Final Report of Åforsk Project (Ref. No. 23-411)

Improved Ni-based Hydro-/oxides for A Sustainable Future: Material Synthesis to Next-generation Aqueous Batteries

Summary

Rechargeable batteries have been paid more attention with the rapid growth of first portable consumer devices, such as laptops and mobile phones, and then later with the production of hybrid as well as electric vehicles, concomitant with the expansion of intermittent solar and wind production that also needs battery storage to facilitate more effective connections to the electric grid. In addition, with today's deteriorating security situation, an ongoing energy crisis, and the transition to completely fossil-free energy production, Europe must become more self-sufficient in strategically relevant supply chains and energy supply. In this new industrial age of clean energy technology manufacturing, it is important to develop the European industry by producing rechargeable batteries. Most of this battery development has been done in Asia leading to the development of the nonaqueous Li-batteries. But we still have battery industries here that are based on aqueous chemistries using alkaline Ni-electrodes in their battery cells. A further improvement of these water-based energy storage devices towards higher energy and power densities will help Europe to become more independent in this area. To meet these demands, it is thus critical and urgent to continuously develop new electrode materials and fully explore their charge carriers and storage mechanisms. Ni-based metal hydro-/oxides (such as $Ni(OH)_2$, NiMn layered double hydroxide (LDH), NiO, and $NiMoO_4$) show very excellent electrochemical potentials due to their high theoretical capacitance, tuned composition and morphology, inexpensive synthesis procedure, high safety, and environmental friendliness. However, also due to their poor conductivities and large volume expansion, these materials still require more thorough investigations related to the effect of the experimental conditions and the change of the crystallographic lattice.

This project focuses on nickel molybdate, exploring methods to improve its conductivity, specific capacity, and cycling stability, aiming to obtain positive electrode materials with excellent electrochemical performance and NiZn batteries with high energy density and good lifetime. The main contents and conclusions of this project are as follows:

- In this project, zinc was introduced to prepare $Ni_{1-x}Zn_xMoO_4$ nanoflake electrodes to increase the energy density and improve the cycling stability for a wider range of applications of aqueous rechargeable nickel-zinc (NiZn) batteries. This was achieved using a facile hydrothermal method followed by thermal annealing, which can be easily scaled up for mass production. Owing to the unique nanoflake structures, improved conductivity, and tunable electronic interaction, excellent electrochemical performance with high specific capacitance and reliable cycling stability can be achieved. When the Zn doping is 25%, the $Ni_{0.75}Zn_{0.25}MoO_4$ nanoflake electrode displays a high specific capacitance of 345.84 mA h g^{-1} (2490 F g^{-1}) at a current density of 1 A g^{-1} and improved cycling stability at a high current density of 10 A g^{-1}. NiZn cells assembled with $Ni_{0.75}Zn_{0.25}MoO_4$ nanoflake electrodes and zinc electrodes have a maximum specific capacity of 344.7 mA h g^{-1} and an energy density of 942.53 W h kg^{-1}.
- In this project, multi-dimensional heterostructured selenized PBA modified Zn-doped $NiMoO_4$ (SNZO) nanoarray electrodes were obtained through a multi-step method. The unique heterostructures present improved conductivity and enhanced electrochemical performance

with high capacity and reliable cycling capability. In this study, ex-situ XPS and XRD analyses reveal the energy storage mechanism referring to several phases in the redox reactions, where their synergistic effects lead to the composite electrodes exhibiting excellent performance. The obtained SNZO electrode has a capacity of 1.33 F cm^{-2} at 0.5 mA cm^{-2}, which is better than the NZO (0.83 F cm^{-2}) and PBA/NZO (0.76 F cm^{-2}) electrodes. Furthermore, the assembled NiZn cell shows a peak energy density of 0.22 mWh cm^{-2} and a power density of 19.98 mW cm^{-2}.

- In this project, we prepared and successfully fabricated Al-doped $Ni(OH)_2$-modified $NiMoO_4$ nanoarrays and investigated their electrochemical performance. It can be seen that this active electrode material exhibits a high capacity, which can be attributed to: (i) the high capacity achieved by coupling two highly electrochemically active materials; (ii) Al doping stabilizes the α-$Ni(OH)_2$ phase structure, resulting in a high capacity; and (iii) the multi-dimensional nanostructure design provides a more stable composite material structure, mitigating volume expansion during repeated charge-discharge cycles and thus improving cycle stability.
- In this project, we prepared P-reinforced carbon decorated NiSe-based nanocomposites and explored their application as electrode materials for NiZn batteries. Based on its enhanced electrochemical performance, we attribute this advantage to: (i) the composite of N-doped carbon materials provides nickel selenide with higher conductivity and more electron transport paths, thereby enhancing its electrochemical activity; in addition, the structural changes enhance the structural stability of the composite material during repeated charge and discharge processes; (ii) the introduction of P not only further enhances the conductivity, but also increases the number of phases, making the electrochemical reaction more complex and causing an enhanced synergistic effect, thereby enhancing the electrochemical performance of the composite material.

This project synthesized high-performance Ni-based cathode materials for NiZn batteries and explored the mechanisms by which they enhance the electrochemical performance of the devices. The project also analyzed in detail the enhancement mechanisms of interfacial conductivity through different design strategies, demonstrating a simple, effective, and universal strategy for improving electrode material performance. Thanks to the support of Åforsk, these design strategies for Ni-based heterostructure nanomaterials enable high-performance aqueous energy storage and unlock more possibilities for future battery systems.

Project outcomes

The project has resulted in two published papers, two manuscripts currently in preparation for submission. The following is the list of outcomes between 2024 and 2026, including publications, conferences, and master's thesis, that contain the appropriate acknowledgement to Åforsk.

Peer-reviewed publications

- ***XingyanZhang***, Dag Noréus. Selenized Zn-doped $NiMoO_4$ modified with the Prussian blue analogue as electrodes for aqueous alkaline NiZn batteries. Chem. Eng. J., 2025, 519, 165666.
- ***XingyanZhang***, Dag Noréus. Zn-doped $NiMoO_4$ enhances the performance of electrode materials in aqueous rechargeable NiZn batteries. Nanoscale, 2024, 16, 18056-18065.

In preparation

- P-doped carbon decorated $NiSe_2$ nanomaterials for aqueous alkaline NiZn batteries,

Xingyan Zhang, Kristofer Bergkvist, Rongfang Feng, and Dag Noréus (in writing)

- Enhancement of hierarchical $NiMoO_4$/Al-doped $Ni(OH)_2$/NF electrode for NiZn batteries, ***Xingyan Zhang***, Rongfang Feng, and Dag Noréus (in writing)

International conferences

- Materials Today Conference 2025, 23-26 Jun 2025, Sitges, Spain
- International Conference on Materials Science and Engineering, 23-24 Feb 2026, Paris, France

Master thesis

- A master's thesis: "Synthesis of $NiSe_2$-based cathodes for rechargeable alkaline NiZn batteries" by Kristofer Bergkvist. Supervision: Dag Noréus and Xingyan Zhang, Stockholm University. (2024).