Lithium-sulphur anode protection through ultra-





Introduction

Development and improvement of different energy storage systems are required due to the growing energy demand from the past 50 years. Among this variety of systems, Lithium-Sulphur (Li-S) started to gain more importance thanks to its multi-electron conversion of sulphur on the cathode, leading to a theoretical capacity of 1672 mAh/g for the cathode, and 3860 mAh/g for the lithium anode (which is over ten times higher than the graphite one (LiC₆, 372 mA h g^{-1}). Unfortunately, Li-S battery presents several drawbacks:

> Dendrite formation can be observed on the anode surface which shortens the lifetime of the battery

The loss of active material caused by the reaction of S with Li+ forming short chains of polysulfides insoluble in the

electrolyte

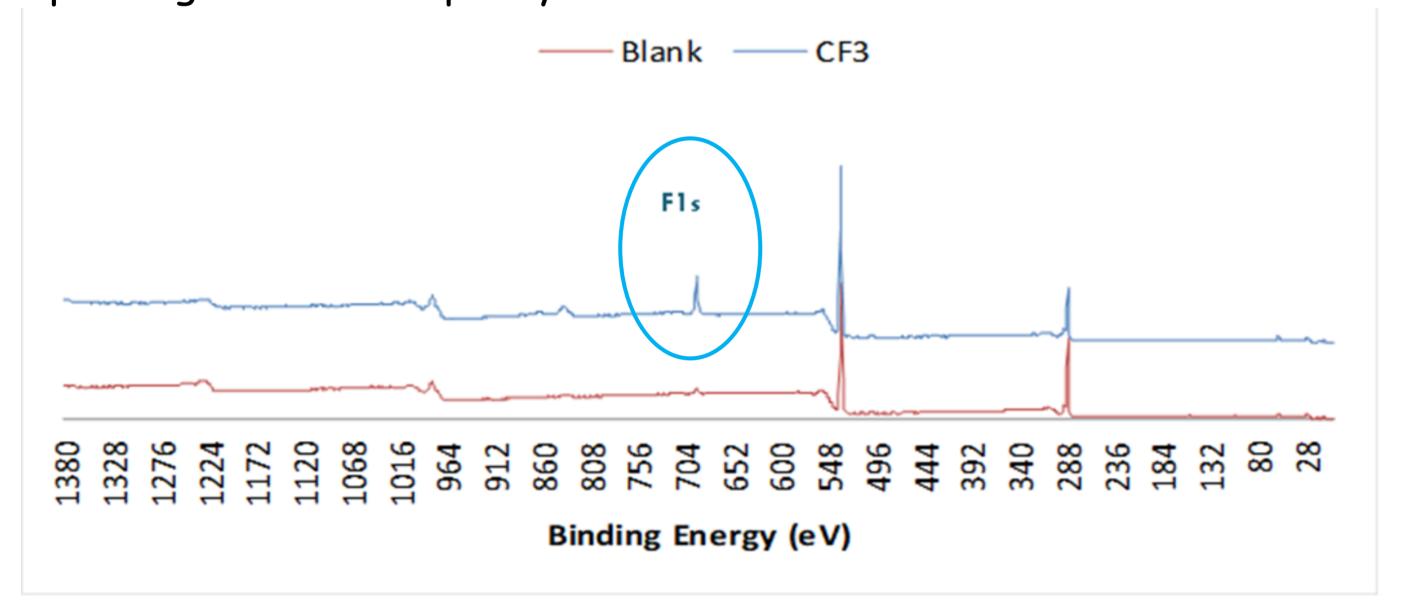
Long-chain polysulfides are formed at the cathode, and shuttle to the anode leading to loss of active material provoking capacity fade

Thermal runaway and cell expansion -> hazard gas evolution (H₂, CH_4 , H_2S , N_2 , NO_2) at (40 °C)

Although so many options can be found in literature, the most promising one corresponds to an organic coating consisting in the stable immobilization (covalent character) on the metallic lithium anode of organic layers, enabling the minimization of the shuttle effect by preventing the diffusion of the polysulfide to the lithium surface (via electrostatic repulsion), and therefore the passivation of the electrode and the parasitic reaction with these anions during discharge.

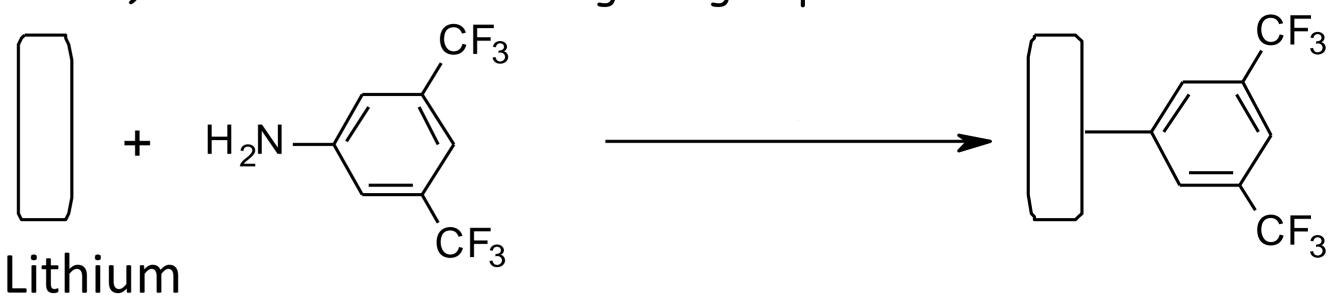
Surface modification

XPS results show, after rinsed with multiple solvents in US, a strong F peak corresponding to the CF3-phenyl functionalized lithium.



How?

Chemically or Electrochemically reduction of aryl diazonium salts, generated in situ, on the lithium surface providing a stable bond (covalent character) with new functional organic groups.



Lifetime, capacity and efficiency improvement in LiS battery CR2016 cells where built with the functionalized lithium and batteries were tested: Cathodic CC Stainless steel spacer C/S Cathode Anodic CC Reference Functionalized Li 90 40 60 120 140 160 180 200 Cycle number 1400 Reference 1200 Reference-cleaned 1000 CF₃-functionalized ٤ capacity 800 600 Discharge 400 200

Conclusions

Through this functionalization on lithium we are able of providing a covalent and stable bond with new functional groups on Li which is able of:

Increase cycle life

Reduce dendrite formation

Reduce drop in coulombic efficiency

Increase discharge capacity

Enhance lithium plating

60

80

120

Cycle number

160

40

Stop PS diffusion 200

180

Next steps

New functionalization groups are being tried Pouch cell system is being built Up-scaling methods are being investigated



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