Design of High Performance, High Energy Cathode Materials

U.S. DEPARTMENT OF ENERGY
Energy Efficiency & Renewable Energy

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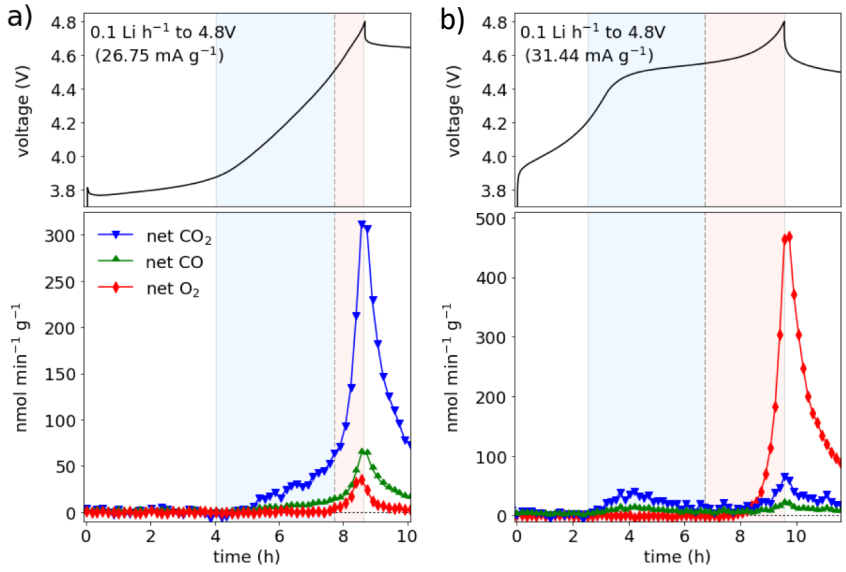
- ***Objective:*** Our project objective is to understand, then control, parasitic processes that result in gas evolution and capacity fade in high energy Ni-rich and Li-rich cathode materials.

Impact:

- Unique ^{18}O isotope labeling of the cathode material and residual lithium carbonate provides a method to decouple gas evolution origins.
- Understanding quantitative, *operando* gas evolution from batteries provides insight to parasitic processes occurring in the cell

Gas evolution from NMC622 (a) and LMR-NMC (b)



Accomplishments:

- Gas evolution analysis completed on numerous high-energy materials, including NMC622, LMR-NMC, $Li_{1.2}Ni_{0.2}Mn_{0.6}O_2$, $Li_{1.2}Ni_{0.2}Ru_{0.6}O_2$, among others.
- Developed a reliable $^{16}O/^{18}O$ isotopic exchange for these transition metal oxides, which discriminately labels the oxide and any residual lithium carbonate left after metal oxide synthesis
- Conclusively showed through gas evolution analysis of these materials that Li_2CO_3 accounts for all CO and CO_2 evolution at <4.8 V during the first charge cycle of all materials.
- Conclusively showed that O_2 release from cathode materials is correlated with the residual lithium carbonate concentration.

FY 18 Milestones:

- Complete DEMS characterization of ^{18}O isotopically labeled $LiNiRuO_2$ and $LiNiMnO_2$ materials series.
- Complete isotope labeling and materials characterization of the Ni-rich NMC series (333, 532, 622).
- Complete long-term cyclability of NM622 with and without residual lithium carbonate.
- Complete DEMS characterization Ni-rich NMC series.

FY18 Deliverables:

3 publications, complete gas evolution analysis of ^{18}O labeled Ni –rich NMC series and $Li_xNi(TM)O_2$ electrodes.

Funding:

— FY18: $50K, FY17: $50K, FY16: $50K