
<p>List of publications with links to them</p>	<ol style="list-style-type: none"> <li>1) Alena A. Starodubtseva, Yaroslav S. Zhigalenok, Kairgali M. Maldybayev, Alina K. Galeyeva, Ivan A. Trussov and Andrey Kurbatov On electrochemistry of metal-organic framework Zn<sub>2</sub>(EDTA)(H<sub>2</sub>O) // RSC Advances. 2023. – V. 13. – P. 4880 – 4889. (WOS - Q2, SCOPUS - 78 процентиль). <a href="https://doi.org/10.1039/d3ra00040k">https://doi.org/10.1039/d3ra00040k</a>.</li> <li>2) Alena A. Starodubtseva, Tatyana V. Kan, Sergey N. Marshenya, Konstantin A. Lyssenko, Stanislav S. Fedotov, Ivan A. Trussov Synthesis and structure of anhydrous Zn<sub>2</sub>EDTA metal-organic framework // Polyhedron. 2024. – V.248. (WOS – Q1, SCOPUS - 69 процентиль). <a href="https://doi.org/10.1016/j.poly.2023.116750">https://doi.org/10.1016/j.poly.2023.116750</a>.</li> </ol>
<p>Patents</p>	

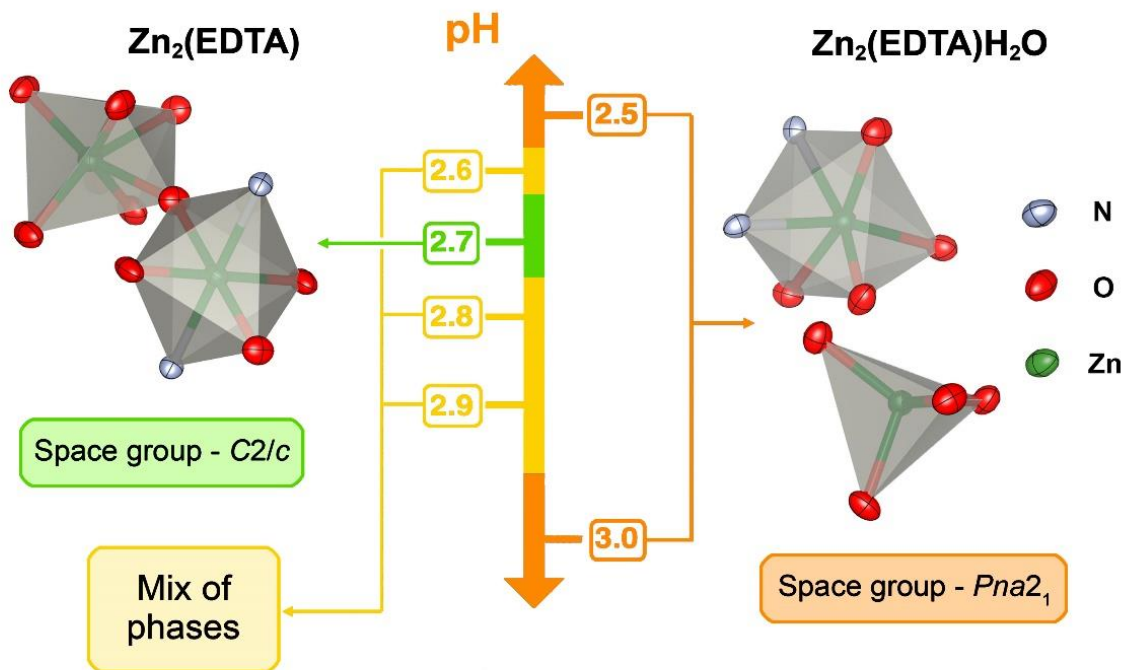


Figure 1 – Effect of pH on the formation of Zn<sub>2</sub>(EDTA) structures

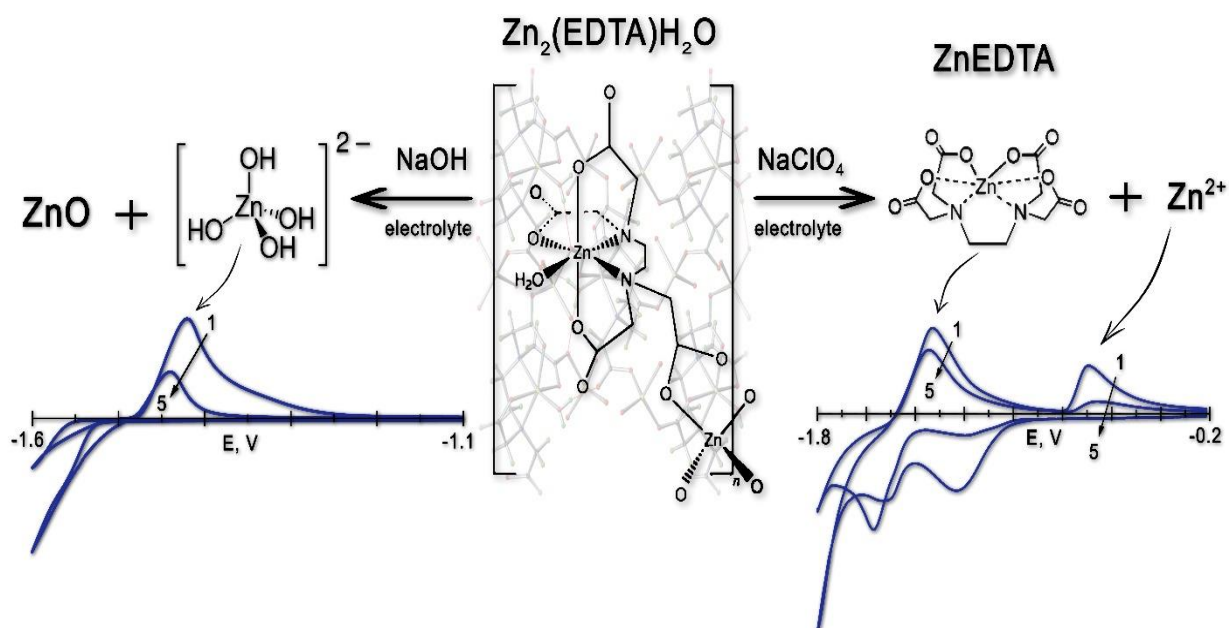


Figure 2 - Electrochemical behavior of Zn<sub>2</sub>(EDTA) in aqueous electrolytes.