OPERANDO XRD STUDY ON THE STRUCTURAL CHANGES OF ZINC HEXACYANOFERRATE IN AQUEOUS ZINC-ION BATTERIES

Dovilė Škarnulytė[1,2], Linas Vilčiauskas[1,2], Jurgis Pilipavičius[1,2]

[1]Vilnius University, Institute of Chemistry, Naugarduko 24, LT-03225, Vilnius, Lithuania
[2]Centre for Physical Sciences and Technology, Sauletekio av. 3, LT-10257, Vilnius, Lithuania
dovile.skarnulyte@chgf.vu.lt

Economic development and rapid population growth are among the factors contributing to the increasing demand for energy. [1] At the same time, growing awareness of the environmental impact of non-renewable resources is accelerating the transition toward renewable energy generation. However, energy supply from weather-dependent sources (sun, wind, etc.), creates imbalance between electricity production and consumption. [2] Possible solution to this problem is the development of large-scale battery parks that can store excess energy and supply it when needed.

Aqueous zinc-ion batteries (AZIBs) have attracted considerable attention as an environmentally benign alternative to widely used lithium-ion systems. [3] A promising cathode material in AZIB systems is a Prussian blue analogue zinc hexacyanoferrate(II, III) (ZnHCF, $Zn_{3+x}[Fe(CN)_6]_2$, $0 < x < 1$), which, depending on synthesis conditions, can crystallize in cubic and rhombohedral structures. [4] The open framework of ZnHCF allows the intercalation of various metal ions such as K^+, Na^+, Zn^{2+}. Nevertheless, practical implementation of these batteries remains challenging, as the mechanism of Zn-ion intercalation is still poorly understood.

This study aims to investigate structural changes occurring during charge/discharge processes using the operando XRD method. The obtained results demonstrate a phase transitions between cubic and rhombohedral crystal phases during cycling. These findings deepen the understanding of the structural and electrochemical properties of ZnHCF and provide guidance for enhancing its performance as a cathode material in safer and more sustainable aqueous zinc-ion batteries.

[1] A. Demirbas, „Energy issues and energy priorities“, Energy Sources, Part B: Economics, Planning, and Policy, vol. 3, no. 1, pp. 41–49, 2007.
[2] K. Hedegaard, P. Meibom, „Wind power impacts and electricity storage – A time scale perspective“, Renew Energy, vol. 37, no. 1, pp. 318–324, 2012.
[3] B. Tang et al., „Issues and opportunities facing aqueous zinc-ion batteries“, Energy Environ Sci, vol. 12, no. 11, pp. 3288–3304, 2019.
[4] J. Rodríguez-Hernández et al., „An atypical coordination in hexacyanometallates: Structure and properties of hexagonal zinc phases“, Journal of Physics and Chemistry of Solids, vol. 68, no. 9, pp. 1630–1642, 2007.