Materials List for

Identification and Quantification of Decomposition Mechanisms in Lithium-Ion Batteries; Input to Heat Flow Simulation for Modeling Thermal Runaway

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Materials

Name	Company	Catalog Number	Comments
Glove box MB 200B	MBraun		Glove box filled with argon to ensure inert atmosphere. H_2O < 0.1 ppm; O_2 < 0.1 ppm
STA 449 F3 Jupiter®	Netzsch		Simultaneous Thermal Analysis for thermal characterization. The STA equipment is located inside the glove box. Type of furnace used: silver
Agilent 7820A GC- Agilent 5977E MS	Agilent		Gas Chromatograph equipped with an quadrupole Mass Spectrometer. GC-MS is coupled to STA via heated lines in order to identify the released gases during thermal characterization
Bruker Vertex 70 V FTIR	Bruker		Fourier Transform Infrared spectrometer equipped with a TG-IR box. FTIR is coupled to STA via heated lines in order to identify the released gases during thermal characterization
18mm graphite electrode disc	Customcell	363586011	graphite electrode disc with an area capacity of 2.24 $mAh.cm^{-2}$
18mm NMC (111) electrode disc	Customcell	363662011	$LiNiMnCoO_2$ electrode disc with stochiometry ratio 111 and an area capacity of 2.0 $mAh.cm^{-2}$
1.0 M $LiPF_6$ in EC/DMC=50/50 (v/v)	Sigma-Aldrich	746711-100ML	Electrolyte
2325 trilayer film separator	Celgard®		Film separator. 22 mm diameter discs should be cut from the film
High precision cutting pliers	EL Cell		1) Used in paragraph 2 for cutting with a fixed 18 mm diameter the bare copper and aluminum foils (non-coated). These current collectors were bought from the same supplier as for the elecrode discs 2) Used

			for cutting 22 mm diameter Cegard separator discs
ECC-PAT-Core (2014 version) kit using: a) reusable stainless steel (SS) upper plunger, b) reusable SS lower plunger of type 50 (size in µm), c) single-use PP insulation sleeves	EL Cell		Electrochemical cell assembly
Maccor Series 4000	Maccor		Battery cycler. It was used to cycle 2 times the electrochemical cell and to adjust afterwards the SOC to 100%
aluminum crucibles with 5 µm laser-pierced lid	Netzsch	6.239.2-64.81.00	Crucible used for the thermal analysis and identification of released gases from cycled electrode material (graphite anode or NMC (111) cathode)
Precision balance AE240 type AE240-S inside Glove box	Mettler Toledo		Battery materials are measured at µg precision
Analogue digital multimeter ABB model MetraWatt M2005	Gossen MetraWatt		Used to measure of the freshly assembled electrochemical cell in paragraph 1.2.6