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**Supplement**

# Mechanism of capacity fade of MCMB/$Li_{1.1}[Ni_{1/3}Mn_{1/3}Co_{1/3}]_{0.9}O_2$ cell at elevated temperature and additives to improve its cycle life

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## Experimental detail for XPS measurements

A lithium-ion button cell using $Li_{1.1}[Mn_{1/3}Ni_{1/3}Co_{1/3}]_{0.9}O_2$ as the cathode and MCMB as the anode was assembled for XPS experiment. The electrolyte used was 1.2 M $LiPF_6$ in mixture solvent of EC/EMC (3:7 by weight). The cell was initially cycled between 3.0 V and 4.1 V for 2 cycles with a constant current of C/10 before being constant-voltage charged to 4.1 V. The charged cell was then stored in a 55$^{o}$C oven for 3 weeks. After aging, the cell was fully discharged, and was disassembled to harvest the aged MCMB anode. The anode was then rinsed with DMC for three times to remove electrolyte residues. After drying in vacuum, XPS experiment was carried out to probe the existence of transition metal on MCMB anode.

All XPS measurements were made using a Kratos™ Axis Ultra DLD surface analysis instrument. The base pressure of the analysis chamber during these experiments was $3x10^{-10}$ Torr, with operating pressures around $1x10^{-9}$ Torr. Spectra were collected using a monochromatic Al Kα source (1486.7 eV) and a 300 x 700 micron spot size. The Al source was operated at 13 mA of emission current with the target anode set to 15 kV, for a resulting power of 195 W. For survey spectra the data were collected using a pass energy of 160 eV (fixed analyzer transmission mode), a step size of 1 eV and a dwell time of 200 ms. High resolution regional spectra were collected using a pass energy of 40 eV (fixed analyzer transmission mode),

a step size of 0.1 eV and a dwell time of 300 ms. For low signal to noise regions, multiple passes were made and the results averaged together as noted. Non-conductive samples showed evidence of differential charging, resulting in peak shifts and broadening. Photoelectron peak positions were shifted back towards their true values and their peak widths were minimized by flooding the samples with low-energy electrons and ions from the charge neutralizer system on the instrument. Further peak position correction was made by referencing the C 1s peak position of adventitious carbon for a respective sample (284.8 eV, PHI Handbook), and shifting all other peaks in the spectrum accordingly.

**Results**

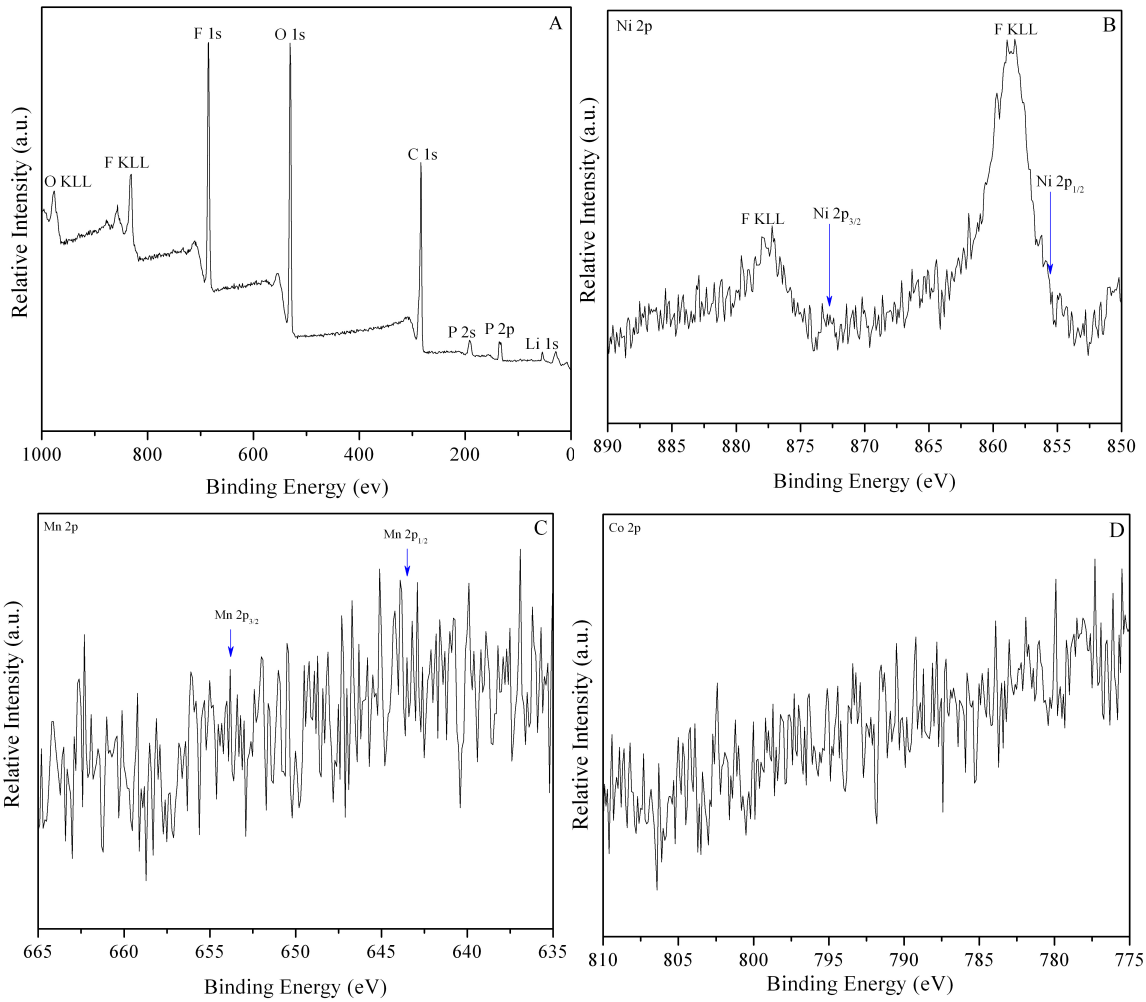


Figure 1S. (A) XPS survey of the MCMB electrode after aging at 55°C for 3 weeks; and high resolution regional spectra of (B) Mn 2p, (C) Ni 2p, (D) Co 2p core peaks for the MCMB anode.

Survey spectrum shows the presence of Li, F, C, O and P. No obvious signal for Mn, Ni, and Co was detected at the survey spectrum. However, trace amount of Ni and Mn may be presented in the sample, as indicated in high resolution regions spectra (Figure 1S.B and 1S.C). Co is still not detected even in the high resolution regions spectrum, as shown in Figure 1S.D)