Charge-Discharge Mechanism of Niobium Pentoxide in Ionic Liquid Electrolyte

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Lithium-ion batteries have gained widespread use in electronic devices such as smartphones, laptops, and electric vehicles owing to their impressive performance of high energy density. However, they often face challenges related to insufficient power density. The demand for next-generation secondary batteries is driven by the necessity for higher energy density as well as high power density, and safety standards.

Niobium pentoxide (Nb_2O_5) has emerged as an interesting candidate for negative electrode material, known for its redox reaction-based pseudocapacitive behavior, providing rapid lithium-ion storage facilitated by its unique structure.[2] Utilizing Nb_2O_5 as a negative electrode material in lithium-ion batteries holds the potential for enhancing fast charge technology. While previous research has delved into the influence of particle size on pseudocapacitive behavior, the impact of temperature on this characteristic remains unexplored.

In this study, we investigated the charge-discharge performance of a Nb_2O_5 electrode using Li[FSA]-[C_2C_1im][FSA] and Li[FSA]-[C_3C_1pyrr][FSA] ([C_2C_1im] = 1-ethyl-3-methylimidazolium, [C_3C_1pyrr] = *N*-methyl-*N*-propylpyrrolidinium, and [FSA] = bis(fluorosulfonyl)amide) ionic liquid electrolytes operating at 90°C. The galvanostatic charge-discharge test reveals a high discharge capacity of ~430 mAh g^{-1} at 90°C (Figure 1).

Changes in oxidation states during charge-discharge processes at 90°C were monitored by Nb L-edge XANES analysis. During the charge-discharge process within the voltage range of 1.0–2.3 V, it is revealed that the storage of lithium ions in Nb_2O_5 drives through reversible oxidation-reduction reactions involving Nb^{V}/Nb^{IV}. However, extending the charging process to 0.01 V resulted in further lithium insertion into Nb_2O_5, despite no discernible alteration in oxidation state being observed.

References

[1] Amine, K.; Belharouak, I.; Chen, Z.; Tran, T.; Yumoto, H.; Ota, N.; Myung, S.-T.; Sun, Y.-K. *Adv. Mater*. **2010**, 22, 3052-3057.2.

[2] Sathasivam, S.; Williamson, B. A. D.; Althabaiti, S. A.; Obaid, A. Y.; Basahel, S. N.; Mokhtar, M.; Scanlon, D. O.; Carmalt, C. J.; Parkin, I. P. *ACS Appl. Mater. Interfaces* **2017**, 9, 18031-18038.

Table 1. List of samples for ex-situ Nb L-edge XAFS measurement.

Samples	Electrode states
1	Pristine
2	charge to 1V (vs Li^+/Li)
3	charge to 0.3V (vs Li^+/Li)
4	charge to 0.01V (vs Li^+/Li)
5	discharge to 2.3V (vs Li^+/Li)

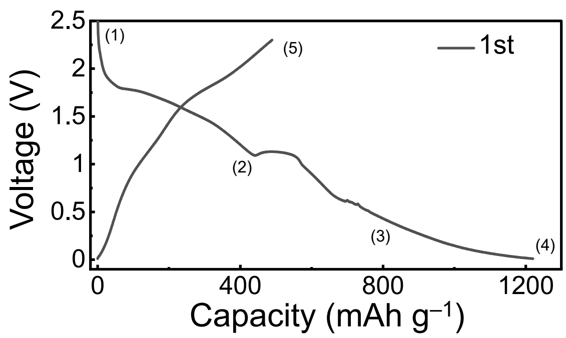

Fig. 1 The first cycle of Nb_2O_5 electrode 90 °C (see Table 1 for the sample list for Nb L-edge XANES spectra).