CONTINUOUS FLOW PROCESS – A TECHNOLOGY PLATFORM FOR MANUFACTURING OF 3,3,3-TRIFLUOROPROPYLENE CARBONATE

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OBJECTIVE

The aim of the project was to develop reliable, cost effective and environmentally friendly process for manufacturing of 3,3,3-trifluoropropylene carbonate (TFPC) , a promising new solvent to enable save, high energy new generation of lithium-ion batteries. Koura will implement the technology in large scale manufacturing.

RELEVANCE AND IMPACT

- The project is relevant to the DOE advanced electrochemical energy storage program by reducing the risk associated with the commercialization of new battery materials.
- The project is a key missing link between invention of new advanced battery materials, evaluation at multiple R&D organization, market evaluation of these materials and high-volume manufacturing.
- This project provides large quantities of materials with consistent quality for industrial validation and prototyping in large format cells.
- To allow battery community access to new materials and advance further research

BARRIERS

- In the quest for better performing LIBs scientists design, synthetize and evaluate more and more complex molecules for advanced electrolyte materials (solvents, salts, additives).
- New, manufacturing techniques are needed to produce experimental materials at scale. High cost of manufacturing advanced materials needs to be addressed.
- Industry typically don't want to invest in new materials before thorough validation and market assessment that requires high purity, uniform quality materials availability at suitable scale.

APPROACH

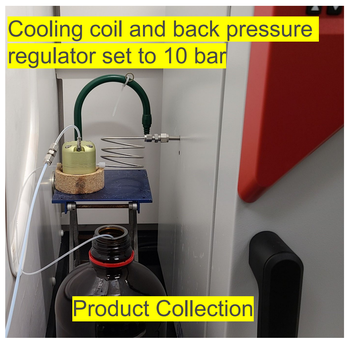
- The objective of this project is to provide a systematic research approach to develop cost-effective, scalable processes for manufacturing of 3,3,3-trifluoropropylene carbonate by more efficient use of feedstock and energy, improved safety and reduced environmental impact.
- Produce and provide high quality and sufficient quantity of material for prototyping and industrial evaluation and to support further research.
- Continuous flow chemistry is an emerging technology that promises to outperform traditional batch manufacturing processes in cost and time.

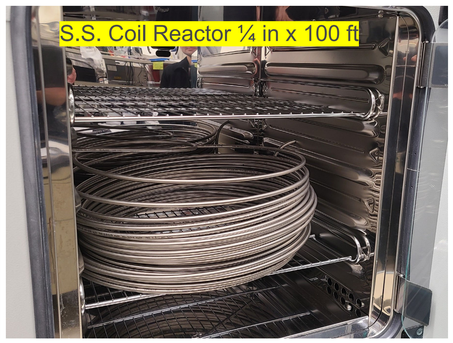
TECHNICAL ACCOMPLISHMENTS

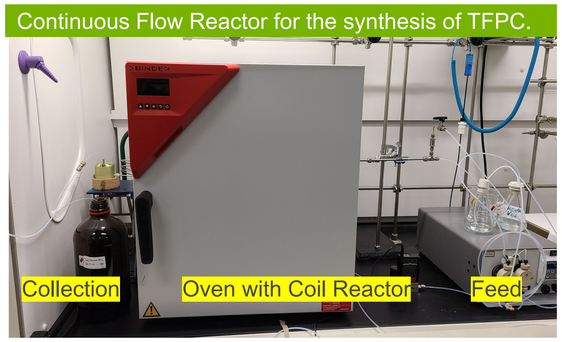
- Koura, the project's industrial partner is in the final stage of developing efficient process for manufacturing 3,3,3-trifluoropropylene oxide (TFPO), a precursor for the title 3,3,3-trifluoropropylene carbonate (TFPC).
- An emerging technology platform (continuous flow chemistry) was developed by Argonne and employed to manufacture TFPC. This green technology is 100% atom efficient minimizing waste and carbon footprint.
- The technology enables efficient production of TFPC and other component of advanced electrolytes for LIB. The proof of concept of the new process was realized by multi kg scale production of high purity TFPC.
- The material was evaluated electrochemically as a component of advanced electrolyte formulation. Preliminary data showed improved cell performance.

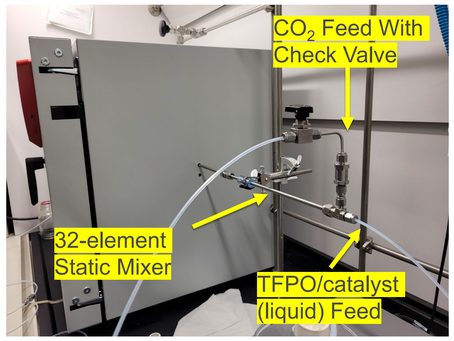
THE NEXT STEP

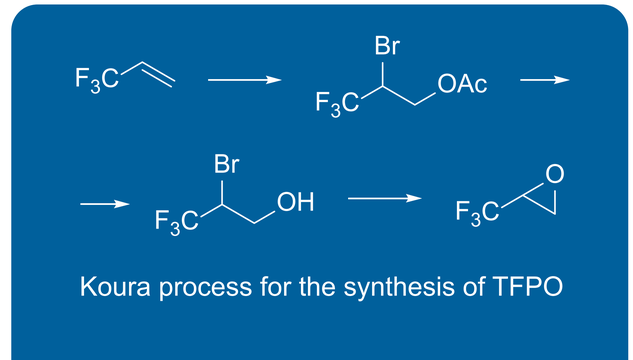
- Argonne will assist the industrial partner (Koura) in implementation and final tuning of the technology in industrial setting as needed.



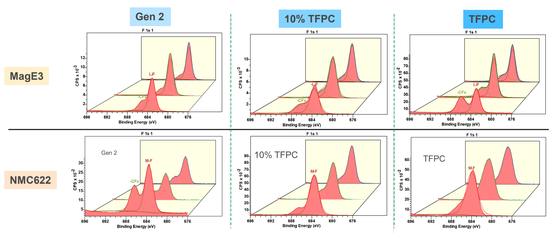








Working mechanism of TFPC on Graphite and NMC622



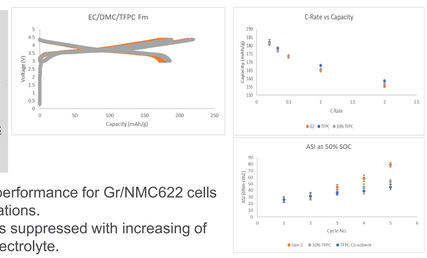
Increase in CFx species on cycled MagE3 anode with increasing TFPC in electrolyte.

Lessened amount of CFx species on cycled NMC622 cathode with increasing TFPC.

TFPC effect on cell impedance

Cathode: NMC622: 9.48 mg/cm2
Anode: MagE3: 6.35 mg/cm2
Electrolyte:
- Gen 2 (1.2M LiPF6 EC/EMC (3:7, w/w)),
- Gen 2 +10 % TFPC (w/w),
- 1 M LiPF6 in EC/DMC/TFPC (1:1:1 w/w)

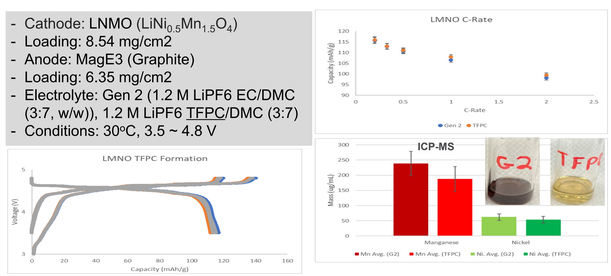
Conditions: 30ºC, 3.0 ~ 4.2 V



Similar formation, rate performance for Gr/NMC622 cells with all electrolyte formations.
Cell impedance rise was suppressed with increasing of TFPC composition in electrolyte.

TFPC effect on high-voltage spinel ($LiNi_{0.5}Mn_{1.5}O_4$)

- Cathode: LNMO ($LiNi_{0.5}Mn_{1.5}O_4$)
- Loading: 8.54 mg/cm2
- Anode: MagE3 (Graphite)
- Loading: 6.35 mg/cm2
- Electrolyte: Gen 2 (1.2 M LiPF6 EC/DMC (3:7, w/w)), 1.2 M LiPF6 TFPC/DMC (3:7)
- Conditions: 30ºC, 3.5 ~ 4.8 V



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