PAUL SCHERRER INSTITUT

ELECTROCHEMISTRY LABORATORY

BATTERIES

Advanced investigation of reaction mechanisms at high potentials during cycling of HE-NCM

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5V cathode material

HE-NCM = Li_2MnO_3·$Li(Ni_xCo_yMn_z)O_2$ ➔ High energy density material.

Oxygen release + cut-off 5 V vs. Li^+/Li ➔ Side-reactions at interfaces.

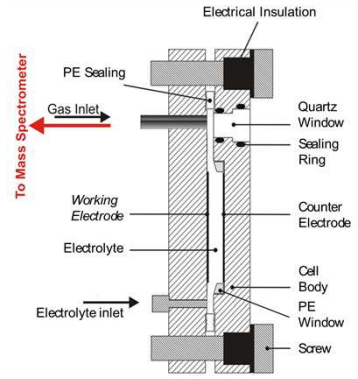
Diagnostics ➔ Gas and solid products investigated by Differential Electrochemical Mass Spectrometry (DEMS), and X-ray Photoelectron Spectroscopy (XPS).

Experimental

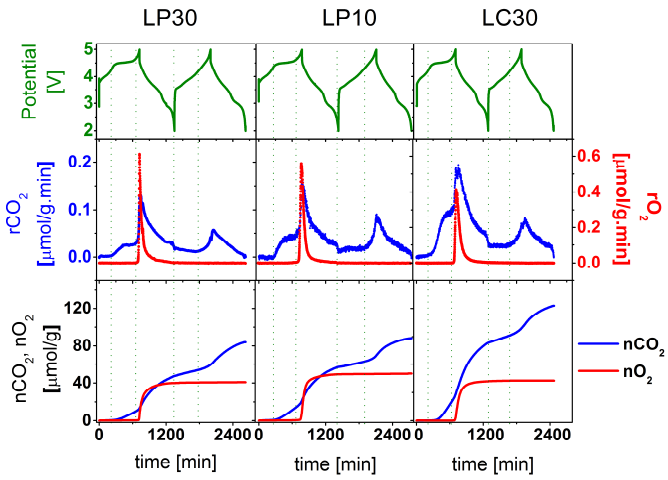
Electrodes of HE-NCM cycled at C/10 between 2 V and 5 V vs. Li^+/Li in:

- **LP30** 1M $LiPF_6$ in EC/DMC, 1:1
- **LP10** 1M $LiPF_6$ in EC/DMC/EMC, 3:3:4
- **LC30** 1M $LiClO_4$ in EC/DMC, 1:1

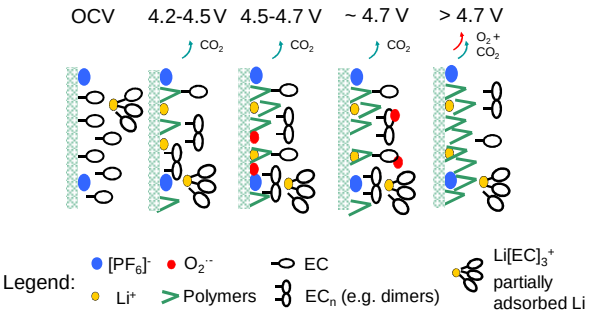
DEMS cell



DEMS: gas evolution

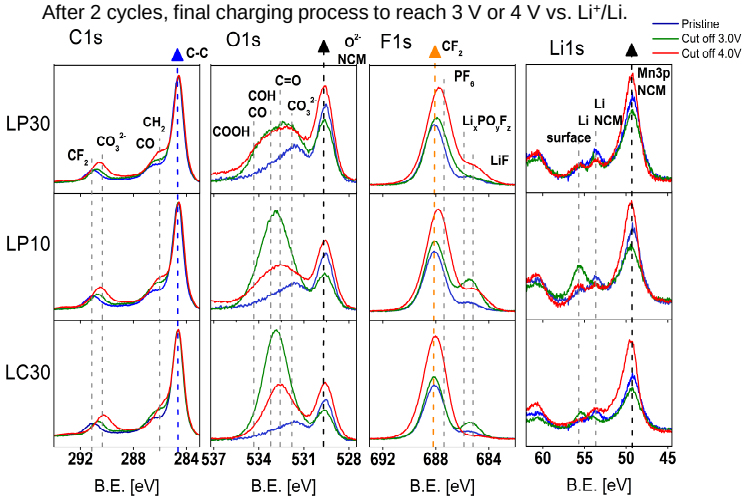


Interpretation

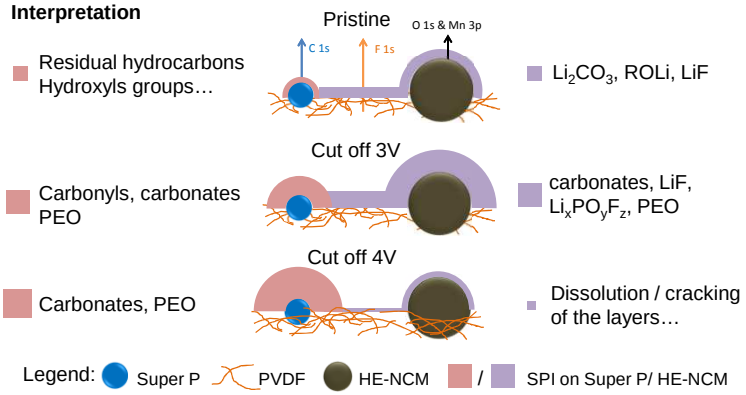


XPS: surface layers

After 2 cycles, final charging process to reach 3 V or 4 V vs. Li^+/Li.



Interpretation



Conclusions

DEMS: The oxygen first is accumulated at the interface, maybe reacting with carbonates. A reaction mechanism releasing both O_2 and CO_2 from the interface is proposed. Gas evolution behavior comparable, whatever the electrolyte.

XPS: Cycle of formation/dissolution of the solid layers covering HE-NCM's electrodes during cycling discovered

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