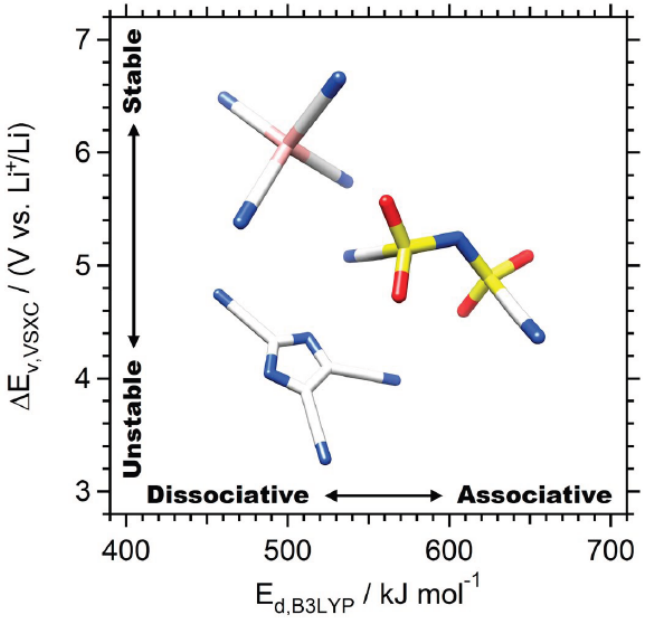
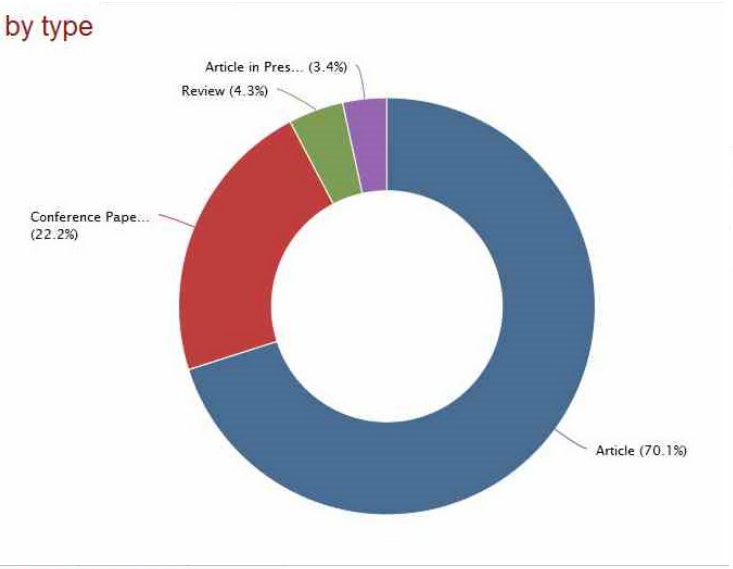
BATTERY (MATERIALS) RESEARCH @ CHALMERS
- FROM FUNDAMENTALS TO SAFETY TESTS

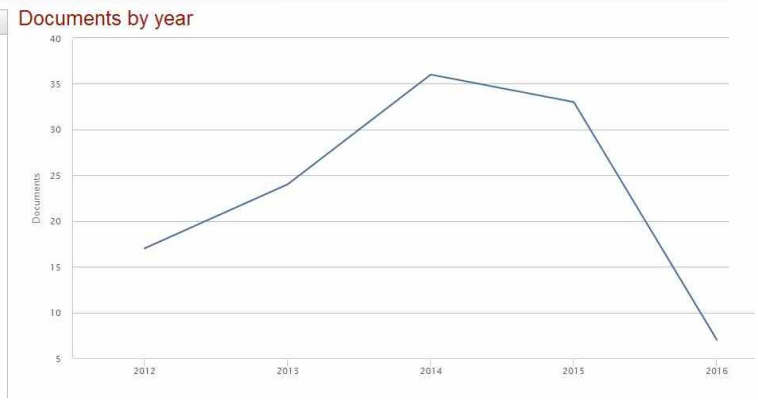


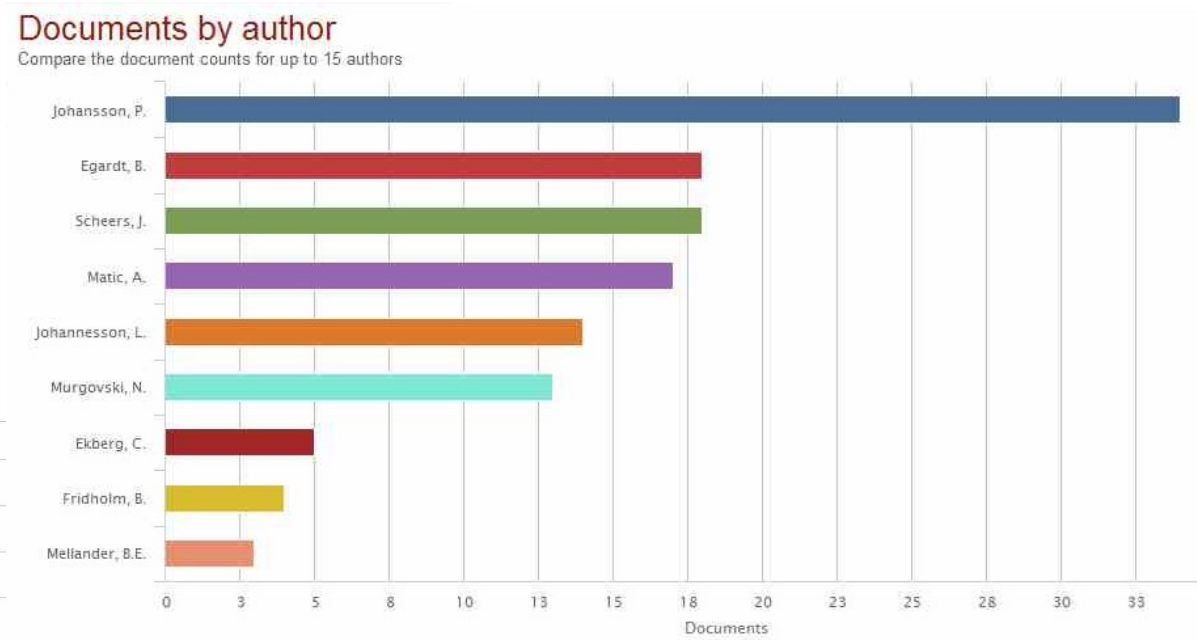
Prof. Patrik Johansson
Physics
Chalmers University of Technology
patrik.johansson@chalmers.se

Who are we – "the battery researchers @ Chalmers"?

Scopus: TITLE-ABS-KEY (battery OR batteries) AND AFFIL (Chalmers) AND PUBYEAR > 2011 => **148 documents => 117 documents**



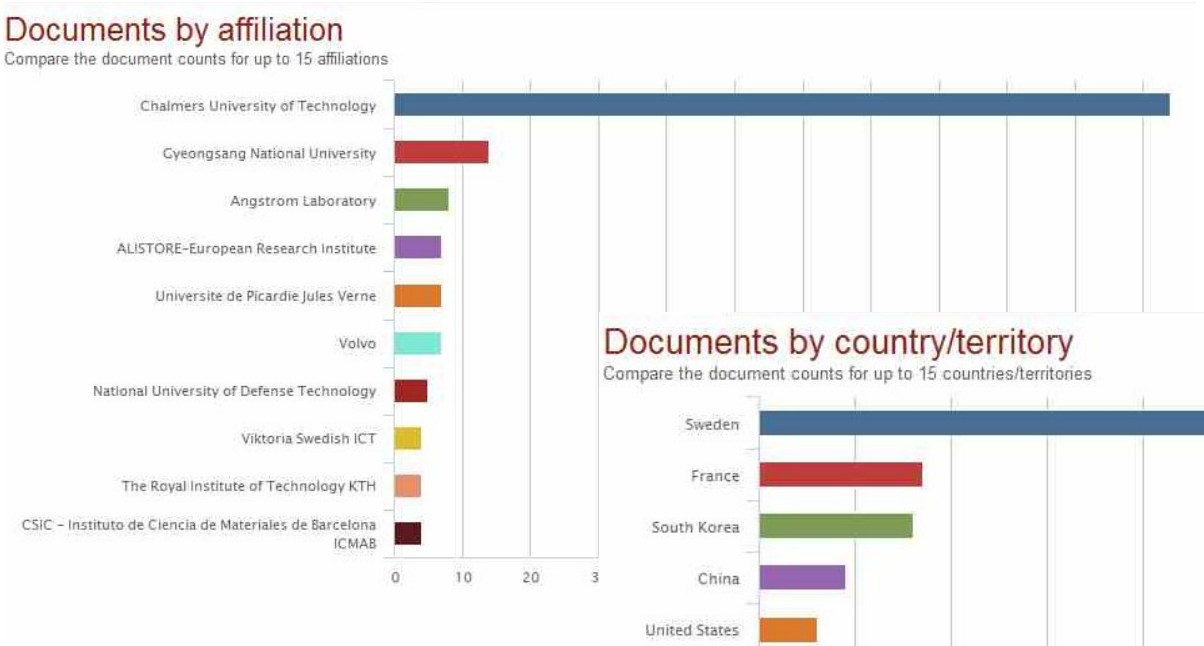


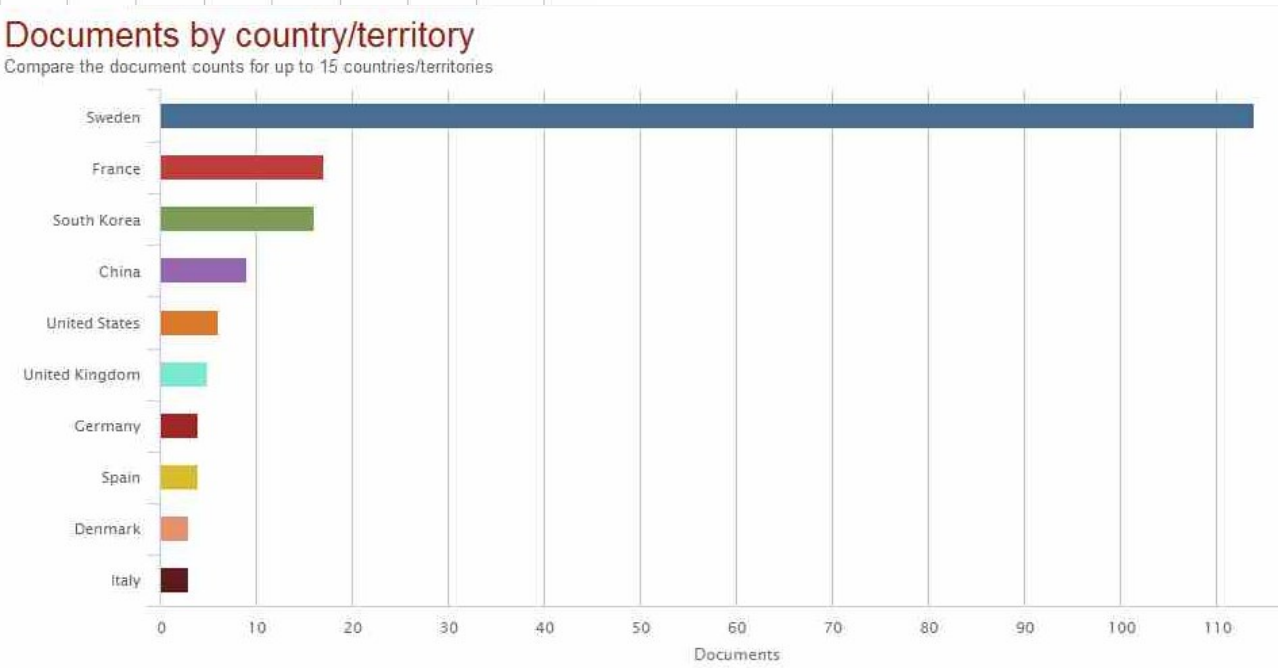


+ *ca.* 50 more

How do we collaborate?

Scopus: TITLE-ABS-KEY (battery OR batteries) AND AFFIL (Chalmers) AND PUBYEAR > 2011 => **148 documents => 117 documents**





CHALMERS
UNIVERSITY OF TECHNOLOGY

Batterifonden @ Chalmers

37671-1	Nästa generation batterier för hybrid- och elfordon	Aleksandar Matic	Chalmers Tekniska Högskola AB, Inst f teknisk Fysik
37684-1	Effektivare insamling av batterier med konsumenterna i fokus	Per EO Berg	Chalmers Tekniska Högskola AB, Inst f Bygg- & miljöteknik
37685-1	Säkrare energilagerlösningar med fluorfria elektrolyter	Patrik Johansson	Chalmers Tekniska Högskola AB, Inst f teknisk Fysik
37711-1	Haverikonsekvensanalys av E-fordonsbatterier	David Sturk	Autoliv Development AB, G42 Battery & EV Safety
37714-1	Hydro och pyrokemisk metallåtervinning från batterier	Christian Ekberg	Chalmers Tekniska Högskola AB, Industriell materialåtervinning / kärnkemi
37718-1	Li-jonbatterier och celler för fordonsapplikationer	Björn Hall	Stena Recycling AB
37722-1	Högtemperaturlitiumbatterier (HT-LiB): Från grundforskning till fordonsimplementering	Patrik Johansson	Chalmers Tekniska Högskola AB, Inst f teknisk Fysik
37725-1	Åldringsmekanismer & hur man förlänger livet på batterier i fordon och stationära applikationer	Theresa Granérus	Volvo Personvagnar AB, Avd 99000 Electric Propulsion System
39042-1	Starkt koncentrerade elektrolyter: Celloptimering och Grunder	Patrik Johansson	Chalmers Tekniska Högskola AB
39045-1	Energi OCH Effekt: Hybridsuperkondensatorer	Patrik Johansson	Chalmers Tekniska Högskola AB
39063-1	Återvinning av NiCd och alkaliska batterier	Christian Ekberg	Chalmers Tekniska Högskola AB
40474-1	Batterier med hög effektsdensitet genom fasta singeljonledande polymerelektrolyter	Patric Jannasch	Lunds universitet, Kemiska institutionen, CAS
40501-1	Snabbladdning av stora energioptimerade Li-ionceller för elektriska drivlinor	Jens Groot	Volvo Technology AB, Avdelning BF40560
40506-1	Flexibel och effektiv hydrometallurgisk återvinning av Li-jon batterier med olika batterikemier	Martina Petranikova	Chalmers, Kärnkemi / industriell materialåtervinning

37670-1	Utveckling av framtidens batterisystem med hjälp av atomistiska beräkningar	Johan Scheers	Chalmers Tekniska Högskola AB, Inst f teknisk Fysik	Bifall utanför progr.
37712-1	Strukturella kompositbatterier för energieffektiva fordon	Göran Lindbergh	Kungliga Tekniska Högskolan, Skolan för kemivetenskap, Tillämpad	Bifall utanför progr.
37724-1	Systemanalys och hydrometallurgisk teknikutveckling för återvinning av förbrukade NiMH-batterisystem inom fordonsindustrin	Kerstin Forsberg	Kungliga Tekniska Högskolan, Inst f kemiteknik Avd f kemisk apparatteknik	Bifall utanför progr.
39049-1	Förstudie av ny batterisensor för mätning av batteristatus i realtid och "on-board"	Bengt Kasemo	Chalmers Tekniska Högskola AB	Bifall utanför progr.

Condensed Matter Physics

Prof. Patrik Johansson
Prof. Aleksandar Matic
Ass. Prof. Johan Scheers

Technology Platforms

- CMP
- Large Scale Facilities
- Others

Research Projects

- LiB
- SiB
- ILs
- LiS
- Structural Batteries
- *In situ*
- Safety
- *Mg/Ca//Al batteries*

Education

- Energy Related Materials
- SHC Battery Days
- Summer Schools
- PhD Battery Technology Course

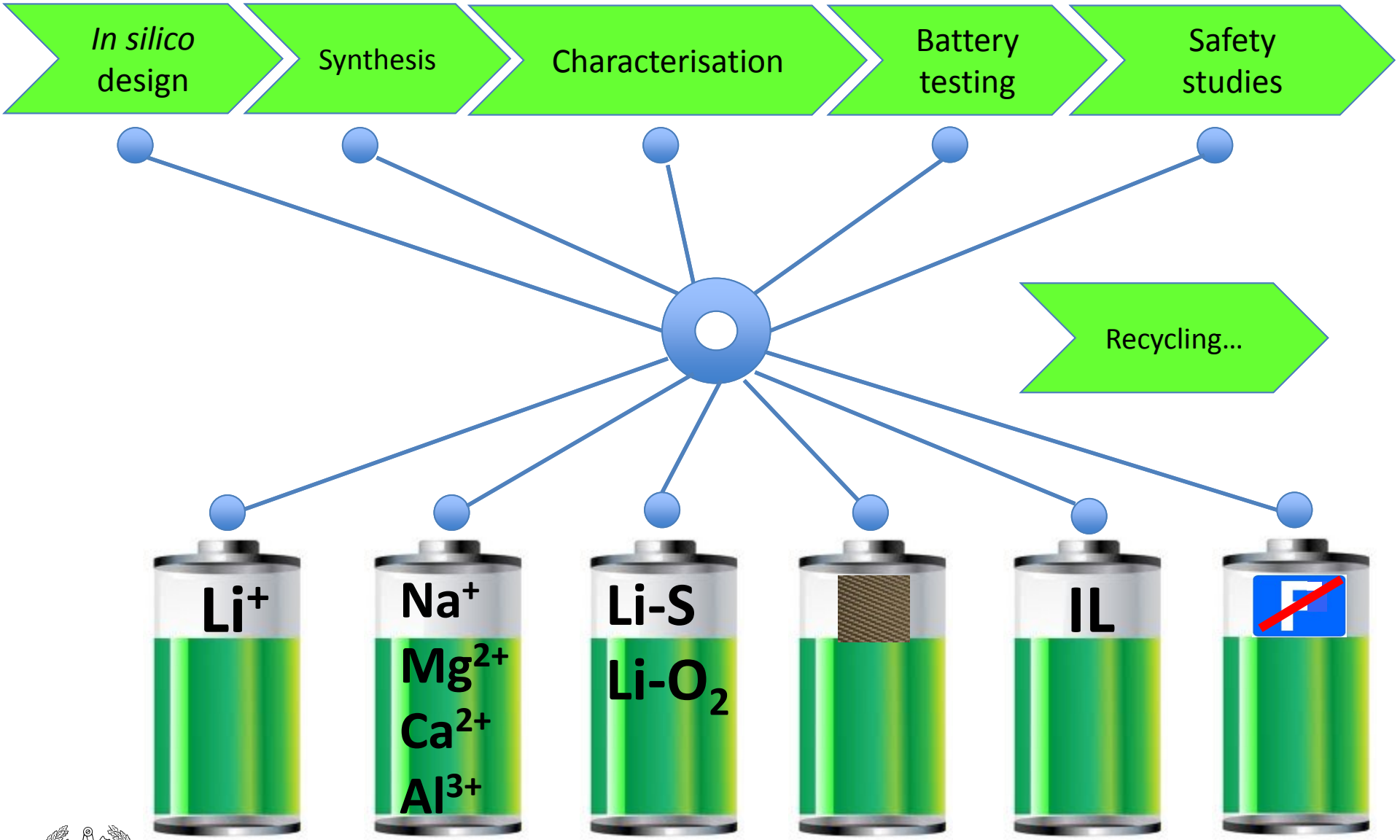
Networks

- Chalmers Areas of Advance
- ALISTORE-ERI
- Swedish Hybrid Vehicle Centre
- H2020/ FP7

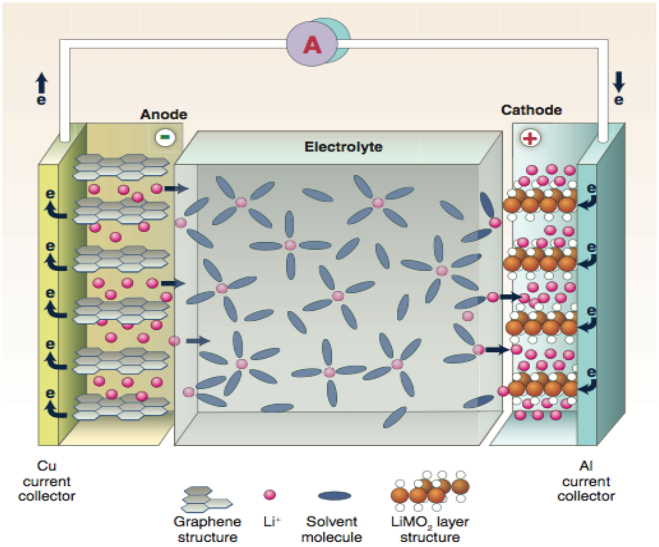
Funding

Vetenskapsrådet
CHALMERS
STINT
Stiftelsen för internationalisering av högre utbildning och forskning
SEVENTH FRAMEWORK PROGRAMME

CMPs' full chain of battery materials research

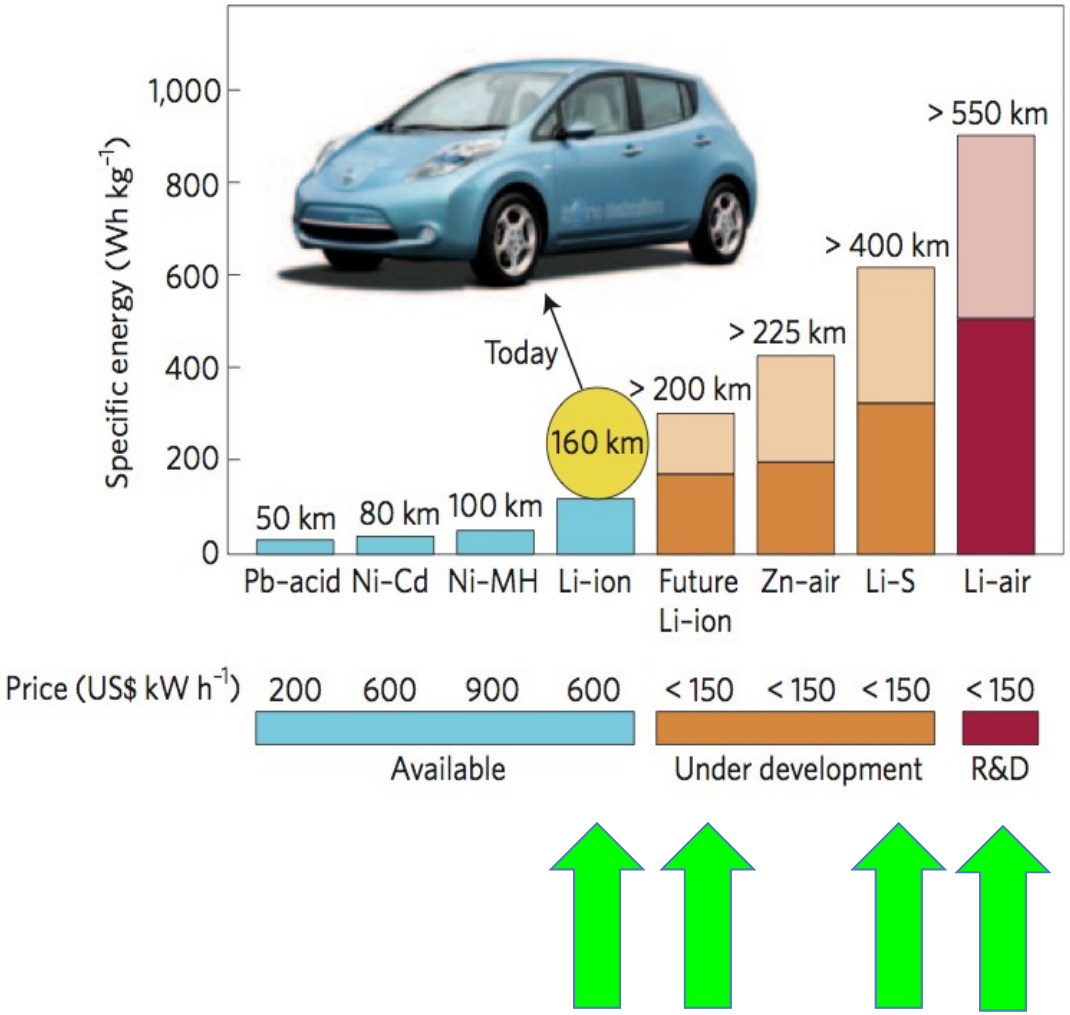


Next generation batteries/battery materials?



$$LiMO_x + C_n \rightleftharpoons Li_{1-y}MO_x + Li_yC_n$$

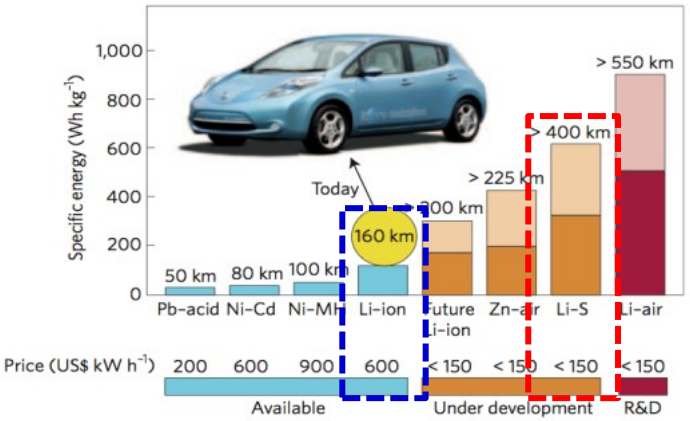
- **High cost!**
  : Co (41,850 US$/ton)
- **Low energy density!**
  : 200 Wh/kg
- **Low safety!**
  : Thermal runaway



Also: Na-ion, Mg, Ca, Al, ….

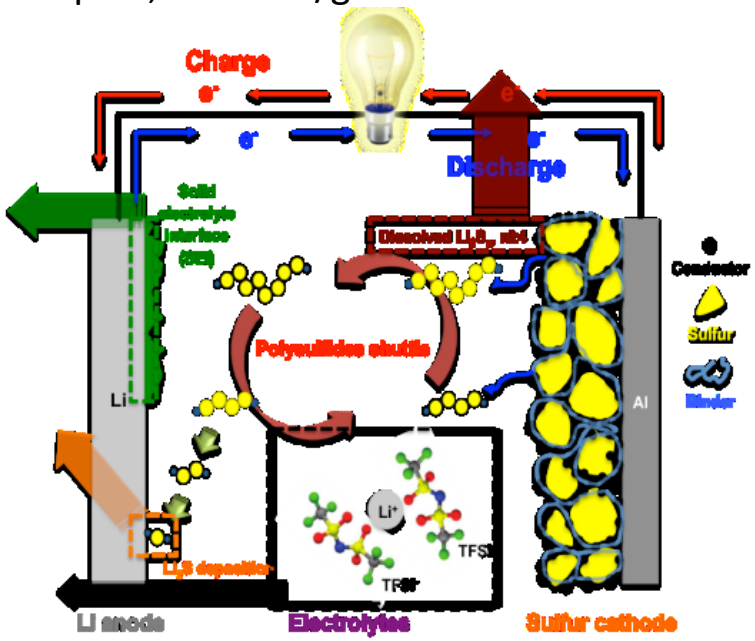
How do we collaborate?

"Success stories": Li-S Batteries



P. G. Bruce et al. Nature materials 11 (2012) 19-29

- Sulphur:
  - 32.06 g/mol & 2.07g/cm^3
  - Non-toxic, "green" material
  - Abundant, cheap (28 US$/ton)
  - Theor. Cap.: 1,675 mAh/g



Cathode materials for LiB and Li-S

Material	Theoretical Capacity (mAhg^{-1})	Specific Capacity (mAhg^{-1})	Relative Price
$LiCoO_2$	275	130-140	1
Li-NMC	~270	150-160	0.59
Li-NCA	~270	170-180	0.89
$LiMn_2O_4$	148	100-120	0.26
$LiFePO_4$	170	140-150	0.37
S	1675	200-1200	0.006

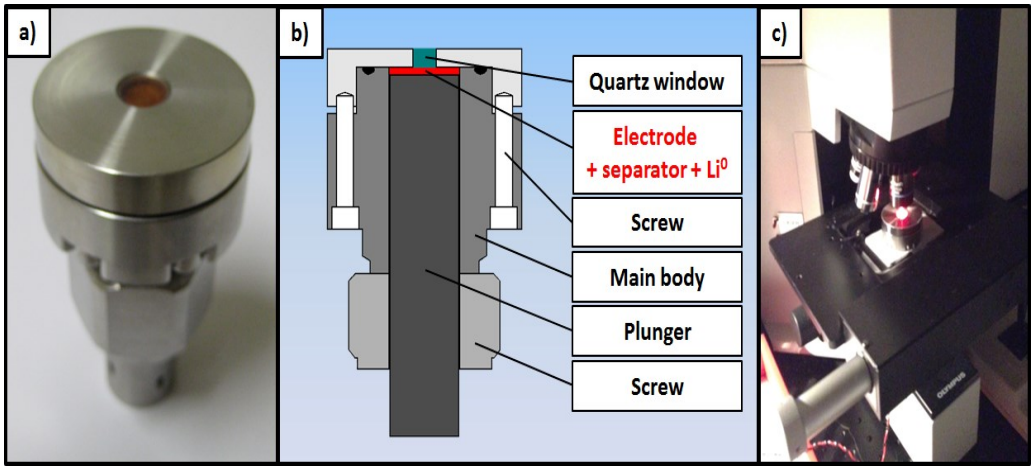
- @ Anode: $2Li \Rightarrow 2Li^+ + 2e^-$
- @ Cathode: $S + 2e^- \Rightarrow S^{2-}$
- Overall: $2Li + S \Rightarrow Li_2S$
- Cell max: 2.15 V

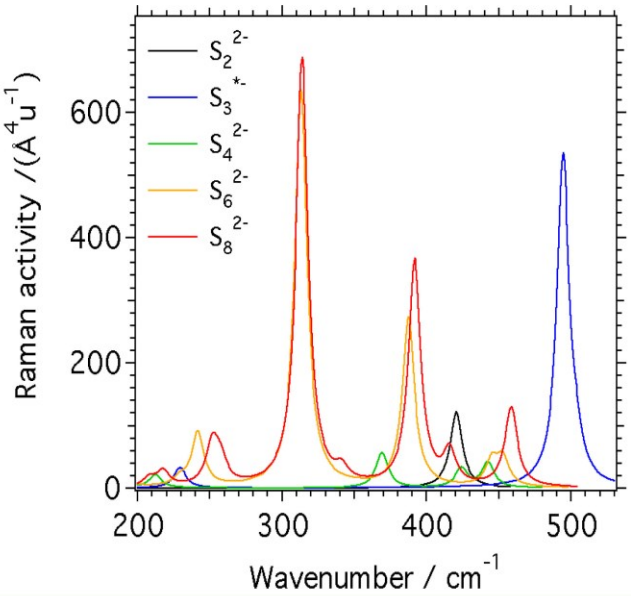
- $Li_{(s)}$: 3,860 mAh/g
- $S_{8(s)}$: 1,675 mAh/g
- => 2567 Wh/kg & 2800 Wh/l
- Today: > 350 Wh/kg (cell)

"Success stories": Li-S Battery Operando Raman

Operando Confocal Raman Spectro-electrochemistry

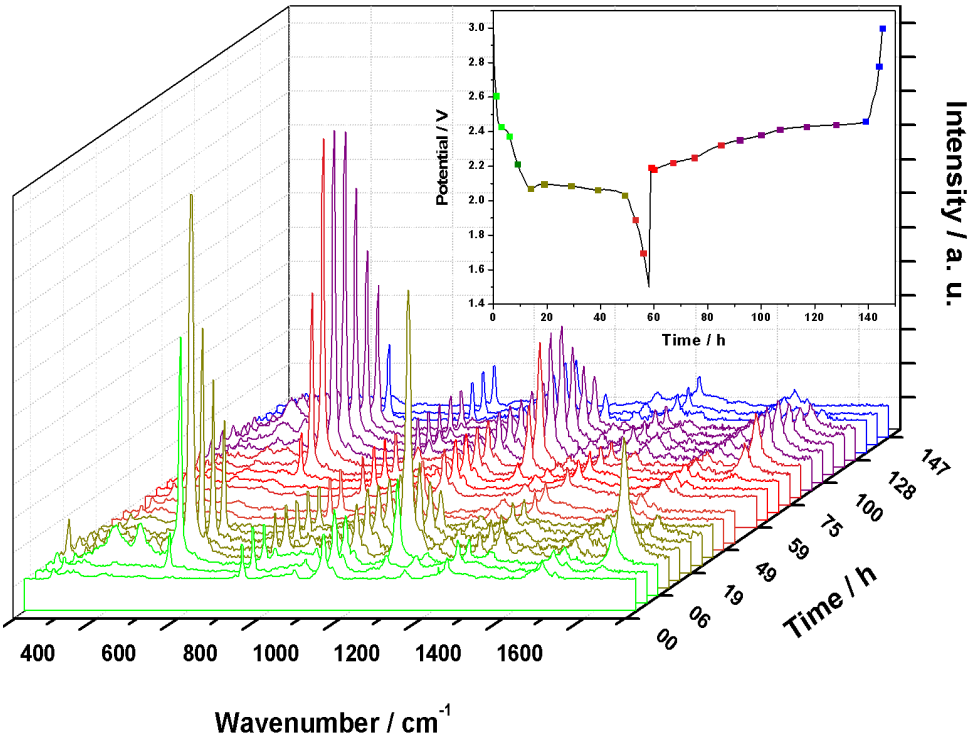
- 1 M LiTFSI in TEGDME:DIOX (1:1)
- Whatman separator
- 60 µL electrolyte/mg_S
- Loading 1 mg_S/cm^2
- 1(!) C/60 charge/discharge cycle
- 4 cm^{-1} resolution, < 10 μm^3 spot
- Spectra collected every 5 min
- PS identification assisted by DFT artificial spectra (B3LYP/6-311G*, PCM ε=15)

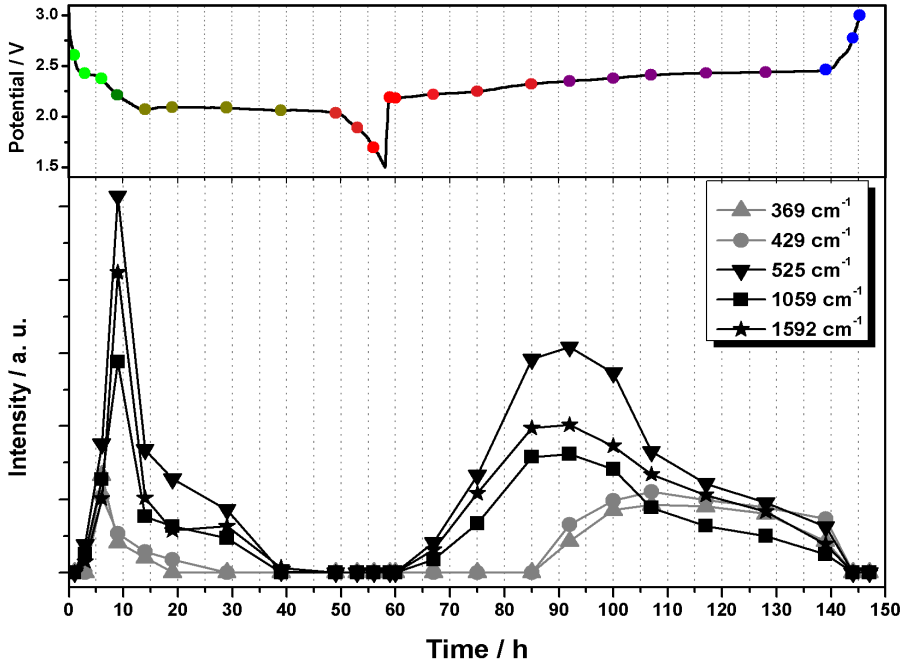




J. Hannauer *et al.*, ChemPhysChem, 2015, 16, 2755-2759.

"Success stories": Li-S Battery Operando Raman





=> Two distinct steps: **1) S_8^{2-} and/or S_6^{2-} *i.e.* "long PS",**
2) Li_2S precipitation & S_3^{*-} radical formation

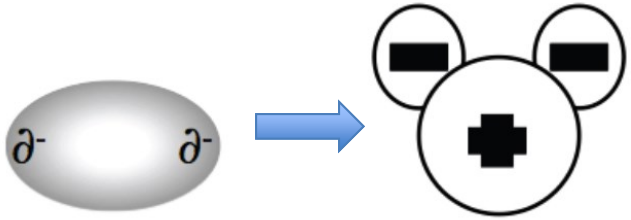
All in several separable bands and nicely reversible

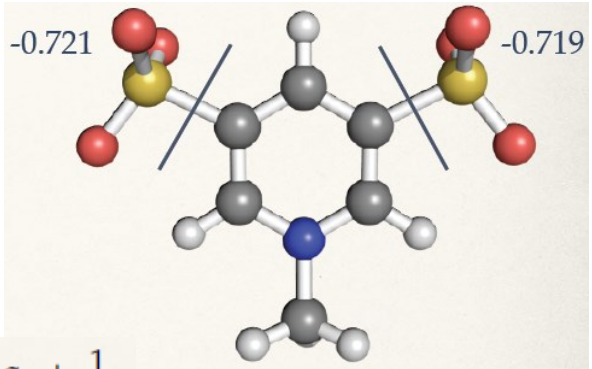
J. Hannauer *et al.*, ChemPhysChem, 2015, 16, 2755-2759.

"Success stories": New Pseudo-delocalized Anions

***In silicio* design of a new type of anions**

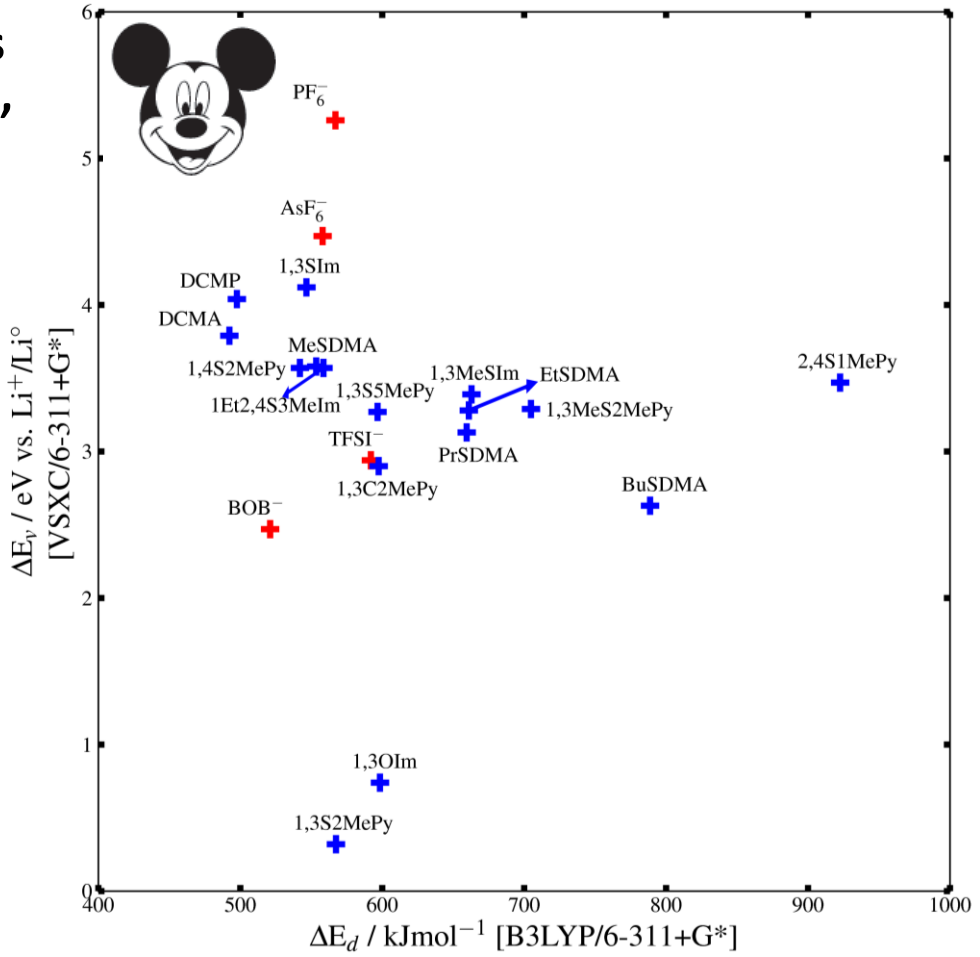
Patented design – "Mickey-Mouse-like"





$$\%_{pd} = \frac{\sum_{i_{cationic}} q_i + \frac{1}{3}}{1\frac{1}{3}}$$

$\%_{pd} = 0.62$



E. Jónsson, M. Armand, P. Johansson PTC /EP2012/072858 (2012)
E. Jónsson, M. Armand, P. Johansson *Phys. Chem. Chem. Phys.* (2012)

"Success stories": Pseudo-delocalized Anions

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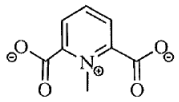
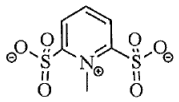
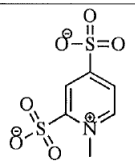
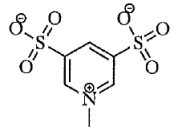
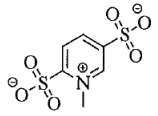
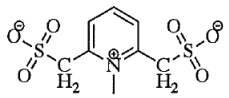
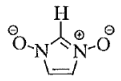
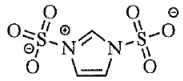
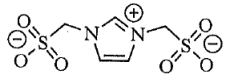
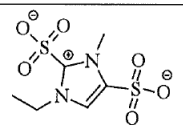
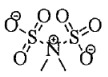
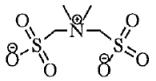
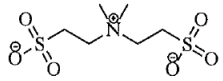
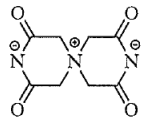
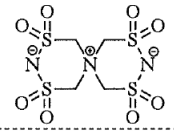
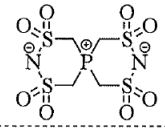
NOTICE OF ALLOWANCE AND FEE(S) DUE

- Cores: -NR_2-, Pyr, Im, Spiro,…
- "Ligands": -CO_2, -SO_3, -O,…
- Chain length & position
- NOW! Synthesis => BF 2014-2017

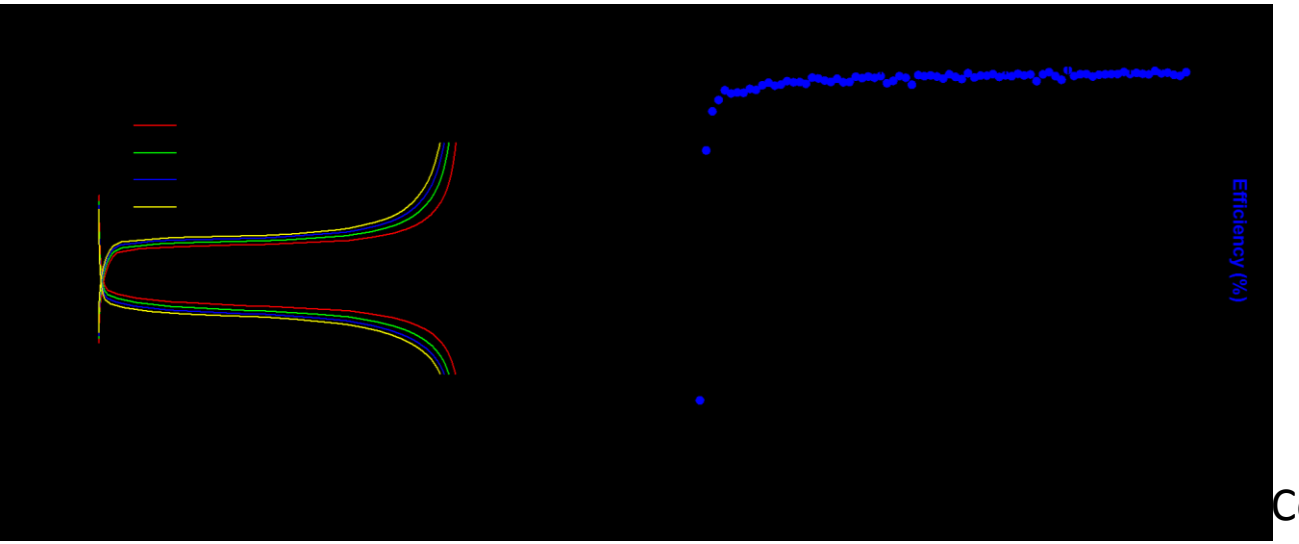
		
2,6-dicarboxy-1-methyl-pyridinium	2,6-disulfonato-1-methyl-pyridinium	1,4-disulfonato-1-methyl-pyridinium
		
3,5-disulfonato-1-methyl-pyridinium	1,5-disulfonato-1-methyl-pyridinium	2,6-bis(sulfonato-methyl)-1-methyl-pyridinium
		
1,3 dioxyimidazolium	1,3 sulfonatoimidazolium	1,3-bis(sulfonato-methyl)-imidazolium

		
1-ethyl-2 methyl-2,4-bis sufonatoimidazolium	bis-sulfonato-dimethyl ammonium	bis(sulfonato-methyl)-dimethyl ammonium
		
bis(sulfonato-2-ethyl)-dimethyl ammonium	spiro-3,5,3'5'tetraoxa-4,4' diaza-bis-piperidinium	spiro-3,5,3',5'tetrathia-4,4' diaza-bis-piperidinium, 3,5,5,5' octaoxide
		
spiro-3,5,3',5'tetrathia-4,4' diaza-bis-piperidinium, 3,5,5,5' octaoxide		

E. Jónsson, M. Armand, P. Johansson PTC /EP2012/072858 (2012)
E. Jónsson, M. Armand, P. Johansson *Phys. Chem. Chem. Phys.* (2012)

"Success stories": HT-LIBs

Goal: Develop new electrolytes, cells, and vehicle design for HT-LIB implementation in hybrid heavy-duty vehicles



Full cell HT-LIB LTO anode & LFP cathode - @80°C!

Cost savings at the vehicle level!

Personell: Dr. Gabriel "Gabi" Oltean, UU => Scania
Dr. Nareerat "Bee" Plylahan, Chalmers => CEVT

"Success stories": Sodium-ion Batteries

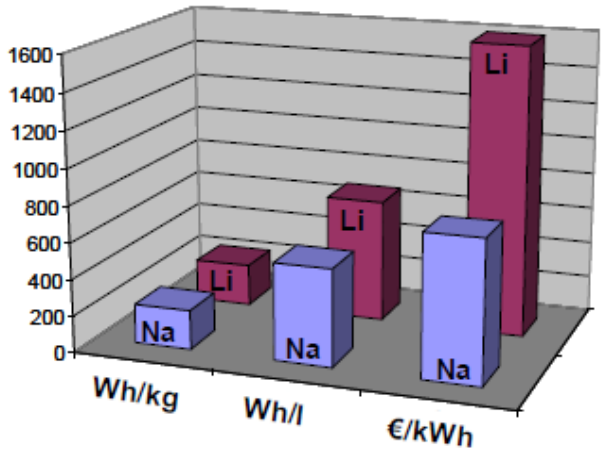
The Problem(s):

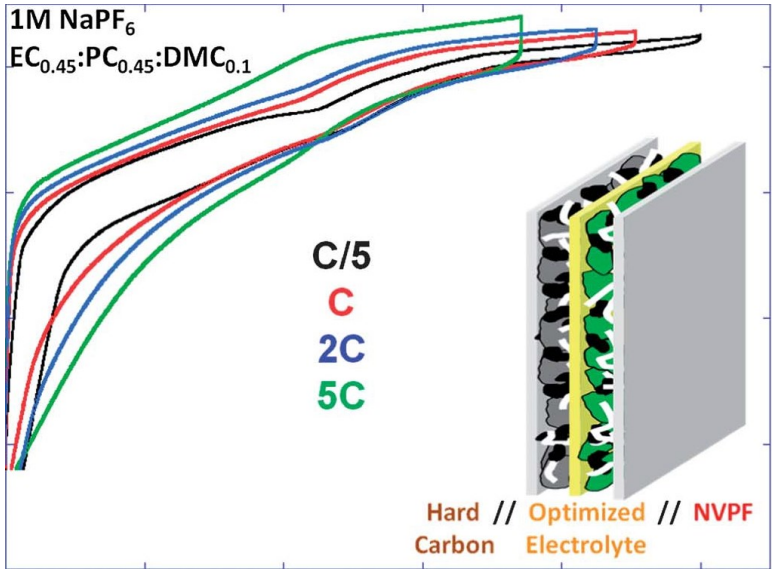
- *Lithium mining is limited & localized*
- *Lithium corrodes Al => Cu curr. collector*
- *For large batteries – Li is expensive*

The Solution(s):

- *Replace Li-ion with Na-ion – use know-how*
- *Cheaper & "predictable"*

	Li	*Na*
El. negativity	-3.04 V	-2.71 V
Price (X_2CO_3)	3.45 $/kg	0.11 $/kg
Earth's crust	20 ppm	23600 ppm
Where?	70% S. Am	"everywhere"
Oceans?	0.18 ppm…	(10800 ppm)
Al corrosion?	Yes	No





A. Ponrouch *et al.*, En. & Env. Sci, 2013, 6, 2361

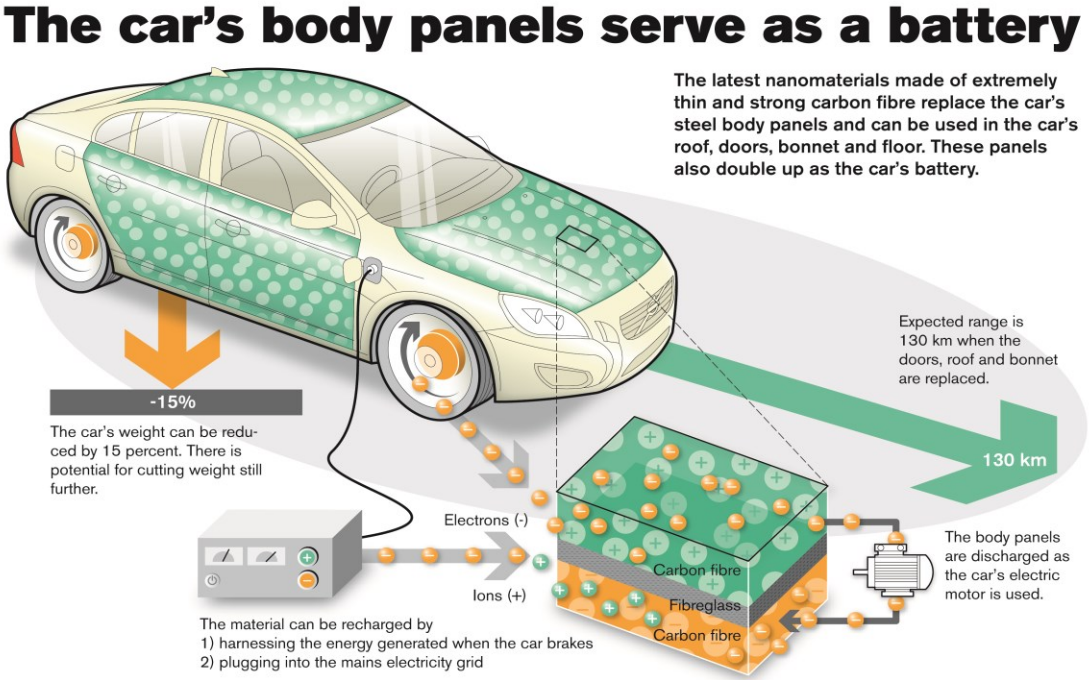
"Success stories": Structural Batteries => KOMBATT II

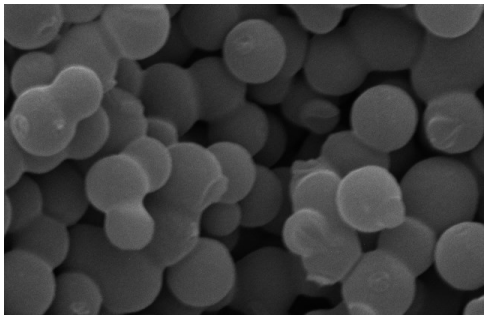
The Problem(s):

- *The storage adds (useless) weight to the car*
- *Safety protection to the battery adds weight*

The Solution(s):

- *Use the storage also for structural load*
- *Safe electrolytes – polymer electrolytes*





http://www.youtube.com/watch?v=RM43llrGbXU&feature=relmfu

"Success stories": Al-batteries

2015 *BASF Open Innovation Contest on Energy Storage* (prize 100.000 €), the only winning team from Europe, focusing on low cost sustainable energy storage solutions.

Acknowledgements

CHALMERS

Areas of Advance

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Materials

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Vetenskapsrådet

HONDA

Thank you!
Questions?