Electronic Supplementary Information for

Towards understanding the role of hyper-branched oligomers coated on cathode in the safety mechanism of lithium ion batteries

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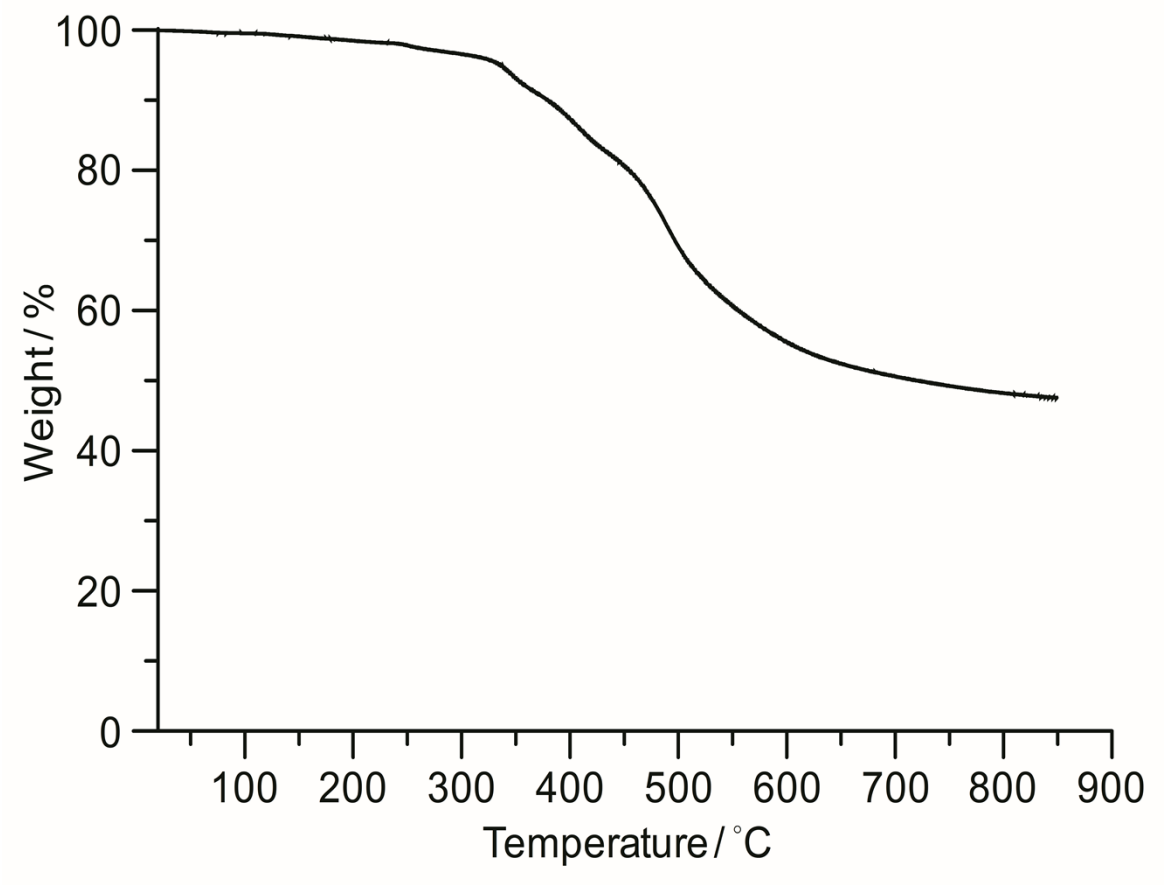


Fig. S1. TGA curve of the STOBA material.

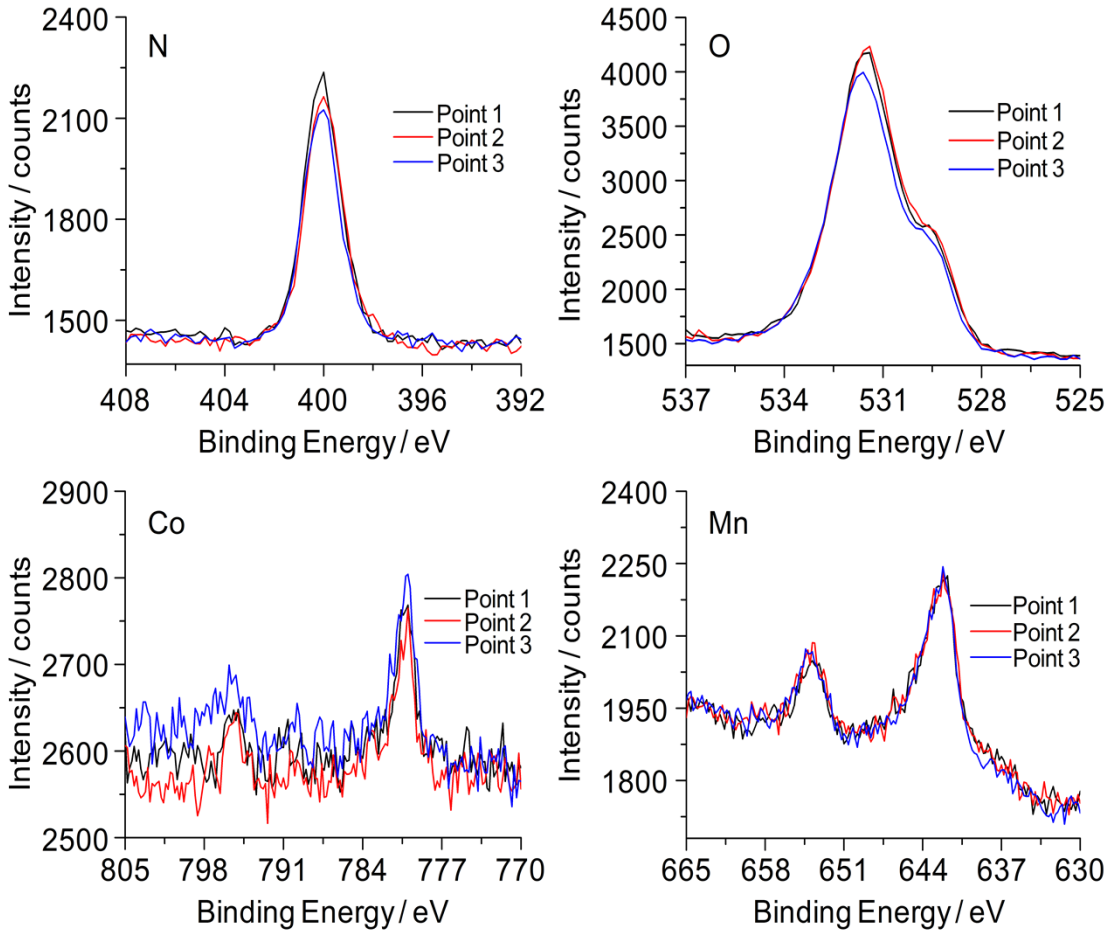


Fig. S2. XPS spectra of the STOBA coated $Li(Ni_{0.4}Co_{0.2}Mn_{0.4})O_2$ cathode with the core peaks at three different points of the sample. (The distances of the selected points are almost 1 cm from each other, sample area = 4 cm^2)

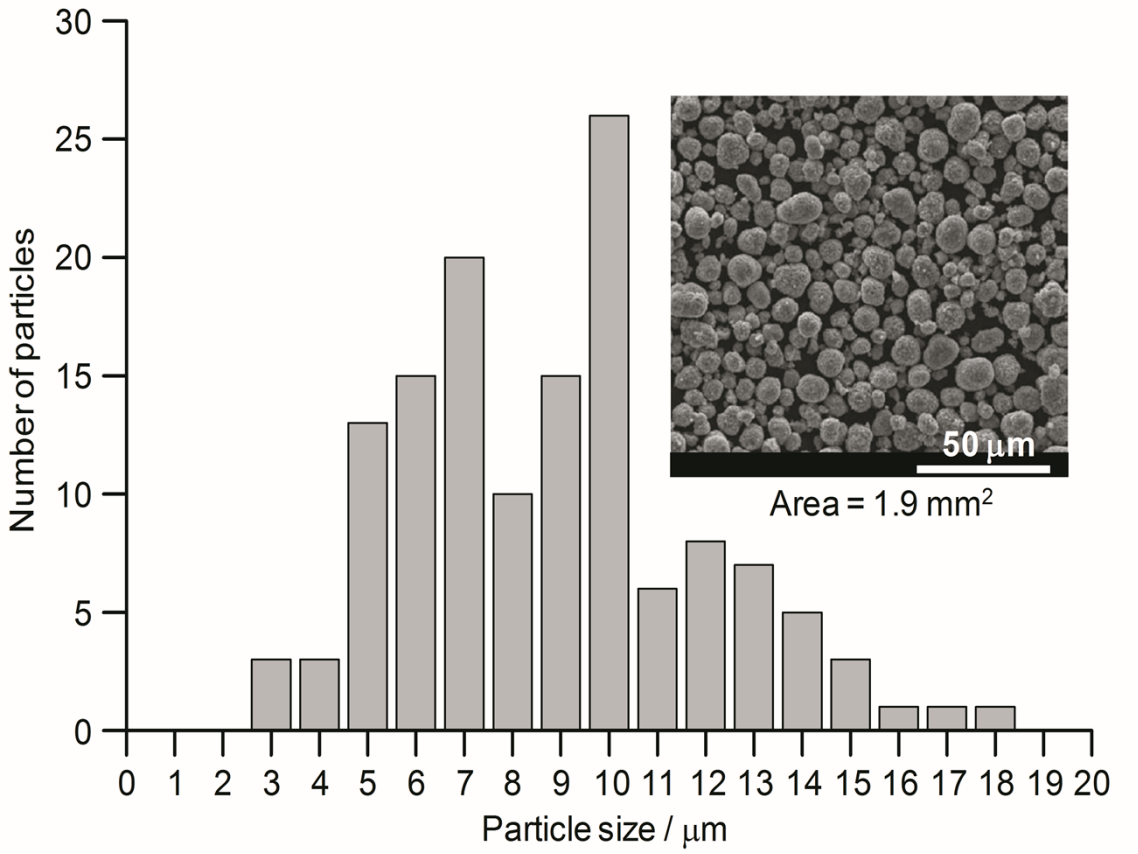


Fig. S3. Histogram of the particle size of the $Li(Ni_{0.4}Co_{0.2}Mn_{0.4})O_2$ cathode. The SEM image (inset) of the bare $Li(Ni_{0.4}Co_{0.2}Mn_{0.4})O_2$ particle was used for counting the particles.

Estimation of minimum amount of STOBA to coat $Li(Ni_{0.4}Co_{0.2}Mn_{0.4})O_2$ particle on the basis of SEM analysis

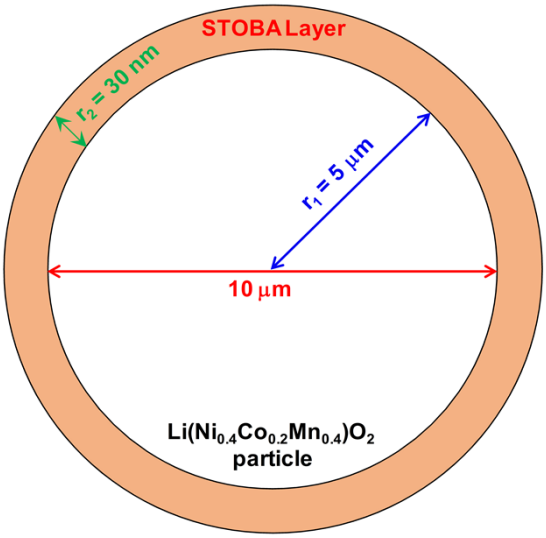
Radius of $Li(Ni_{0.4}Co_{0.2}Mn_{0.4})O_2$ particle, $r_1 = 5\ \mu m = 5 \times 10^{-6}$ m

Average STOBA layer thickness = 30 nm

Therefore, total radius of STOBA coated $Li(Ni_{0.4}Co_{0.2}Mn_{0.4})O_2$ particle,

$$r_2 = 5\ \mu m + 30\ nm = 5.03 \times 10^{-6}\ m$$

STOBA volume (ΔV) = volume of STOBA coated $Li(Ni_{0.4}Co_{0.2}Mn_{0.4})O_2$ particle (V_2) – volume of $Li(Ni_{0.4}Co_{0.2}Mn_{0.4})O_2$ particle (V_1)



$$\Delta V = V_2 - V_1$$

$$= \frac{4}{3}\pi {r_2}^3 - \frac{4}{3}\pi {r_1}^3$$

$$= \frac{4}{3}\pi\left({r_2}^3 - {r_1}^3\right)$$

$$= \frac{4}{3}\pi\left(5.03^3 - 5^3\right) \times 10^{-18}\ m^3$$

Minimum amount of STOBA required to coat the $Li(Ni_{0.4}Co_{0.2}Mn_{0.4})O_2$ particle is

$$\frac{\Delta V}{V_1} = \frac{STOBA\ volume}{Li(Ni_{0.4}Co_{0.2}Mn_{0.4})O_2\ volume}$$

$$= \frac{\frac{4}{3}\pi\left(5.03^3 - 5^3\right) \times 10^{-18}}{\frac{4}{3}\pi 5^3 \times 10^{-18}}$$

$$= \frac{\left(5.03^3 - 5^3\right)}{5^3}$$

$$\approx 0.018$$

$$= 1.8\%\ (volume\ percentage)$$

Therefore, the minimum amount of STOBA required to coat the $Li(Ni_{0.4}Co_{0.2}Mn_{0.4})O_2$ particle in weight percentage is

Density of STOBA = 1 g cm^{-3}

Density of $Li(Ni_{0.4}Co_{0.2}Mn_{0.4})O_2$ = 2.3 g cm^{-3}

$$\frac{\Delta w}{w_1} = \frac{STOBA\ volume \times density}{Li(Ni_{0.4}Co_{0.2}Mn_{0.4})O_2\ volume \times density}$$

$$= \frac{\frac{4}{3}\pi\left(5.03^3 - 5^3\right) \times 10^{-18} \times 1}{\frac{4}{3}\pi 5^3 \times 10^{-18} \times 2.3}$$

$$\approx 0.0078$$

$$= 0.78\% \ (weight\ percentage)$$

The estimation of the minimum amount of STOBA to coat the $Li(Ni_{0.4}Co_{0.2}Mn_{0.4})O_2$ particle is based on ideal spherical particles. In practice, the particles are not completely spherical and the size of particles varies (inset, Fig. S3). As shown in the SEM image (Fig. 4e), the coating layer is not uniform in the thickness, which varies from about 24 to 43 nm. In the calculation as shown above, we have considered the average thickness of the coating layer to be 30 nm. Therefore, some errors are present while calculating the minimum STOBA amount due to the assumptions of the shape and size of the $Li(Ni_{0.4}Co_{0.2}Mn_{0.4})O_2$ particle as well as the coating thickness. As the actual amount of STOBA used in the coating process (2 wt.%) is more than twice the minimum amount calculated, the effect of the above-mentioned errors will be compensated by the actual amount added.