METAL-ORGANIC FRAMEWORK AS POSITIVE ELECTRODE MATERIAL OF LITHIUM AND SODIUM ION BATTERIES FOR LARGE-SCALE APPLICATIONS

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Considering large-scale applications such as electric vehicles (EVs) or energy storage systems (ESSs), low cost of whole battery system as well as energy density is important due to widespread use. Conventional cathode materials, however, are suffered from high raw material cost, complexity of the synthetic process at high temperature. For this reason, metal–organic frameworks (MOFs) have been intensively investigated as cathode materials. Among MOFs, Prussian Blue analogues (PBAs) show impressive electrochemical performance. They also possess several advantages, including easy synthetic procedures at low temperature. [1, 2]

Furthermore, Na-ion batteries (SIBs) can be more suitable than Li-ion batteries (LIBs) for large-scale applications because the cost of raw materials for SIBs is estimated to be about 30 times cheaper than those of LIBs. [3]

In this study, we present the cell performances on non-aqueous Li-ion and Na-ion battery with sodium zinc hexacyanoferrate (NZH), Na2Zn(Fe(CN)6)·xH2O, which is substantially improved PBA structure by simply replacing the existing Fe3+ with Zn2+. The well-defined open framework enabled by cyanide ligands bridging the octahedral Fe sites and the tetrahedral Zn sites endows enlarged ionic channels compared to those of typical PBAs. The sufficiently large channel of NZH can accommodate diffusion of Na ions as well as Li ions. NZH shows good electrochemical activity of a reversible capacity of about 60 mA h g−1 in the redox potential range of 2.0–4.0 V vs. Na/Na+ and 2.0–4.2 V vs. Li/Li+. In addition, in order to understand the mechanism of guest ion insertion to the NZH compound, additional experiments such as Ex-situ X-ray photoelectron spectroscopy (XPS), Ex-situ X-ray diffraction (XRD) and solvent comparison test were performed.

![Fig. 1. Crystal structure of NZH](image)

![Fig. 2.](image)

**References**