LIBchallenge
To challenge processes that limit life in Li-ion batteries

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LIB challenge
Goals in a Nutshell

- Develop a high energy density model cell
- Study and understand the ageing effects which limit performance and life
Specific Energy Targets for EV Applications

Strategies to Increase Energy Density

- Increase capacity of cathode material
- Increase capacity of anode material
- Increase cell voltage i.e. increase cathode potential
- Improve electrode and cell design
### The Materials

<table>
<thead>
<tr>
<th>Component</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Anode:</td>
<td>Graphite / Silicon composite&lt;br&gt;Up to 10 wt.% Si&lt;br&gt;From project SiLiCoat</td>
</tr>
<tr>
<td>Cathode:</td>
<td>Ni-rich NMC: 532, 622 or 811&lt;br&gt;Layered oxide Li[Ni(_x)Mn(_y)Co(_z)]O(_2)&lt;br&gt;Optionally coated (e.g. with ZrO(_2), AlO(_x), or AlPO(_4))</td>
</tr>
<tr>
<td>Electrolyte:</td>
<td>Base electrolyte with functional additives for anode and cathode</td>
</tr>
</tbody>
</table>
Ni-Rich NMCs

Layered oxide Li[Ni$_x$Mn$_y$Co$_z$]O$_2$ with Ni $\geq$ 0.5
Ni-Rich NMCs

With increasing Ni content
- the capacity increases
- the cycling stability decreases
- the thermal stability decreases
(for a given cut-off voltage)

3.0 – 4.3 V vs. Li/Li$^+$

Ni-Rich NMCs

"For long-range EVs
NMC622 at 4.35 V
is competing with
NMC811 at 4.2 V"

P. Spurk (Umicore), Graz Battery Days 2016.
Functional Electrolytes

Additives for cathode:
- Fluoroethylene carbonate (FEC),
- Lithium bis(oxalato)borate (LiBOB),
- Trimethylboroxine (TMB),
- Tris(hexafluoro-iso-propyl) phosphate (HFiP)
- Lithium 4,5-dicyano-2-(trifluoromethyl) imidazolide (LiTDI)
- etc.

Additives for anode:
- Fluoroethylene carbonate (FEC)
- VINylene carbonate (VC)
- etc.

**Functional Electrolytes**

**LiTDI as Additive**

Lithium 4,5-dicyano-2-(trifluoromethyl) imidazolide

- Scavenges $\text{H}_2\text{O}$
- Creates protective film on NMC cathode
- Takes part in SEI formation at graphite anode
- Improves cycling stability
- Slows down impedance increase

Electrode Balancing and Cell Manufacture

- Single layer pouch cells with full cell configuration
- With help of LiFeSiZE (Uppsala)
**Electrode Balancing**

**Influence of Unstable Interfaces**

E.g. Protective solid electrolyte interphase at anode / electrolyte interface (SEI)

### Case 1: SEI is fully formed in first cycle and stable afterwards

- **Anode:**
  - Rev. cap. in 1st cycle: 600 mAh/g
  - Coul. eff. in 1st cycle: 80%
  - Coul. eff. in following cycles: 99.5%
  - Capacity loss per cycle: 0.5%

- **Cathode:**
  - Rev. cap. in 1st cycle: 170 mAh/g
  - Coul. eff. in 1st cycle: 80%
  - Coul. eff. in following cycles: 99.95%
  - Capacity loss per cycle: 0.05%

### Case 2: SEI is unstable and needs to be partially reformed in every cycle

- **Anode:**
  - Rev. cap. in 1st cycle: 600 mAh/g
  - Coul. eff. in 1st cycle: 80%
  - Coul. eff. in following cycles: 99.5%
  - Capacity loss per cycle: 0.5%

- **Cathode:**
  - Rev. cap. in 1st cycle: 170 mAh/g
  - Coul. eff. in 1st cycle: 80%
  - Coul. eff. in following cycles: 99.95%
  - Capacity loss per cycle: 0.05%
Ageing Phenomena in Li-Ion Cells

Source: EPG - Oxford
Ageing Studies & 
*Post Mortem* Analysis

- Electrochemical performance at different cycling and storage conditions
- *Operando* XRD and ND studies
- Tear-down and *post mortem* analysis (SEM, XRD, PES, …)
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Thank you for your attention!

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