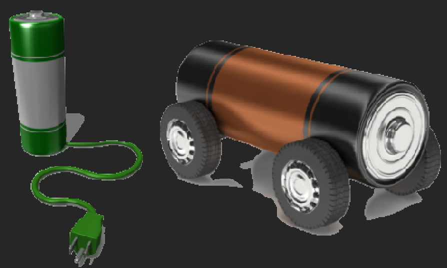
Pregl colloquium
NIC
Ljubljana, Slovenia
December 14, 2016

Mesostructure-performance relationships in batteries: challenging the dogma with multiscale computations

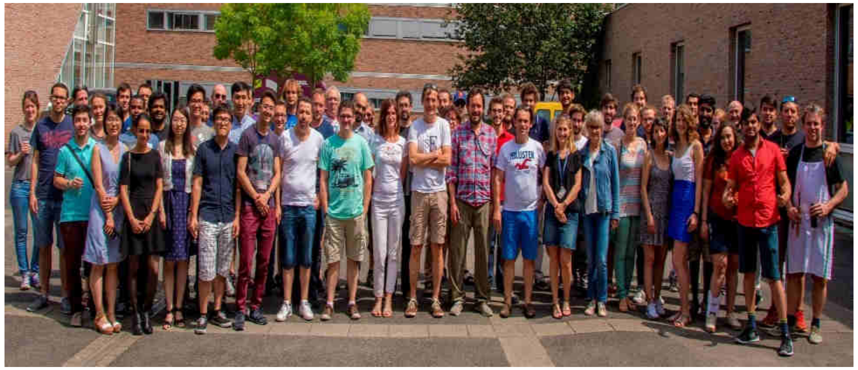


Prof. Alejandro A. Franco[1,2,3,4]

[1]LRCS, Université de Picardie Jules Verne & CNRS – Amiens, France
[2]Réseau sur le Stockage Electrochimique de l'Energie (RS2E)
[3]ALISTORE European Research Institute
[4]Institut Universitaire de France

LABORATOIRE DE REACTIVITE ET CHIMIE DE SOLIDES


New building (rue St. Leu, since 2017)

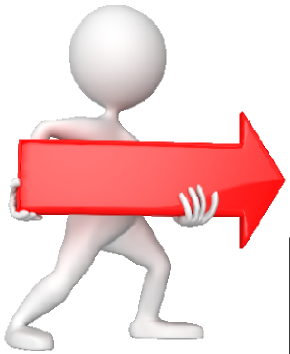


LRCS (UMR UPJV/CNRS 7314) ≅ 80 people
(Director: M. Morcrette)

- ***Electrochemical conversion and storage***
- Solid state materials chemistry
- Nanostructured materials
- Advanced characterization techniques
- Theory

ENERGIE RS2E

ALISTORE European research institute



→ **LRCS** (Prof. J.M. Tarascon): lead the foundation of the national **RS2E** network and of the **ALISTORE** European Research Institute.

LRCS

Prof. Alejandro A. Franco
Mesostructure-performance relationships in batteries…
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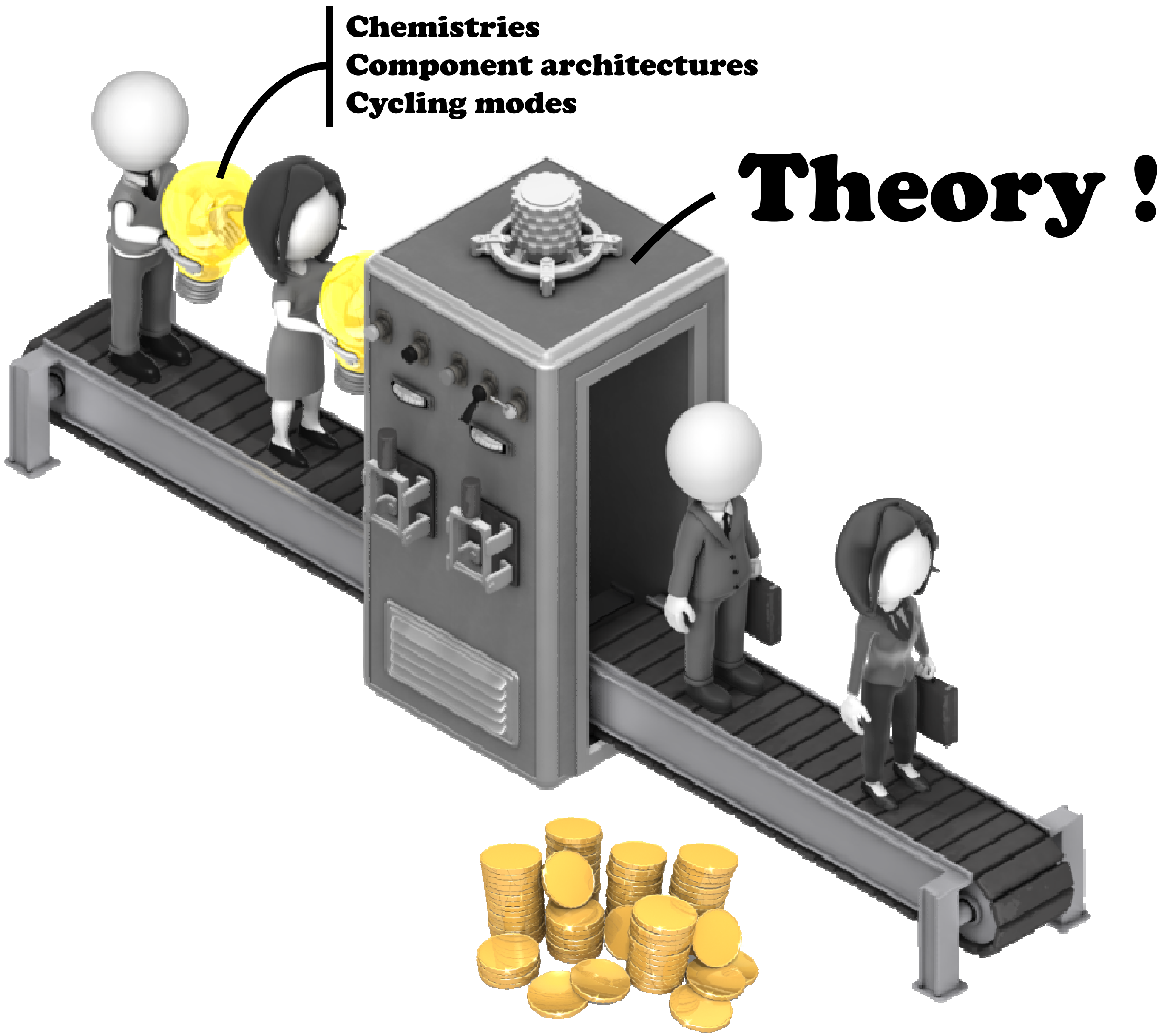
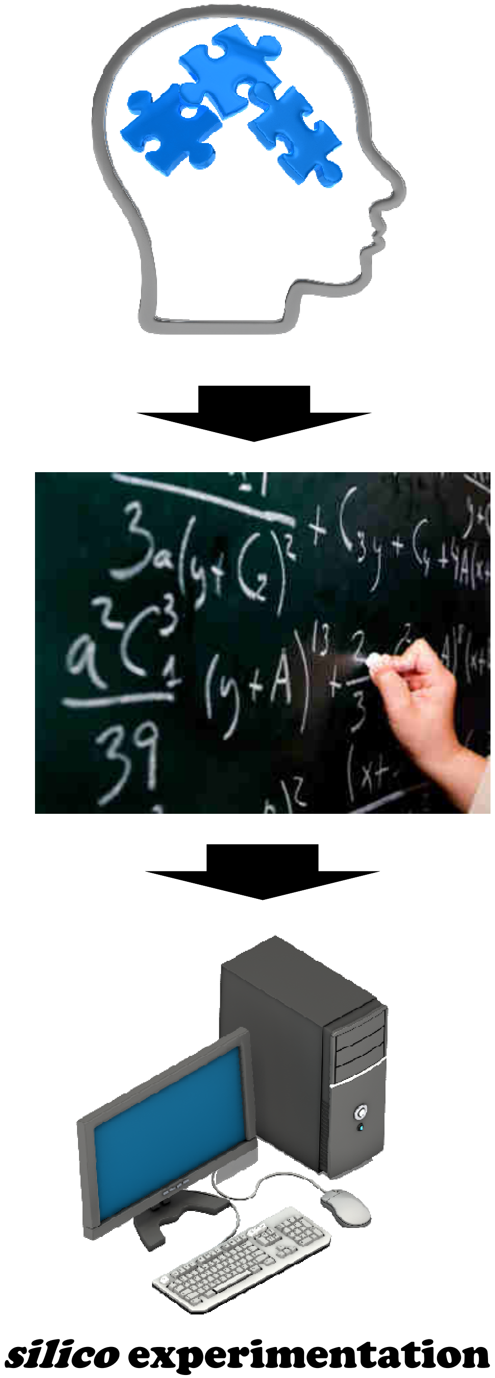
NIC - Ljubljana, Slovenia
December 14, 2016

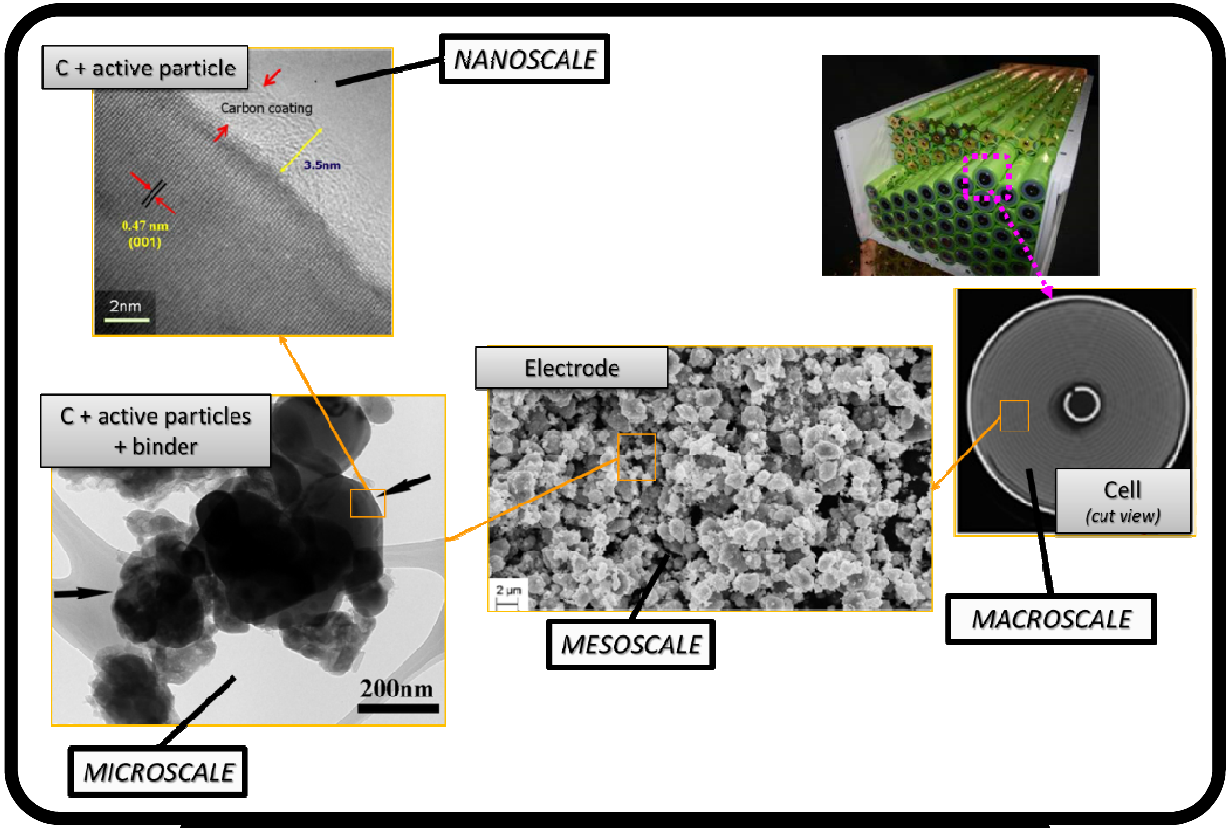
IUF cnrs www.cnrs.fr UNIVERSITÉ de Picardie Jules Verne





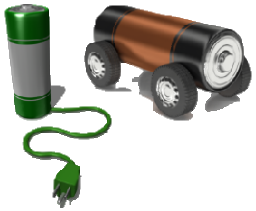
A.A. Franco in: A.A. Franco, M.L. Doublet, W. Bessler, Eds., *Physical Multiscale Modeling and Numerical Simulation of Electrochemical Devices for Energy Conversion and Storage*, Springer London (2016).

MULTISCALE COMPLEXITY IN BATTERIES



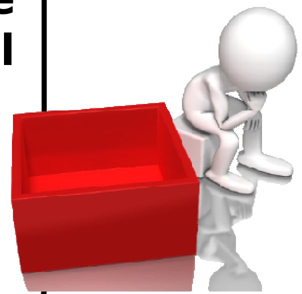
➔ **<u>MULTIPLE</u> MATERIALS & MECHANISMS**

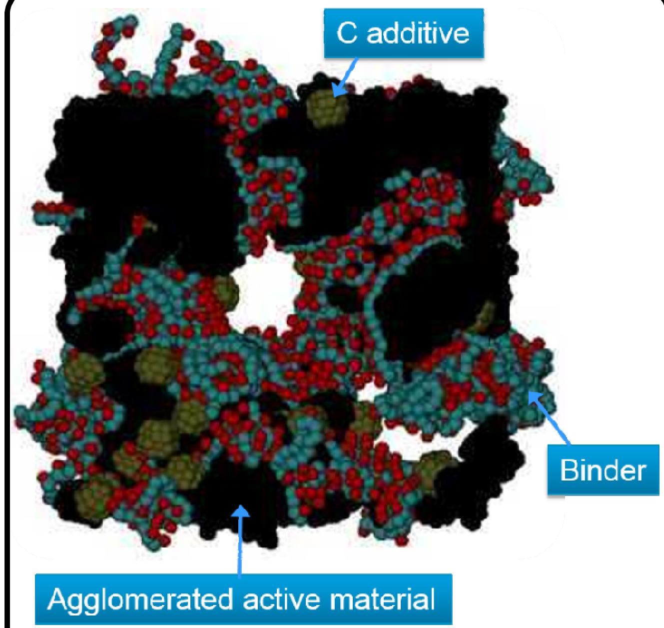
A.A. Franco, *RSC Adv.* **3** (2013) 13027.
A.A. Franco, in: Encyclopedia of Applied Electrochemistry, G. Kreysa, K. Ota, R. F. Savinell (Eds.), Springer, New York (2014).
A.A. Franco, M.L. Doublet, W. Bessler, Eds., *Physical Multiscale Modeling and Numerical Simulation of Electrochemical Devices for Energy Conversion and Storage*, Springer London (2016).



OUR MULTISCALE MODELING PLATFORM

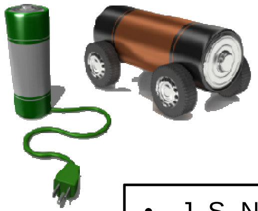
- **Flexible computational platform (adaptable to a wide diversity of systems, e.g. Li-Ion, Na-Ion, Li-Air, Li-S, Fuel Cells, etc.)**
  - ↳ to investigate electrode mesoscale properties impact on cell performance;
  - ↳ to discover optimal compositions, architectures and cycling modes.





Mesoscopic ≈ few μm

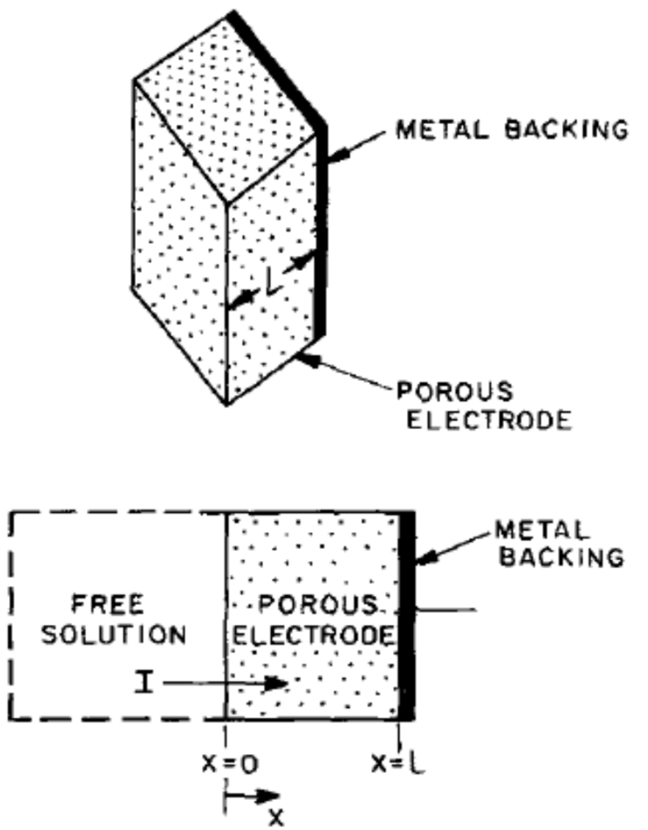
From left to right: R. Zhao, Dr. M. Quiroga, A. Torayev, G. Shukla, Y. Yin, A. Geng, Prof. A..A Franco, M. Maiza, V. Thangavel, R. Andersson, C. Gaya, A. Shodiyev.



STATE-OF-THE-ART MATHEMATICAL MODELING OF RECHARGEABLE BATTERIES

POROUS ELECTRODE THEORY

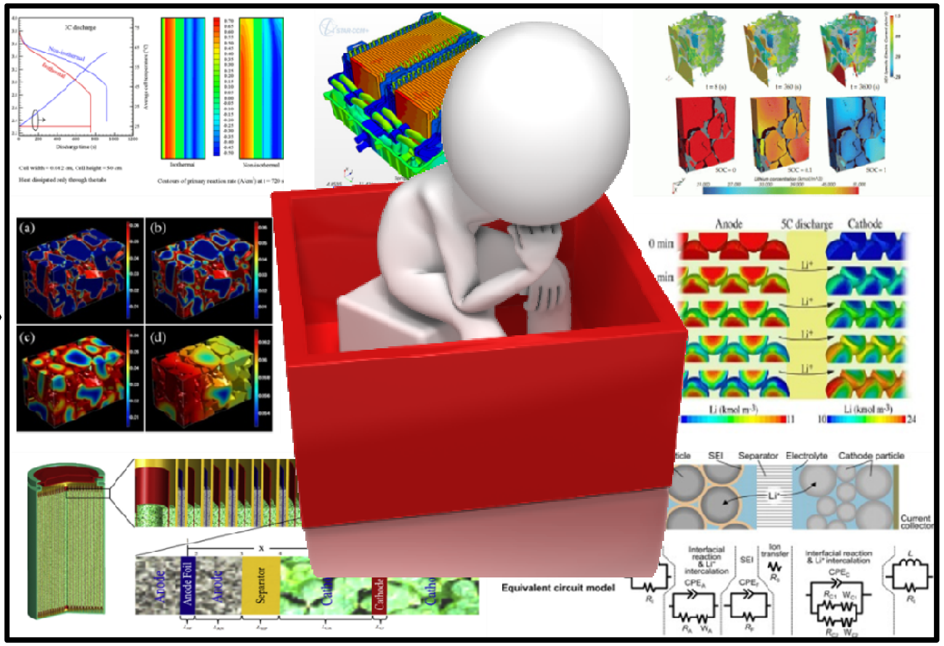
- J. S. Newman, C. W. Tobias, *J. Electrochem. Soc.*, **109** (12) (1962) 1183.
- J. S. Newman, W. Tiedemann, *AIChE Journal*, **21** (1) (1975) 25.



$$\vec{J}_{Li^+}(\vec{x},t) = -D_{Li^+}\nabla C_{Li^+}(\vec{x},t)$$

$$D_{Li^+} = \varepsilon^{\nu} D^{bulk}_{Li^+}$$

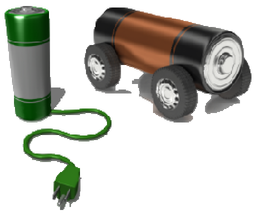
~ 50 years of rechargeable battery models based on Newman's approach…

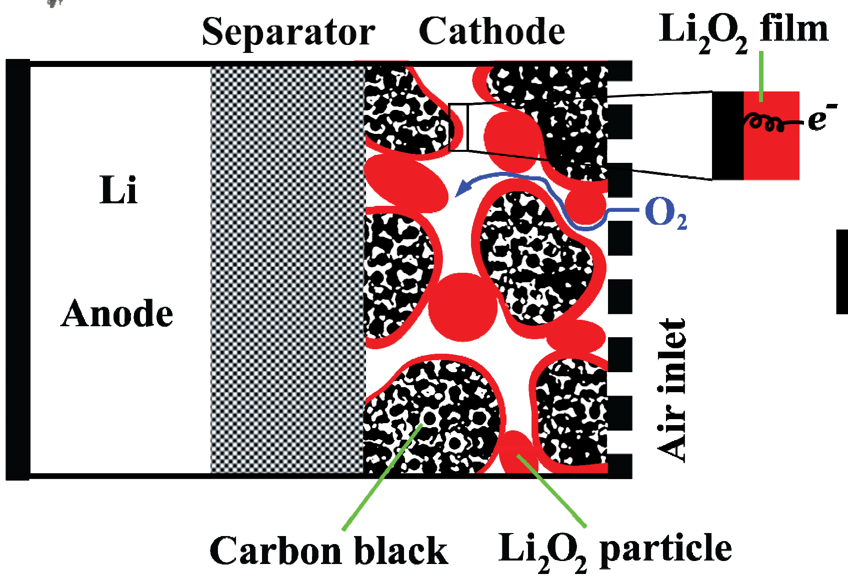


→ Macroscopic description of the porosity and the tortuosity.

1. LITHIUM-O_2 BATTERIES

LITHIUM AIR BATTERIES: PRACTICAL ISSUES

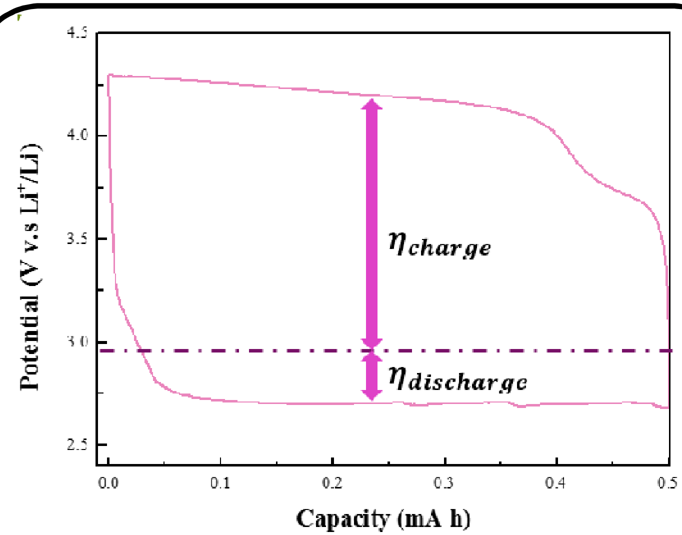




DISCHARGE $O_2 + 2Li^+ + 2e^- \rightarrow Li_2O_2$ (solid)

CHARGE Li_2O_2 (solid) $\rightarrow O_2 + 2Li^+ + 2e^-$

O_2 ? AIR



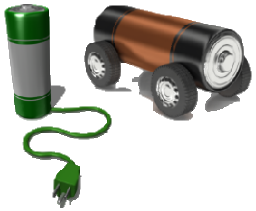
Low Round-trip Efficiency:

$$RTE = \frac{E_{out}}{E_{inp}}$$

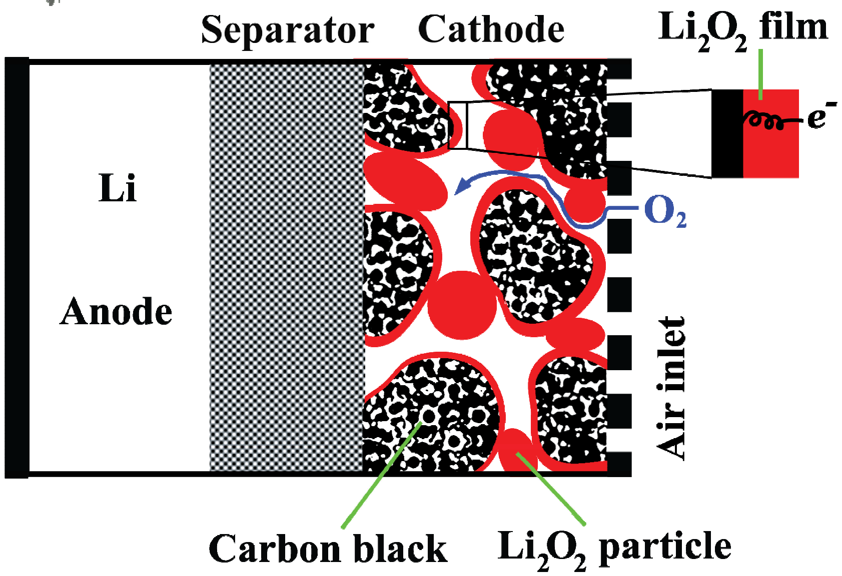
$$E = Q \times U$$

RTE of LAB: <70% (LIB: > 90%)

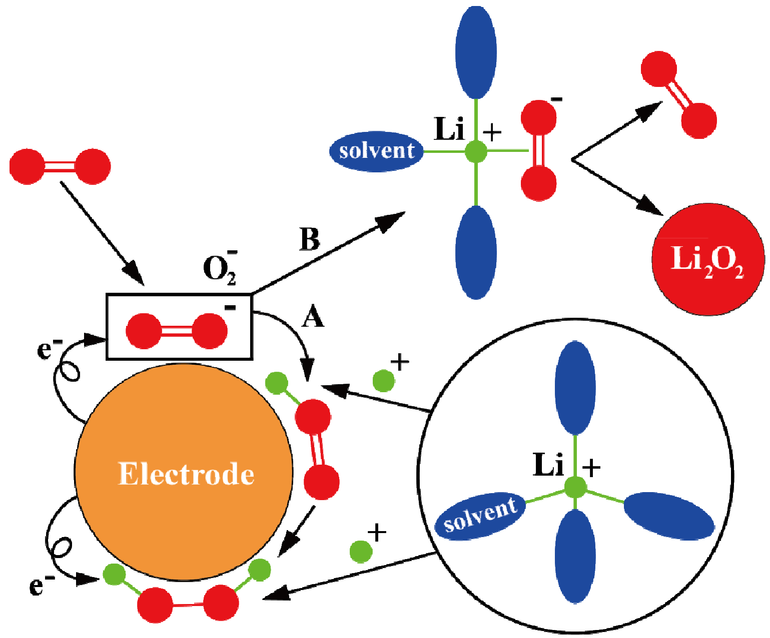
- Electronic transport
- Ionic transport
- Oxygen solubility & diffusivity
- Pore clogging
- Electrode passivation
- Materials degradation



OXYGEN REDUCTION REACTION (ORR) @ LI-O_2 BATTERIES



$$O_2 + 2Li^+ + 2e^- \rightarrow Li_2O_2 \text{ (solid)}$$



Route A: Insulating thin film formation on the active surface

Consequence		
	Decrease of oxygen diffusion coefficient:	Yes
	Comsumption of active surface area:	Yes

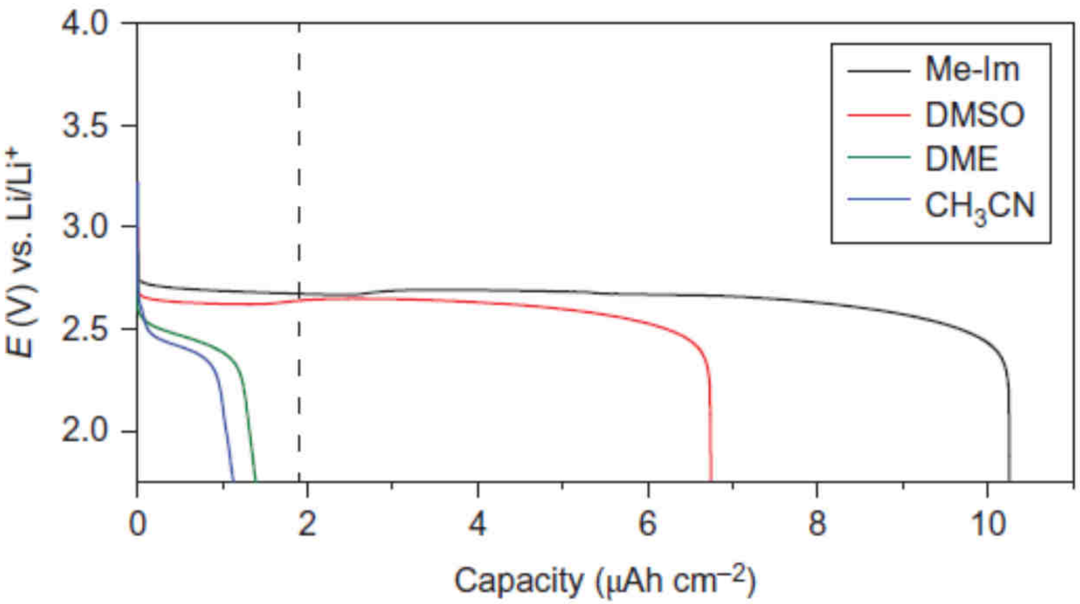
Route B: Solution phase nucleation-growth of Li_2O_2 particles

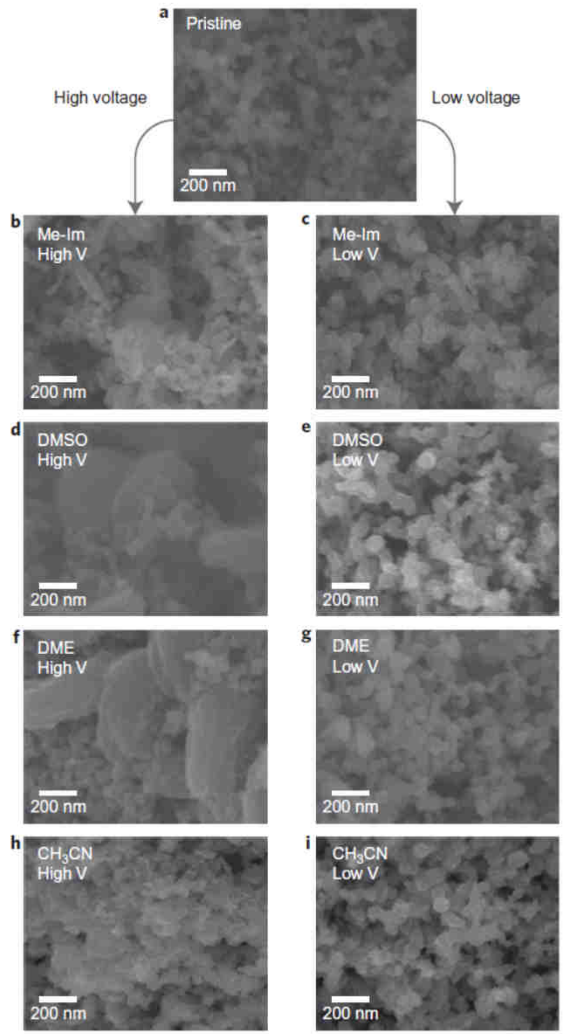
Consequence		
	Decrease of oxygen diffusion coefficient:	Yes
	Comsumption of active surface area:	No

A.A. Franco, K.H. Xue, *ECS J. Solid State Science and Tech.*, **2** (10) (2013) M3084.
L. Johnson, C. Li, Z. Liu, Y. Chen, S. A. Freunberger, P. C. Ashok, B. B. Praveen, K. Dholakia, J.-M. Tarascon, and P. G. Bruce, *Nature Chemistry* **6** (2014) 1091.

SOLUTION PHASE VS. THIN FILM ORR MECHANISMS

➔ Solvent influences the capacity and the Li_2O_2 deposit morphology.

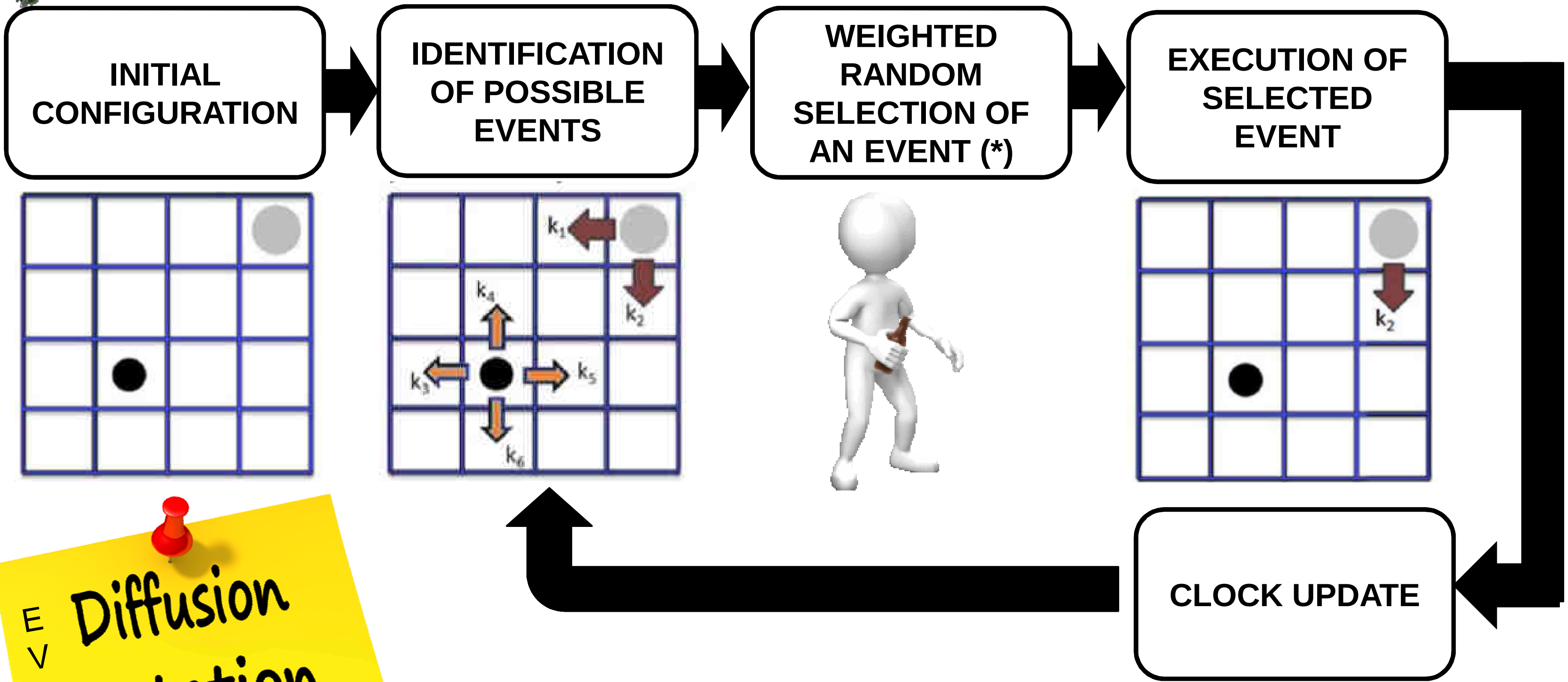


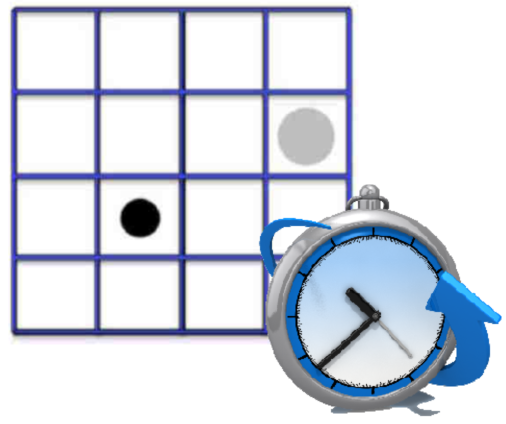


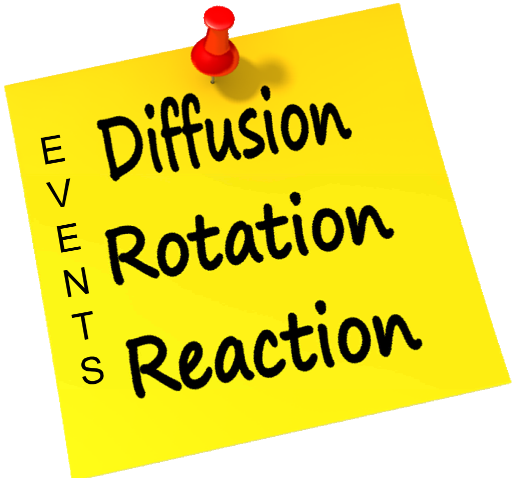
L. Johnson, C. Li, Z. Liu, Y. Chen, S. A. Freunberger, P. C. Ashok, B. B. Praveen, K. Dholakia, J.-M. Tarascon, and P. G. Bruce, *Nature Chemistry* **6** (2014) 1091.


Monte Carlo Electrochemistry
Simulation Software for Innovation
MESSI

KINETIC MONTE CARLO MODEL: LINKING CHEMISTRY WITH REACTIONS & DIFFUSION







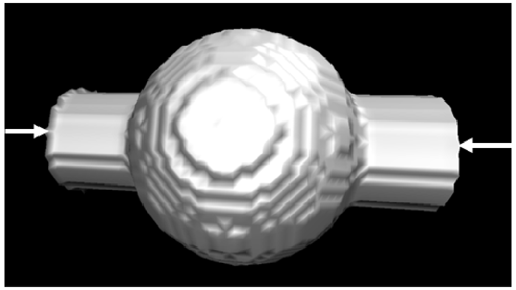
- Typical total simulation time $\approx$ seconds to hours.

(*) Electrochemical Variable Step Size Method
M.A. Quiroga, A.A. Franco, *J. Electrochem. Soc.*, **162** (7) (2015) E73.
M.A. Quiroga, K. Malek, A.A. Franco, *J. Electrochem. Soc.*, **163** (2) (2016) F59.

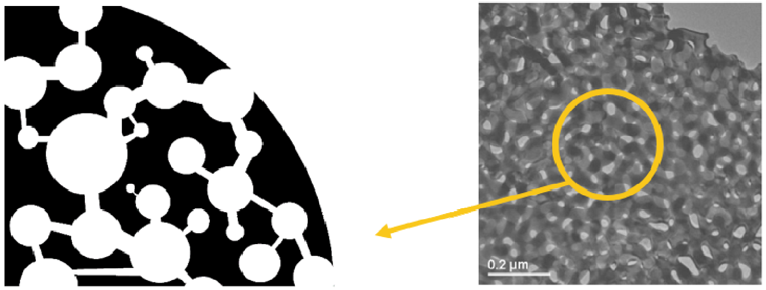
NANOPORE (1/5): KMC MODELING OF THE ORR

GEOMETRICAL CONSIDERATIONS

Pore size: 10-30 nm

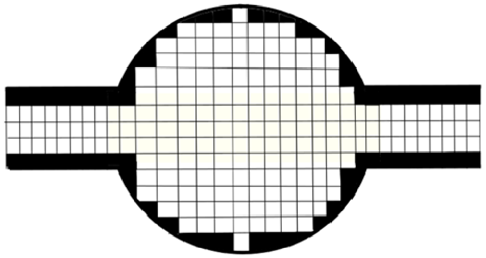


NanoPorous Gold Electrode



Z.Peng *et al.* *Science* **337**, 563–566 (2012)

Grid size: 5 Å



REACTIONS

$$Li^+ + O_{2(sol)} + e^- \xrightarrow{k_1} LiO_2^* \quad (1)$$

$$LiO_2^* \underset{k_{-2}}{\overset{k_2}{\longleftrightarrow}} LiO_{2(sol)} \quad (2)$$

$$LiO_2^* + Li^+ + e^- \xrightarrow{k_3} Li_2O_2^* \quad (3)$$

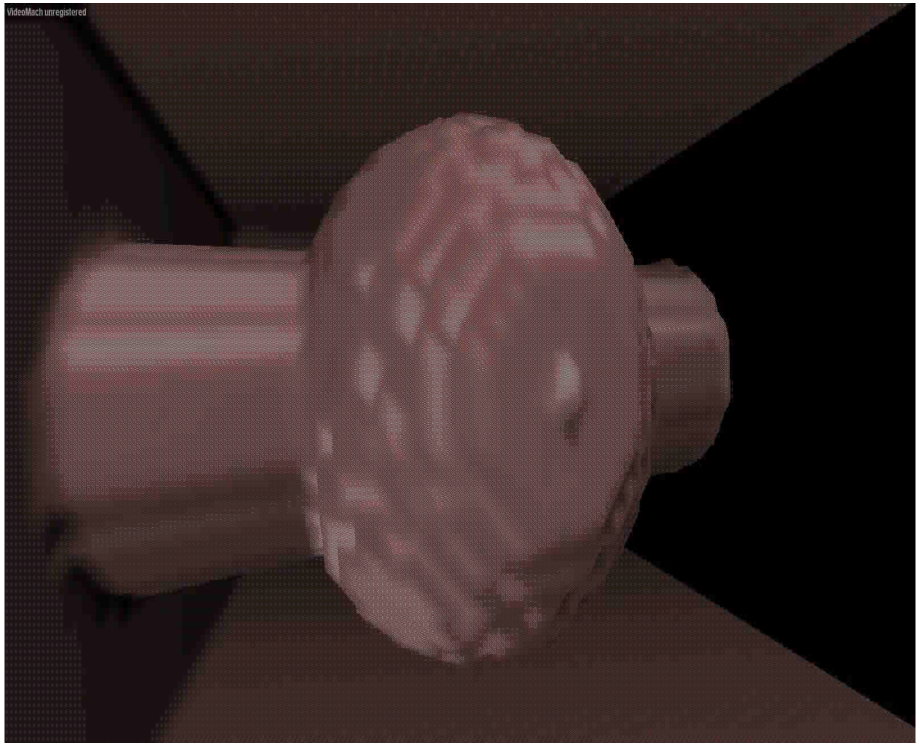
$$LiO_{2(sol)} \xrightarrow{k_4} \frac{1}{2}Li_2O_2 + \frac{1}{2}O_2 \quad (4)$$

G. Blanquer, Y. Yin, M.A. Quiroga, A.A. Franco, *J. Electrochem. Soc*, **163** (3) (2016) A329.

NANOPORE (2/5): KMC MODELING OF THE ORR

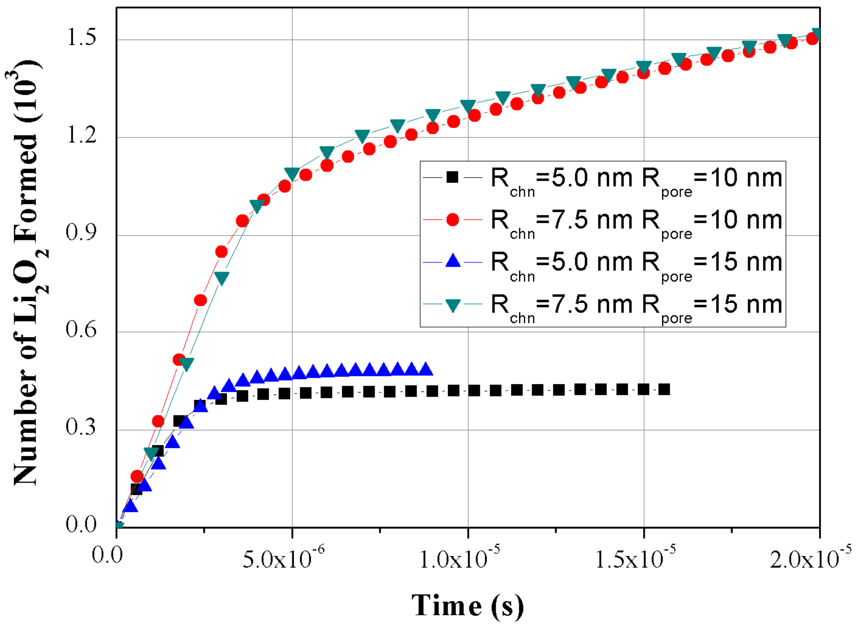
Li^+ and O_2 transport

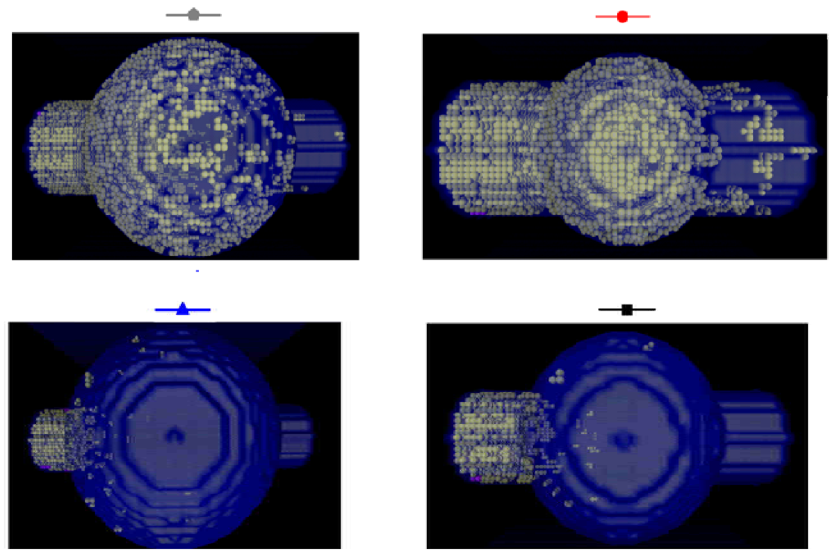
Li_2O_2 formation



G. Blanquer, Y. Yin, M. Quiroga, A.A. Franco, *J. Electrochem. Soc*, **163** (3) (2016) A329.

NANOPORE (3/5): CALCULATED IMPACT OF THE PORE GEOMETRY





Discharge process is limited by channel clogging → **Increase the capacity by enlarging the channel size**

G. Blanquer, Y. Yin, M.A. Quiroga, A.A. Franco, *J. Electrochem. Soc*, **163** (3) (2016) A329.

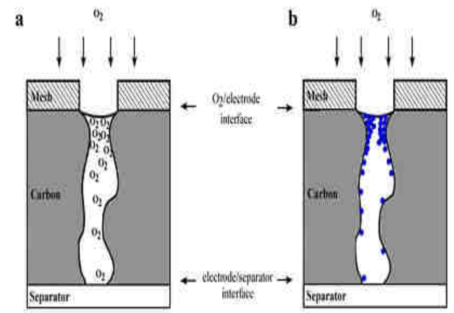
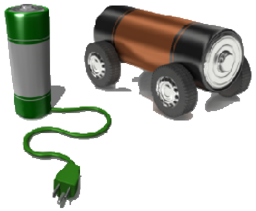
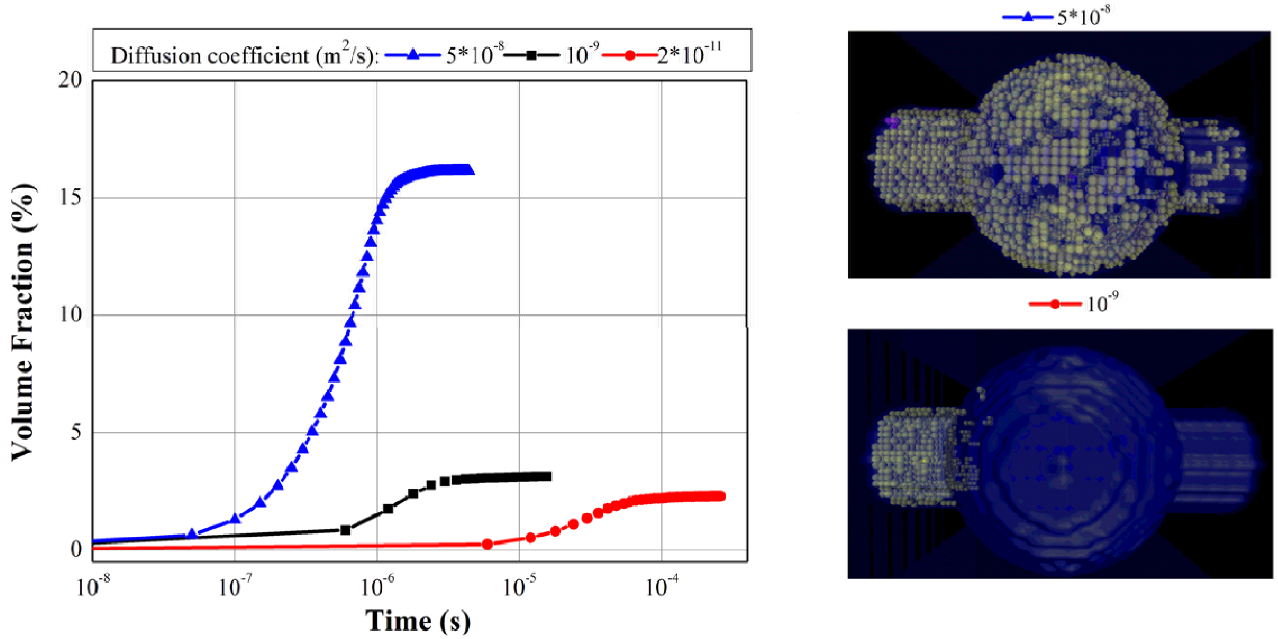


Figure 2. Schematic representation of the oxygen electrode a) before discharge and b) after discharge.

I. Landa-Medrano *et al.*, *J. Electrochem. Soc.*, **162** (2015) A3126.



NANOPORE (4/5): CALCULATED IMPACT OF THE O_2 DIFUSSION COEFFICIENT



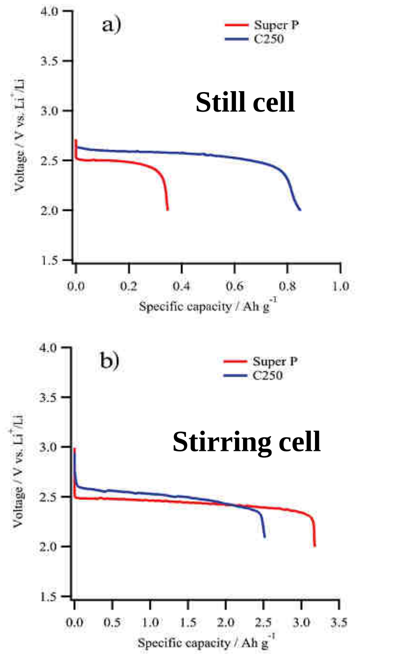


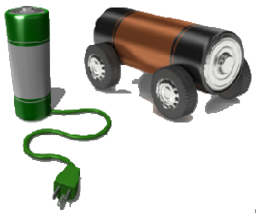
Figure 1. Discharge profiles of Super P and C250 electrodes at 60 °C under a current density of 0.1 mA cm⁻² in a (a) still- and (b) stirred-electrolyte cell.

M. Aklalouch *et al.*, *ChemSusChem*. (2015).

Higher diffusion coefficient
Higher capacity

→ **Decrease viscosity of electrolyte**

G. Blanquer, Y. Yin, M.A. Quiroga, A.A. Franco, *J. Electrochem. Soc*, **163** (3) (2016) A329.

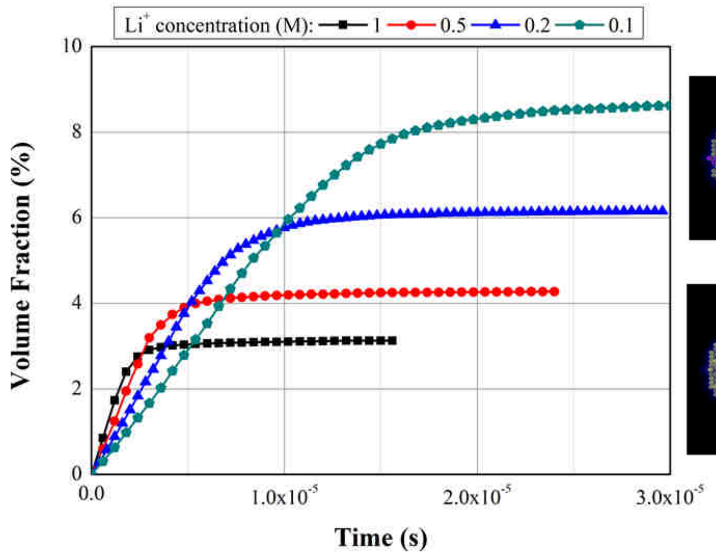


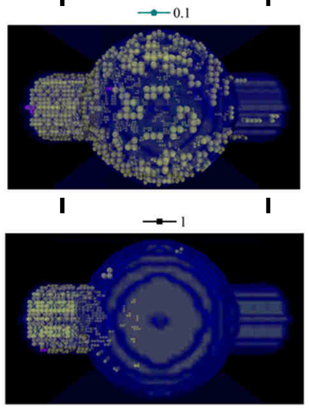
NANOPORE (5/5): IMPACT OF THE SALT CONCENTRATION ON THE ORR IN PORES

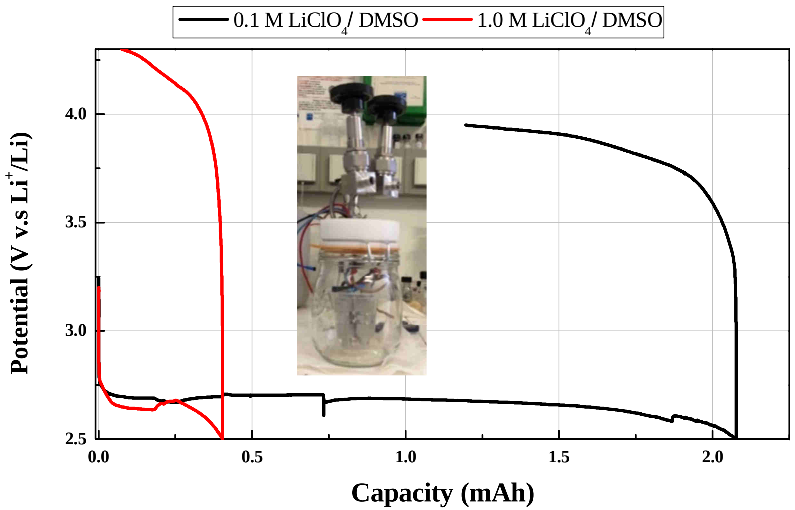
MODELING

Pore size: 10-30 nm

EXPERIMENTS(*)







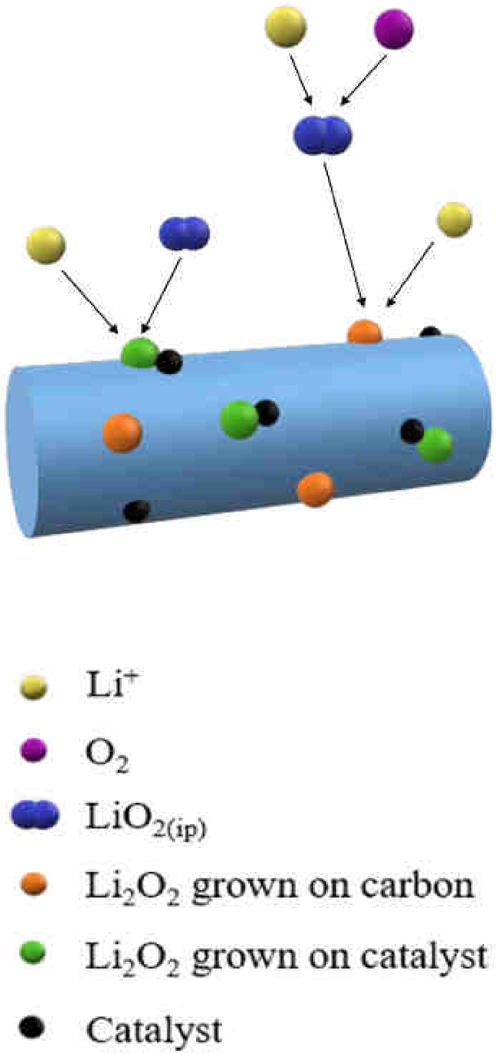
90%C_{sp} + 10% PVdF-HFP – 2.5 mg – 1 bar O_2 – 100 μA/cm^2 – 2.2-4.5 V

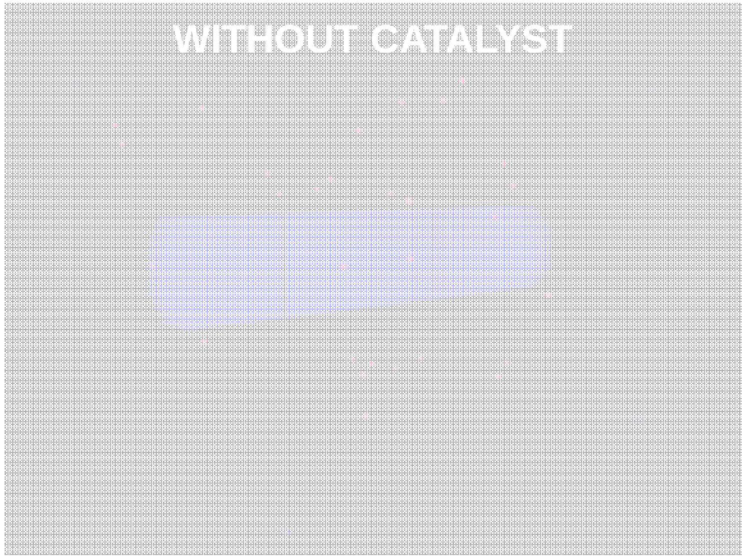
High Li^+ concentration hinders O_2 transport and accelerates pore clogging.

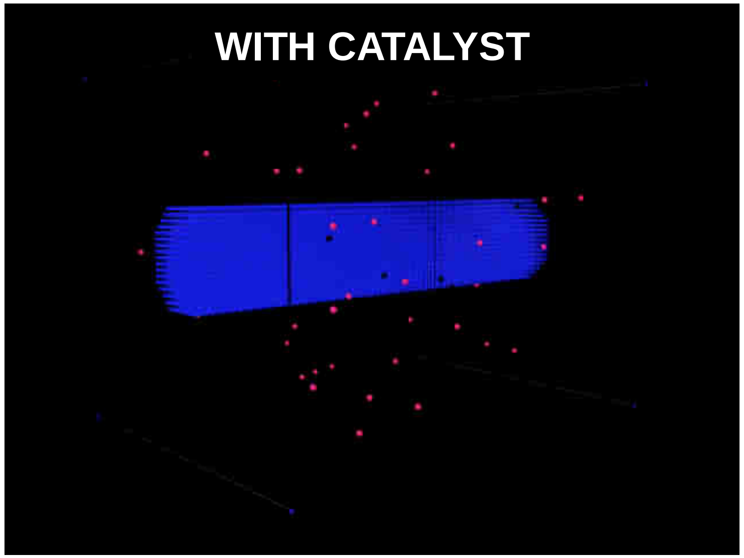
G. Blanquer, Y. Yin, M.A. Quiroga, A.A. Franco, *J. Electrochem. Soc*, **163** (3) (2016) A329.

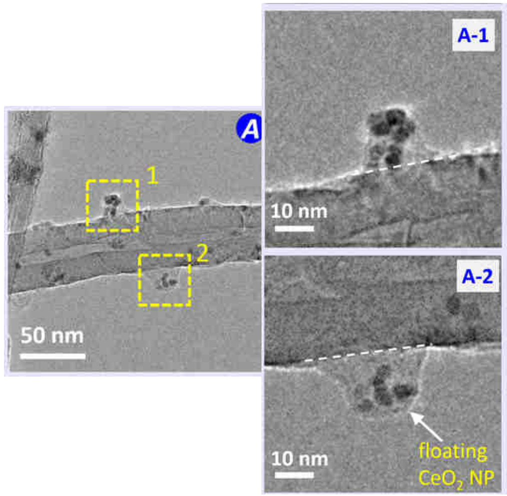
(*) **Unpublished in house data.** Similar trend also reported in J. Read *et al.*, *J. Electrochem. Soc.*, **150** (2003) A1351.

CARBON FIBER (1/2): IMPACT OF CATALYST ON THE OXYGEN REDUCTION REACTION

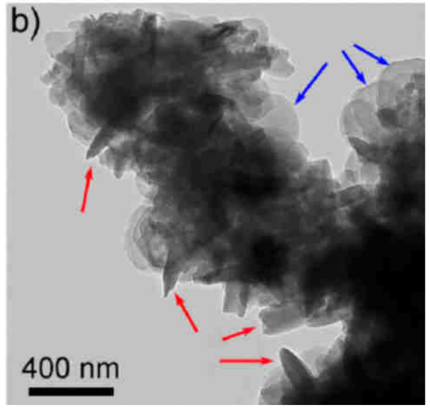








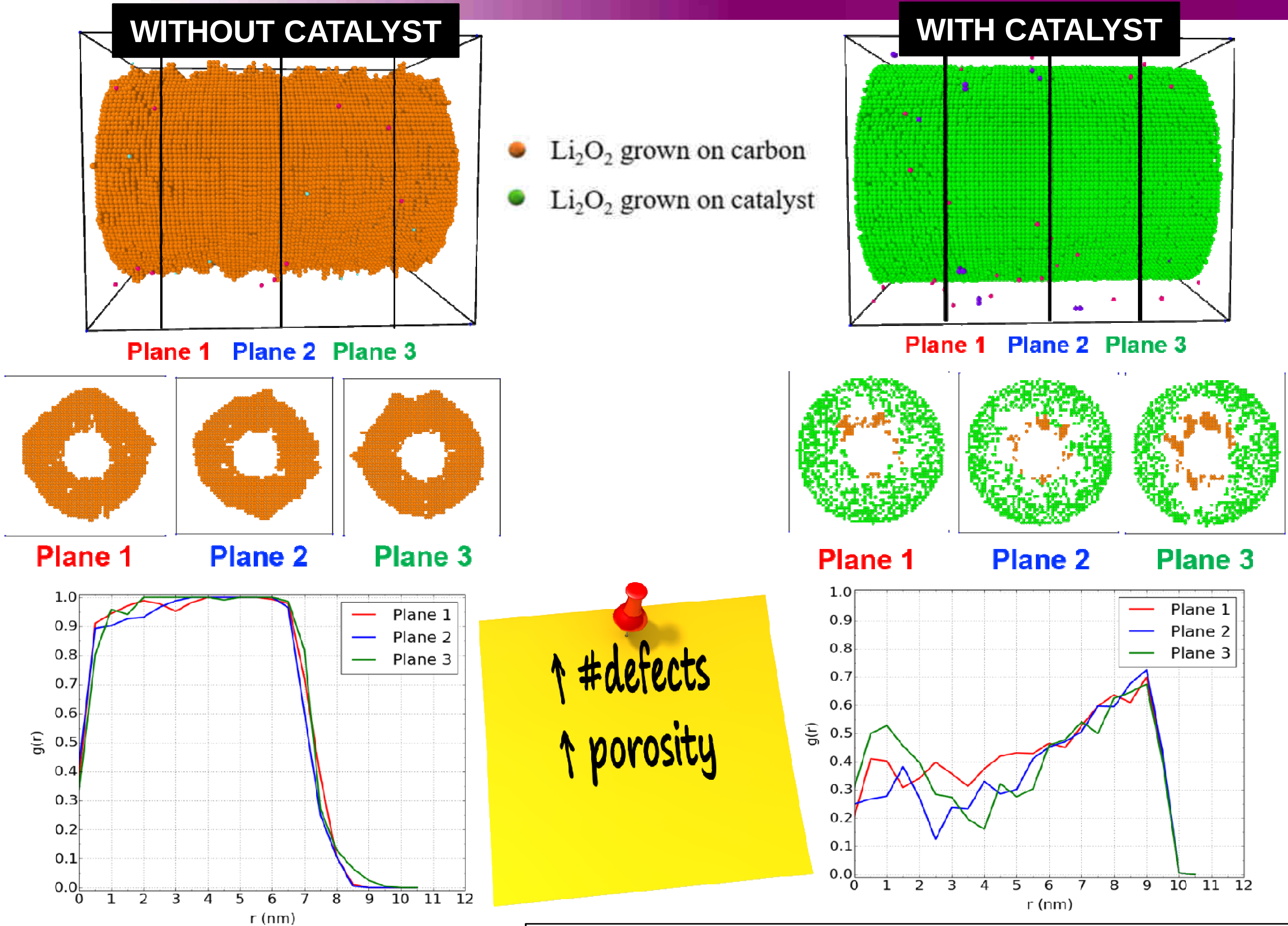
Yang *et al.*, *Nano Lett.*, 16 (2016) 2969.



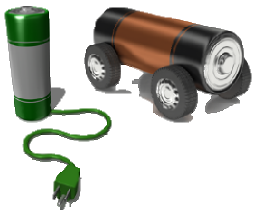
Shui *et al.*, ACS Nano, **8** (2014)' 3015

Y. Yin, R. Zhao, Y. Deng, A.A. Franco, *J. Phys. Chem. Letters*, under revision (2016).
G. Blanquer, Y. Yin, M.A. Quiroga, A.A. Franco, *J. Electrochem. Soc*, **163** (3) (2016) A329.

CARBON FIBER (2/2): IMPACT OF CATALYST ON THE OXYGEN REDUCTION REACTION

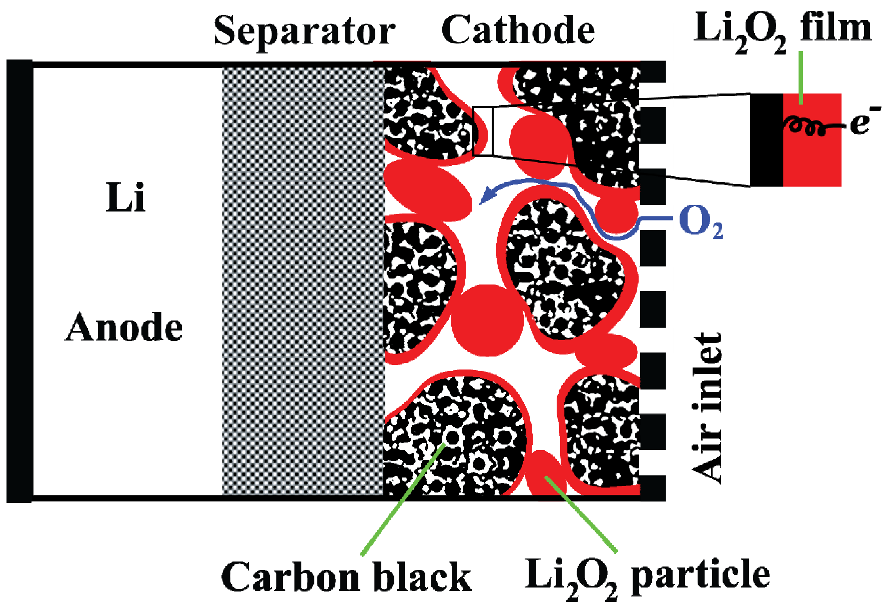


Y. Yin, R. Zhao, Y. Deng, A.A. Franco, *J. Phys. Chem. Letters*, under revision (2016).
G. Blanquer, Y. Yin, M.A. Quiroga, A.A. Franco, *J. Electrochem. Soc*, **163** (3) (2016) A329.



POROUS ELECTRODES IN LITHIUM-O_2 BATTERIES

Lithium O_2 Battery at discharge

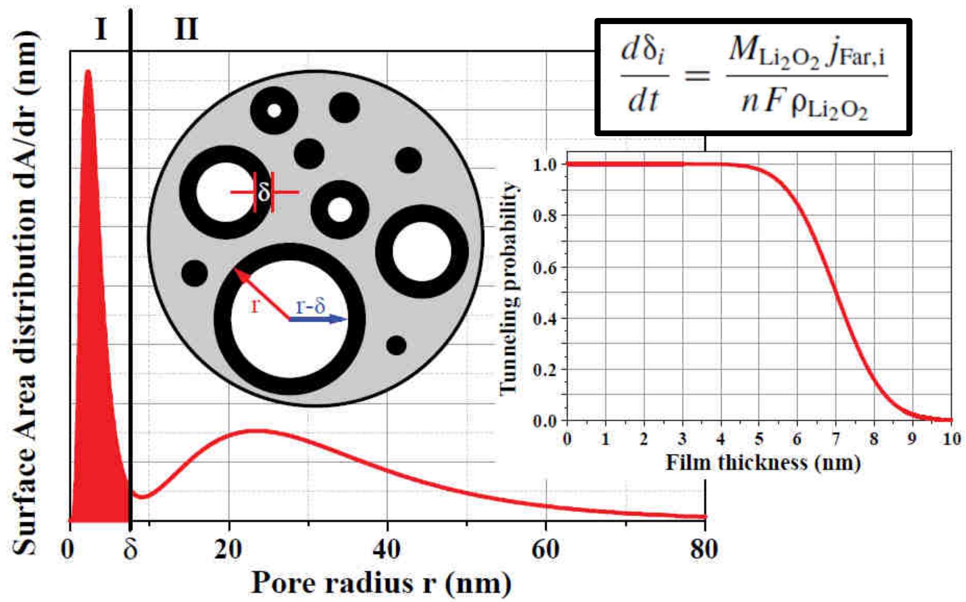


$O_2 + 2Li^+ + 2e^- \rightarrow Li_2O_2$ (solid)

Thin film mechanism

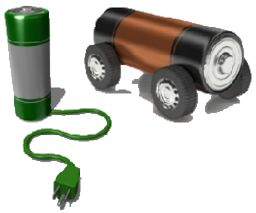
$$a_i = \left[\frac{1 - erf(\delta - 7)}{2}\right] a_i^0$$

$$\frac{d\delta_i}{dt} = \frac{M_{Li_2O_2}\, j_{Far,i}}{n F \rho_{Li_2O_2}}$$



➔ Porosity vs. Electronic tunneling probability vs. Reactive surface area.

A.A. Franco, K.H. Xue, *ECS J. Solid State Science and Tech.*, **2** (10) (2013) M3084.
K.H. Xue, T.K. Nguyen, A.A. Franco, *J. Electrochem. Soc.*, **161** (8) (2014) E3028.



CONTINUUM SIMULATION OF SPECIES TRANSPORT @ MACROSCALE

DIFFUSION EQUATION

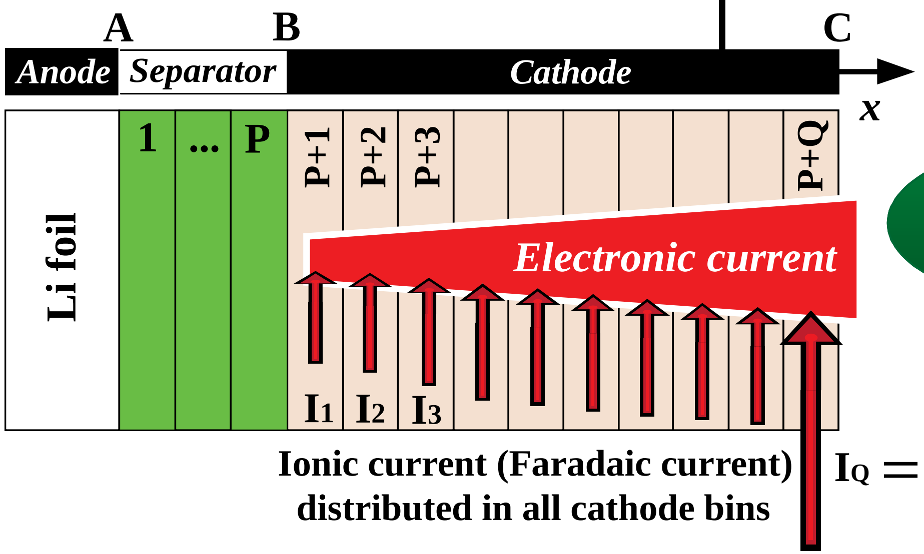
$$\frac{\partial(\varepsilon\, C(x,t))}{\partial t} = \frac{\partial}{\partial x}\left(D\,\frac{\partial C(x,t)}{\partial x}\right) + \gamma . j(x,t)$$

$$D = \left(\frac{\epsilon}{\tau}\right) D_0$$

$$\epsilon = (1 - s)\,\epsilon_0$$

$$s \approx \int j(x,t)\,dt$$

Specific surface area (m^2/m^3)



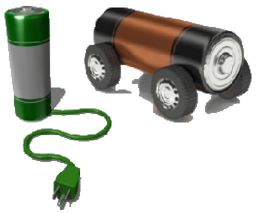
Ionic current (Faradaic current) distributed in all cathode bins

$$I_Q = j(x,t) = f\left(C_{Li^+}, C_j \ldots\right)$$

Function calculated by the kinetic model (e.g. KMC or Butler-Volmer)

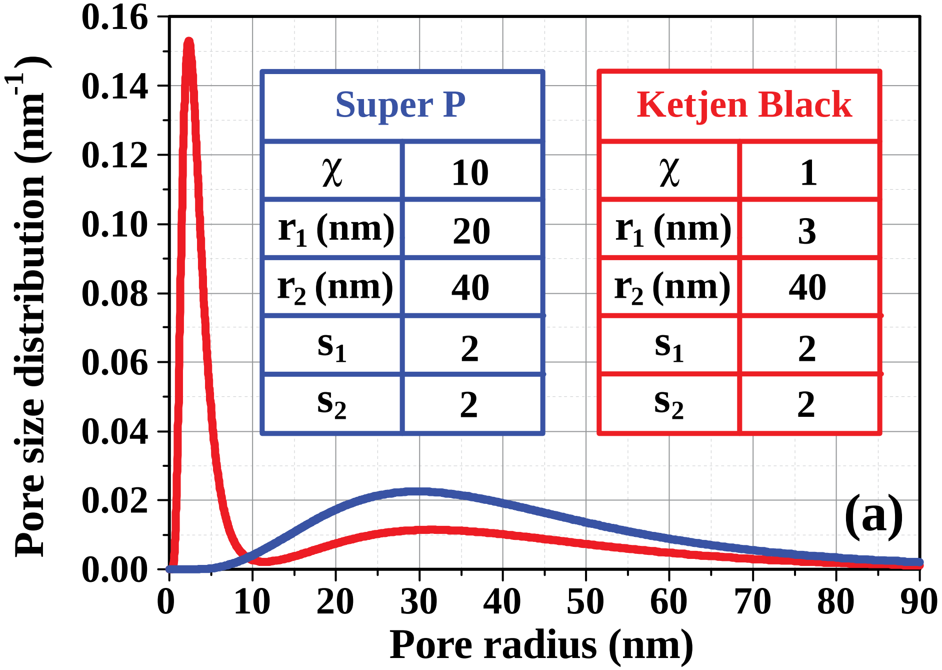
Finite Volume Method

MS LIBER-T



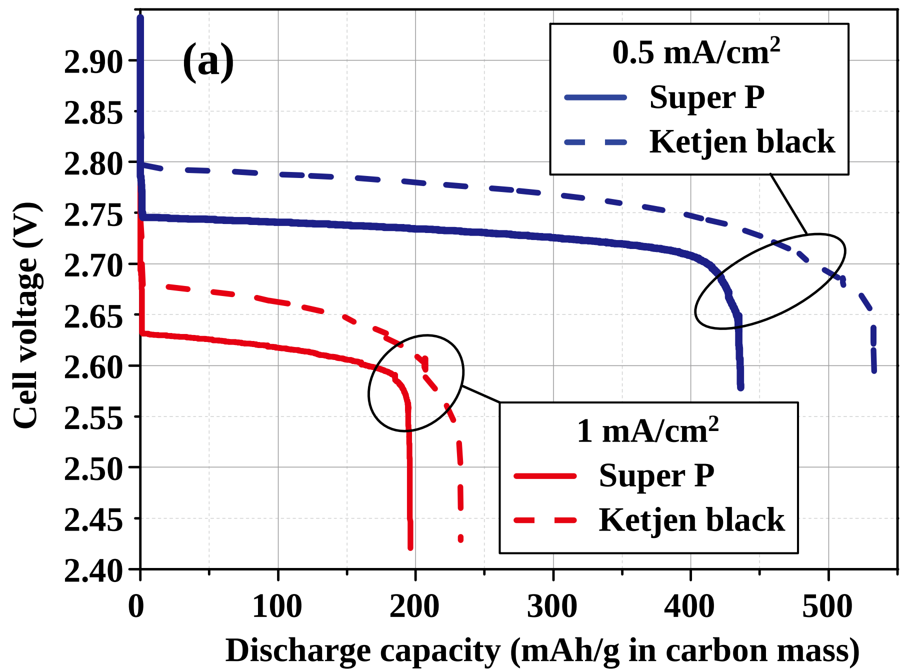
IMPACT OF THE PSD ON THE DISCHARGE CURVE

➔ For intermediate and high current densities, KB provides lower overpotential and higher capacity than SP.

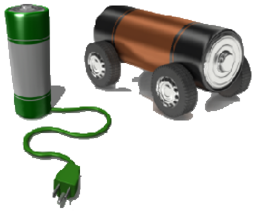


Super P	
χ	10
r_1 (nm)	20
r_2 (nm)	40
s_1	2
s_2	2

Ketjen Black	
χ	1
r_1 (nm)	3
r_2 (nm)	40
s_1	2
s_2	2



- A.A. Franco, K.H. Xue, *ECS J. Solid State Science and Tech.*, **2** (10) (2013) M3084.
- K.H. Xue, T.K. Nguyen, A.A. Franco, *J. Electrochem. Soc.*, **161** (8) (2014) E3028.



SOLUTION PHASE: O_2^- ESCAPE PROBABILITY

First reduction

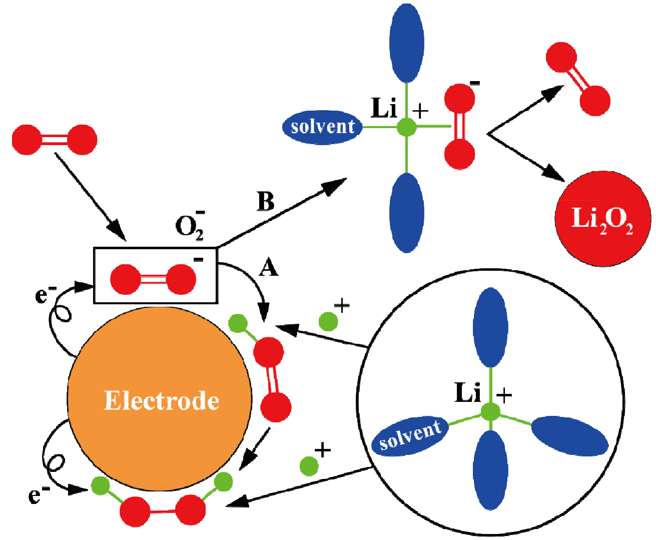
$$O_{2\,(sol)} + e^- \xrightarrow{\text{surface}} O^-_{2\,(sol)}$$

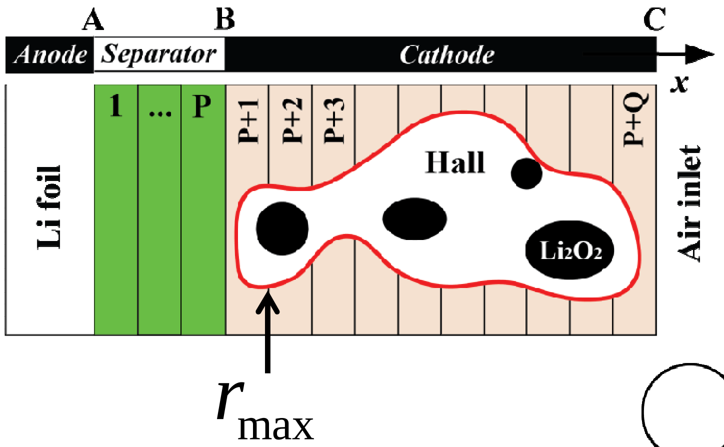
Second reduction

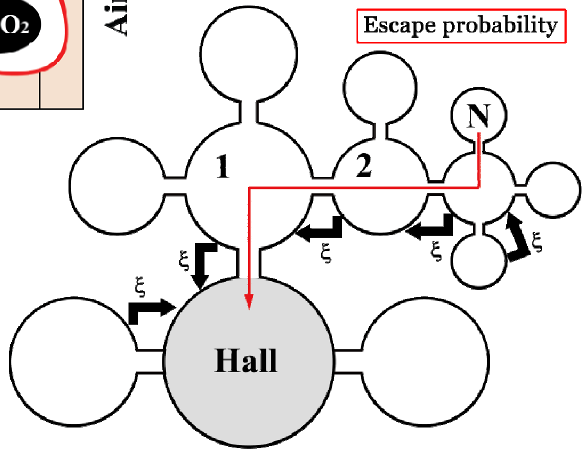
$$O^-_{2\,(sol)} \longrightarrow \chi(r)\, O^-_{2\,(sol)} + [1-\chi(r)]\, O_2^{-\,*}$$

Route A: $[1-\chi(r)]\, O_2^{-\,*} + 2[1-\chi(r)]\, Li^{+\,*} + [1-\chi(r)]\, e^- \xrightarrow{\text{surface}} [1-\chi(r)]\, Li_2O_{2\,(film)}$

Route B: $\chi(r)\, O^-_{2\,(sol)} + \chi(r)\, Li^+_{(sol)} \longrightarrow \left[\frac{\chi(r)}{2}\right] Li_2O_{2\,(particle)} + \left[\frac{\chi(r)}{2}\right] O_2 \uparrow$







Escape function

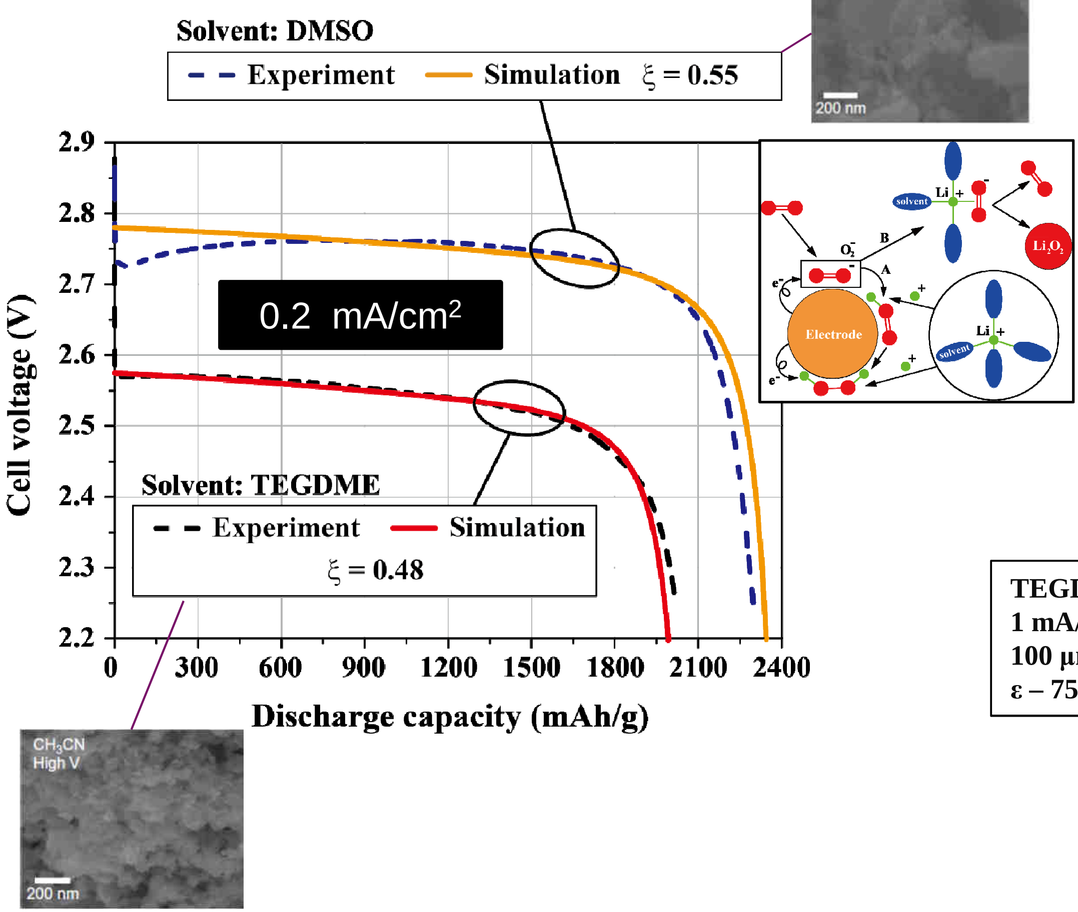
$$\chi(r) = \xi^N = \xi^{\frac{r_{max} - r}{r_{max}}}$$

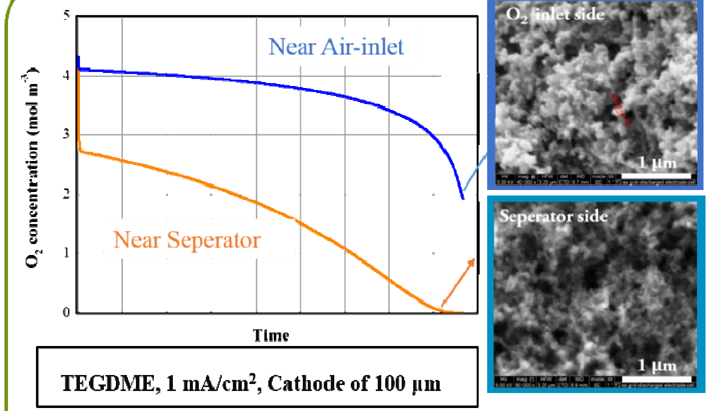
ξ increases with the donor number

K.-H. Xue, E. McTurk, L. Johnson, P. G. Bruce, and A. A. Franco, *Journal of the Electrochemical Society*, **162** (4) (2015) A614.

SOLVENT & ARCHITECTURE IMPACTS ON DISCHARGE

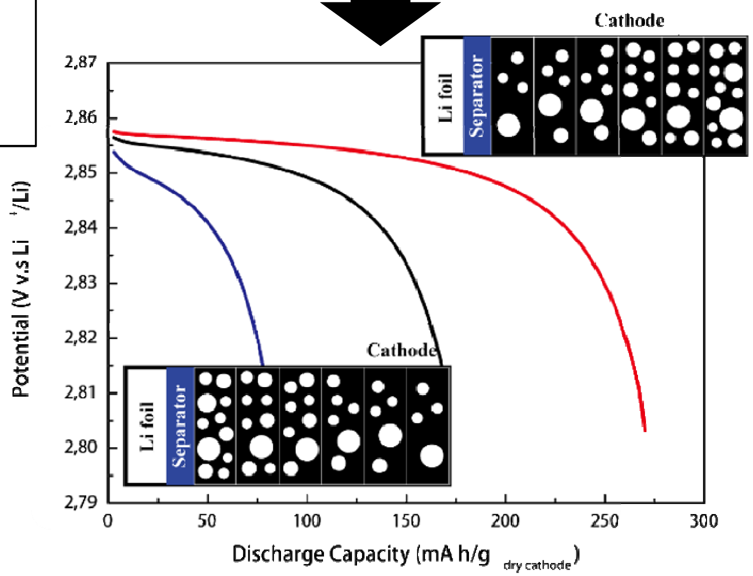
Impact of solvent



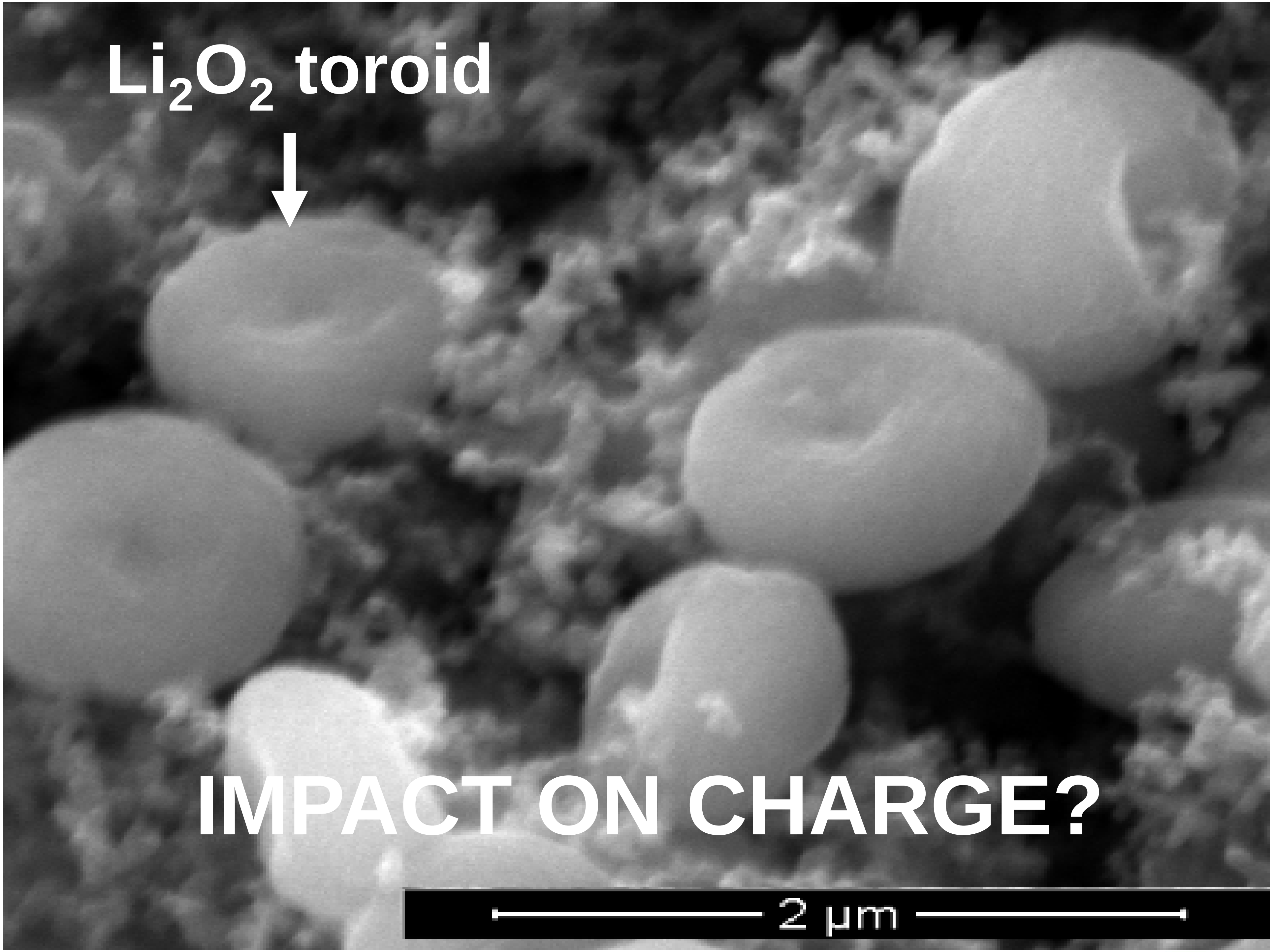


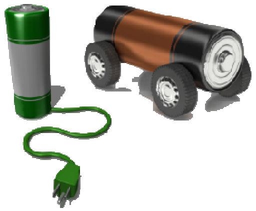
More Li_2O_2 formed close to the O_2 inlet. Insuffiсent discharge of inner part mainly due to poor O_2 transport.

TEGDME
1 mA/cm²
100 µm
ε – 75%



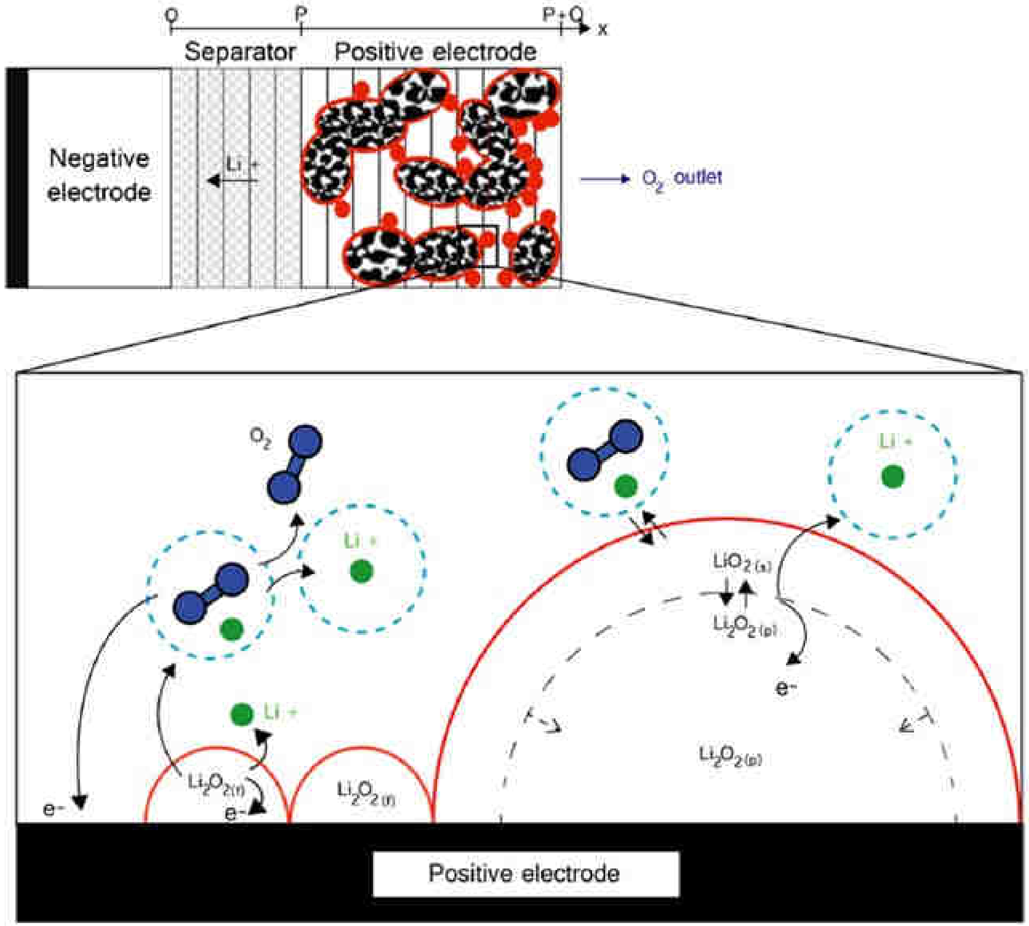
- K.H. Xue, T.K. Nguyen, A.A. Franco, *J. Electrochem. Soc.*, **161** (8) (2014) E3028.
- K.-H. Xue, E. McTurk, L. Johnson, P. G. Bruce, A. A. Franco, *J. Electrochem. Soc.*, **162** (4) (2015) A614 .
- SEM images from: L. Johnson *et al.*, *Nature Chemistry* **6** (2014) 1091


Li_2O_2 toroid
IMPACT ON CHARGE?
2 µm



IMPACT OF DISCHARGE PRODUCTS MORPHOLOGY ON THE CHARGE PROCESS (1/2)

Y. Yin, C. Gaya, A. Torayev, V. Thangavel, A.A. Franco, *The Journal of Physical Chemistry Letters*, **7**(19) (2016) 3897.



Oxidation of Thin-film

$$Li_2O_{2(f)} \rightarrow Li^+ + LiO_{2(ip)} + e^-$$
$$LiO_{2(ip)} \rightarrow Li^+ + O_{2(sol)} + e^-$$

Oxidation of Large-particle

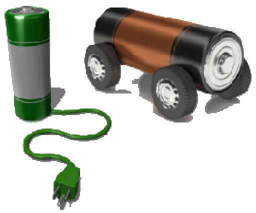
$$Li_2O_{2(p)} \rightarrow Li^+ + LiO_{2(ad)} + e^-$$
$$LiO_{2(ad)} \rightarrow LiO_{2(ip)}$$
$$LiO_{2(ip)} \rightarrow Li^+ + O_{2(sol)} + e^-$$

➔ **Extension of the cell model for charge:** capturing impact of Li_2O_2 particle size distribution on charge kinetics.

LRCS

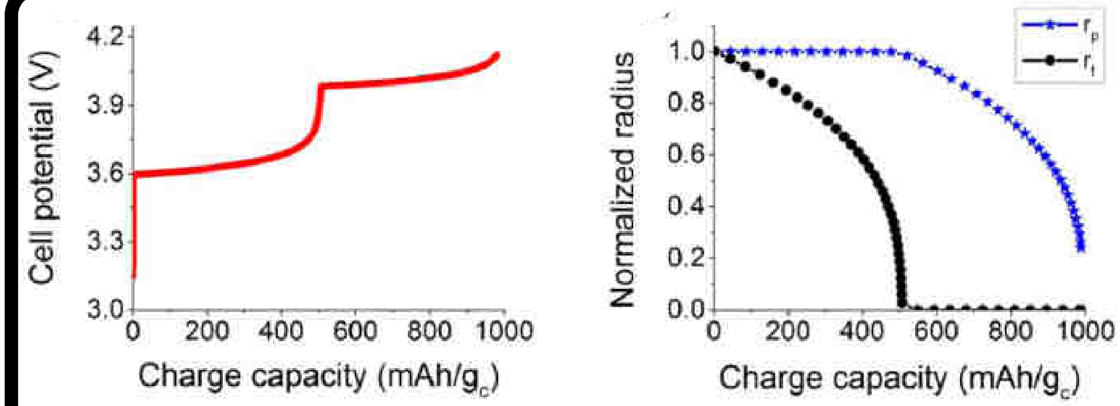
Prof. Alejandro A. Franco
Mesostructure-performance relationships in batteries…
Pregl colloquium
NIC - Ljubljana, Slovenia
December 14, 2016

IUF cnrs www.cnrs.fr UNIVERSITÉ de Picardie Jules Verne



IMPACT OF DISCHARGE PRODUCTS MORPHOLOGY ON THE CHARGE PROCESS (2/2)

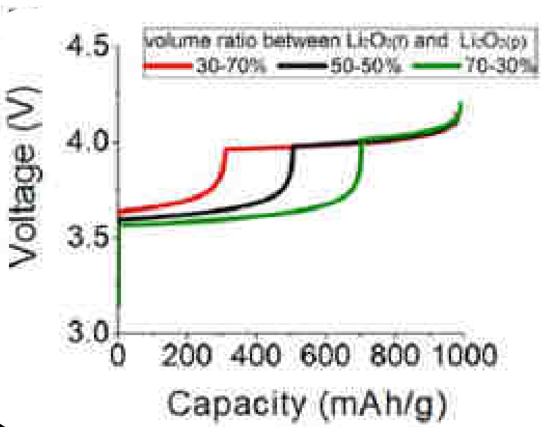
Y. Yin, C. Gaya, A. Torayev, V. Thangavel, A.A. Franco, *The Journal of Physical Chemistry Letters*, **7**(19) (2016) 3897.



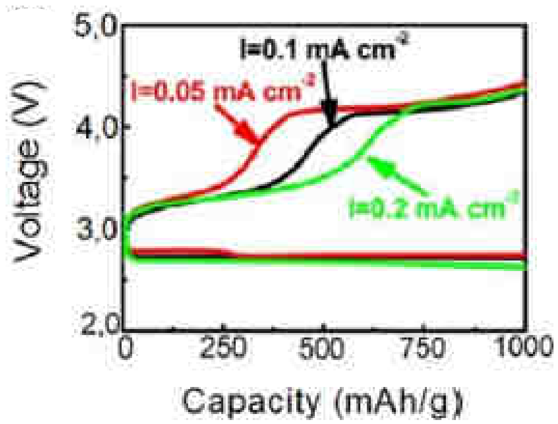
➔ **Two potential plateaus calculated:** linked to the two size of particles consumption.

➔ **Impact of discharge current density on the charge potential:** good agreement with experiment.

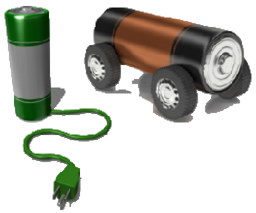
MODEL



EXPERIMENT(*)

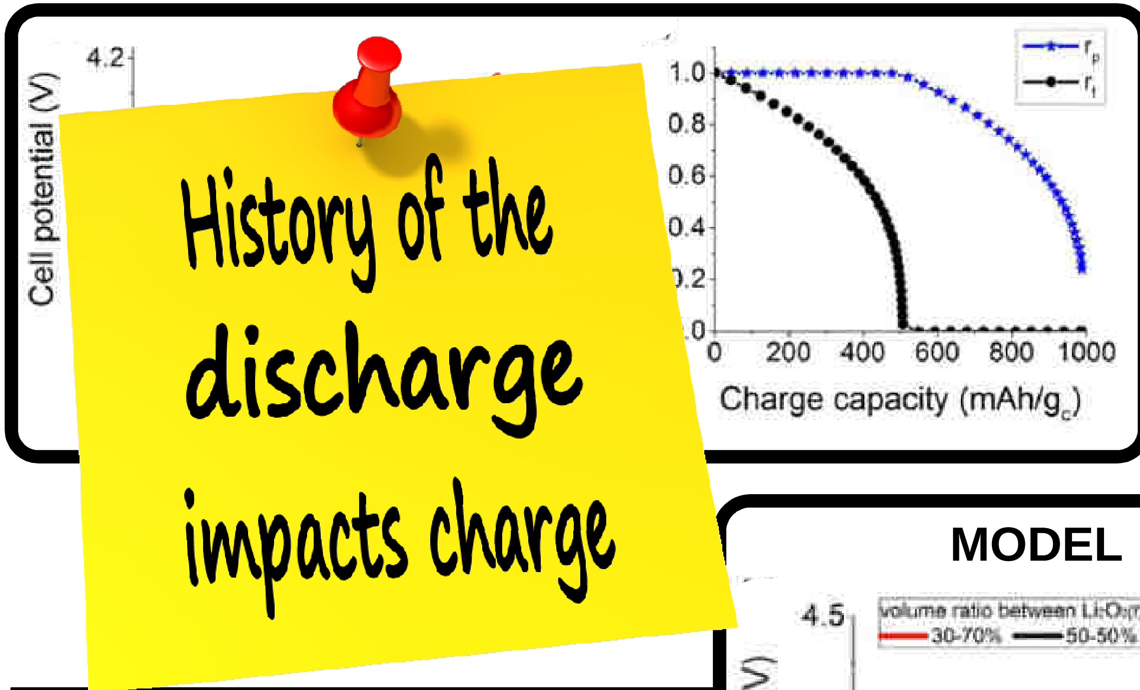


(*) D. Zhai, H. Wang, J. Yang, K.C. Lau, K. Li, K. Amine, L.A. Curtiss, J. Am. Chem. Soc. **135** (2013) 15364.



IMPACT OF DISCHARGE PRODUCTS MORPHOLOGY ON THE CHARGE PROCESS (2/2)

Y. Yin, C. Gaya, A. Torayev, V. Thangavel, A.A. Franco, *The Journal of Physical Chemistry Letters*, **7**(19) (2016) 3897.



➔ **Two potential plateaus calculated:** linked to the two size of particles consumption.

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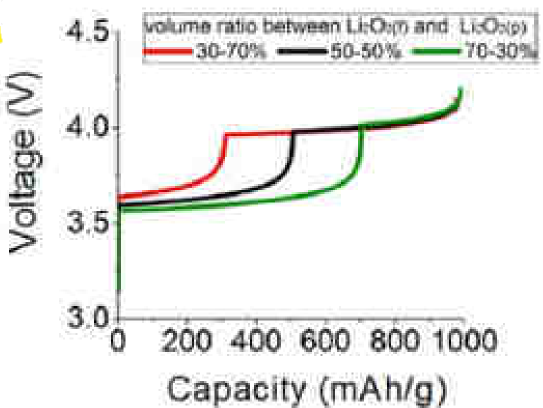
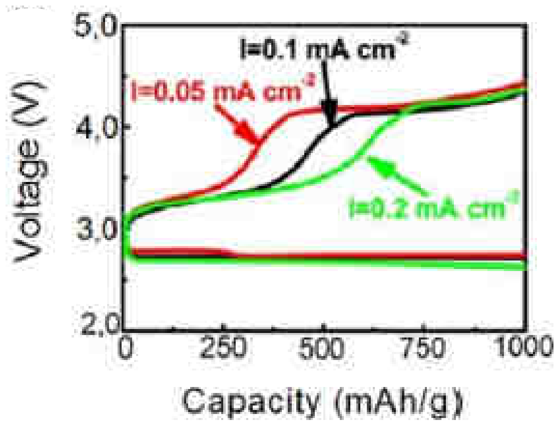
MODEL



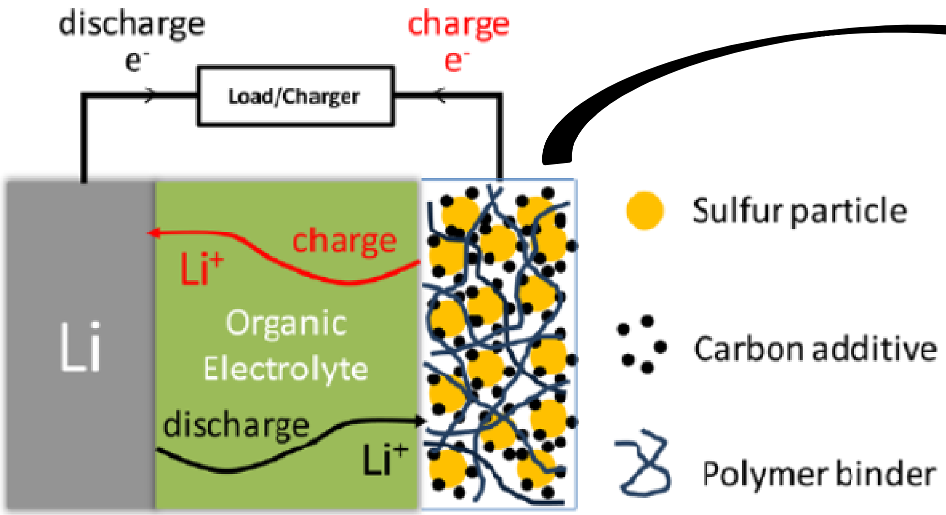
EXPERIMENT(*)

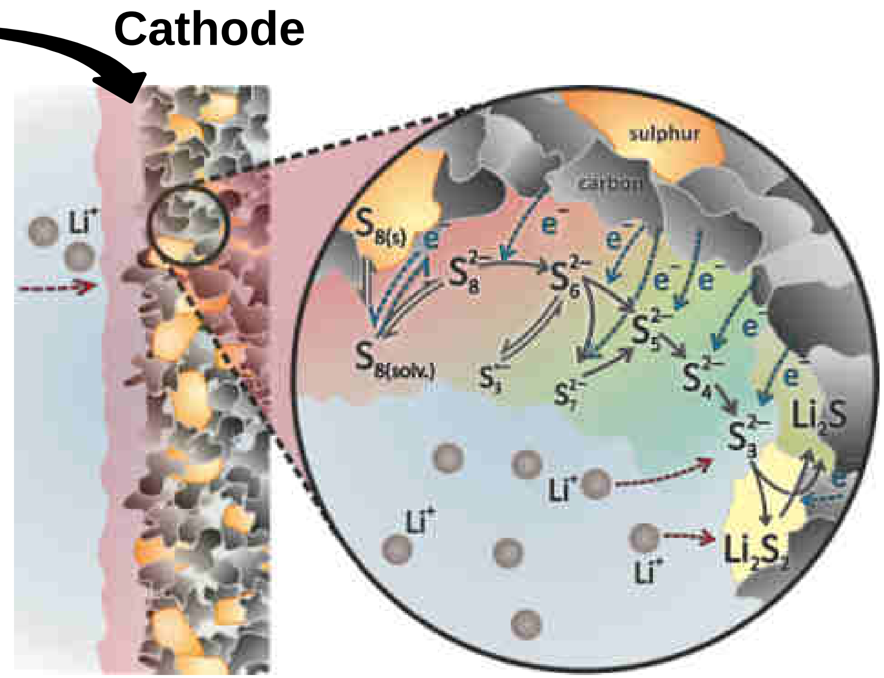


(*) D. Zhai, H. Wang, J. Yang, K.C. Lau, K. Li, K. Amine, L.A. Curtiss, J. Am. Chem. Soc. **135** (2013) 15364.

2. LITHIUM-S BATTERIES

LITHIUM-SULFUR BATTERIES: MOTIVATION



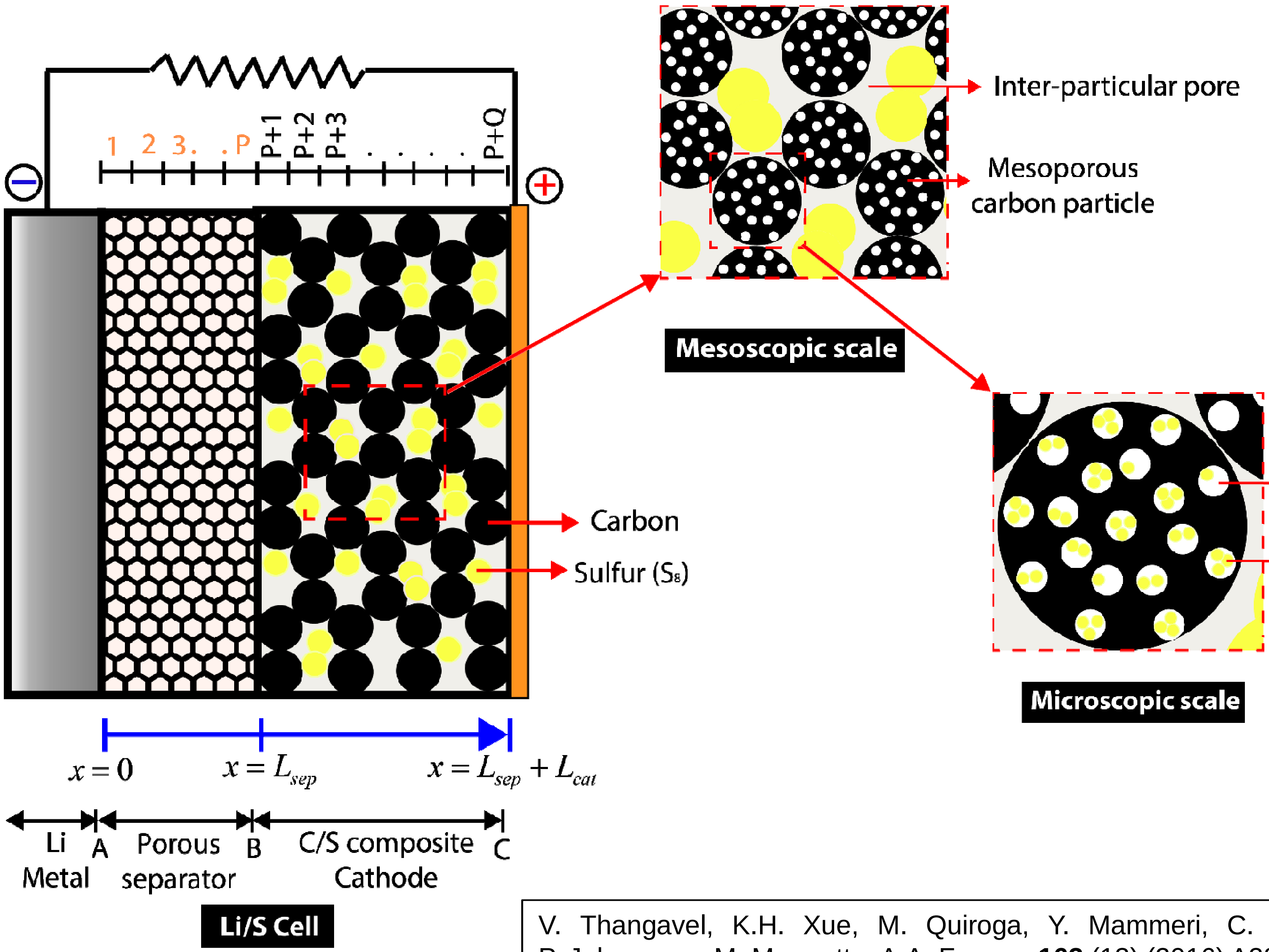


P.G. Bruce *et al.*, *Nat. Mater.* **11** (2012) 19.
A. Manthiram *et al.*, *Chem. Rev.* **114** (2014) 11751.

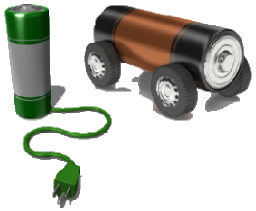
➔ **Key to enhance LiS batteries:** deeper insights about the electrolyte composition and porous electrode microstructure impact on the cell performance.

↳ e.g. sulfur repartition between different scales of porosity, Li_2S location…

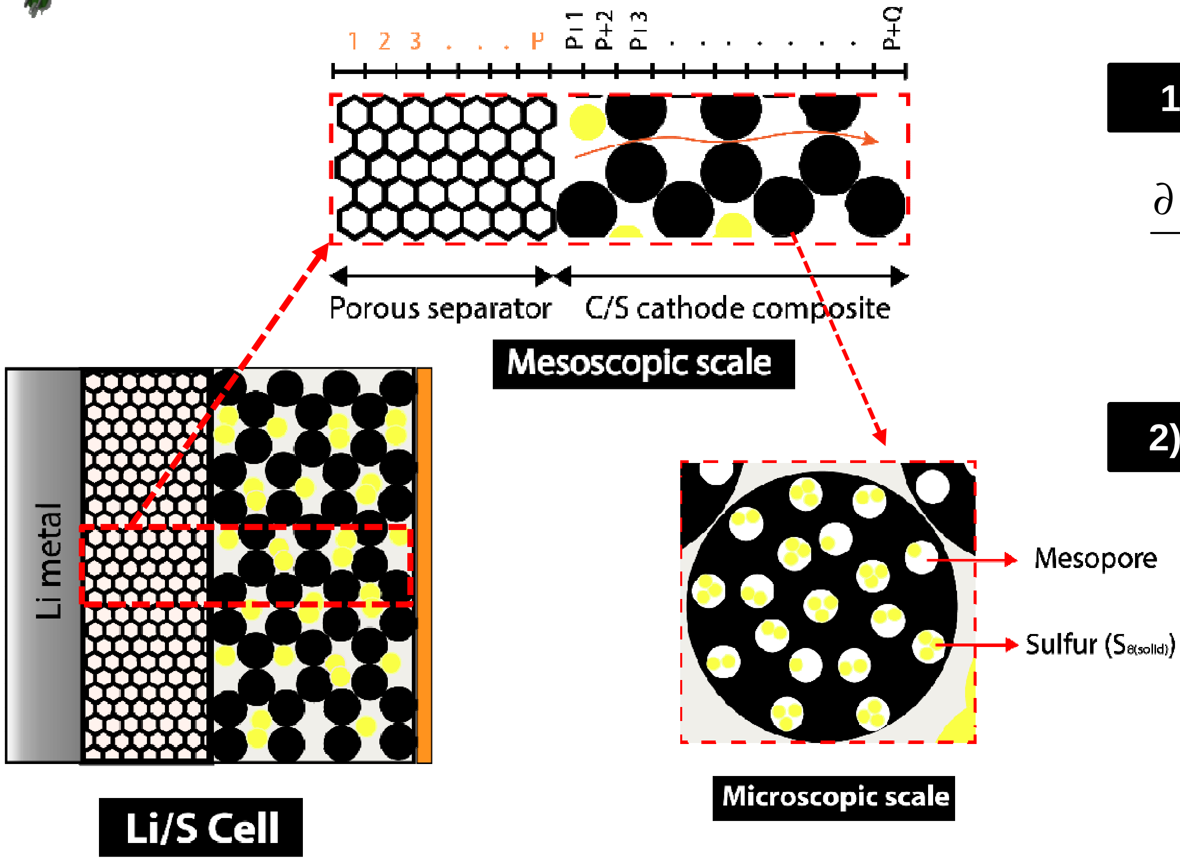
1D-CONTINUUM CELL MODEL



V. Thangavel, K.H. Xue, M. Quiroga, Y. Mammeri, C. Guery, A. Moustari, P. Johansson, M. Morcrette, A.A. Franco, **163** (13) (2016) A2817.



SULFUR-BASED SPECIES TRANSPORT

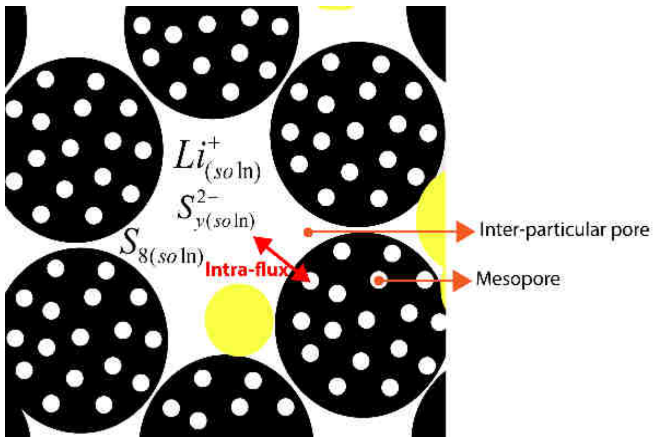


1) Mass conservation for mesoscale

$$\frac{\partial(\varepsilon_1 c_1)}{\partial t} = \frac{\partial}{\partial x}\left[(\varepsilon_1)^{1.5} D\left(\frac{\partial c_1}{\partial x}\right)\right] + r_1 - R_1 + f$$

2) Mass conservation for microscale

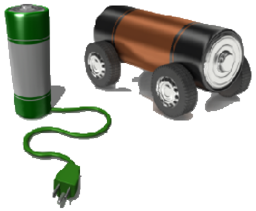
$$\frac{\partial(\varepsilon_2 c_2)}{\partial t} = r_2 - R_2 - f$$



3) Intra-flux between two scales

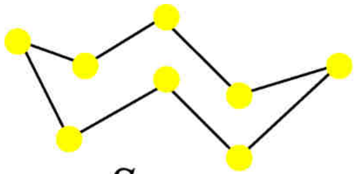
$$f \propto K_{flux}(c_2 - c_1)\,\Xi(\delta_1)$$

r : generation rate through electrochemical reactions
R : sink rate due to chemical dissolution/precipitation
f : species intra-flux between the two scales

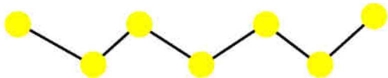


SULFUR-BASED SPECIES TRANSPORT

↳ During the initial stage of discharge long chain polysulfides are produced which can increase the viscosity of the electrolyte.



$S_{8(soln)}$



$S^{2-}_{8(soln)}$

↳ Diffusion coefficient is inversely proportional to viscosity according to Stokes-Einstein equation.

$$D \propto \frac{1}{\mu}$$

↳ Viscosity of the electrolyte can be determined from Einstein's theory of suspension.

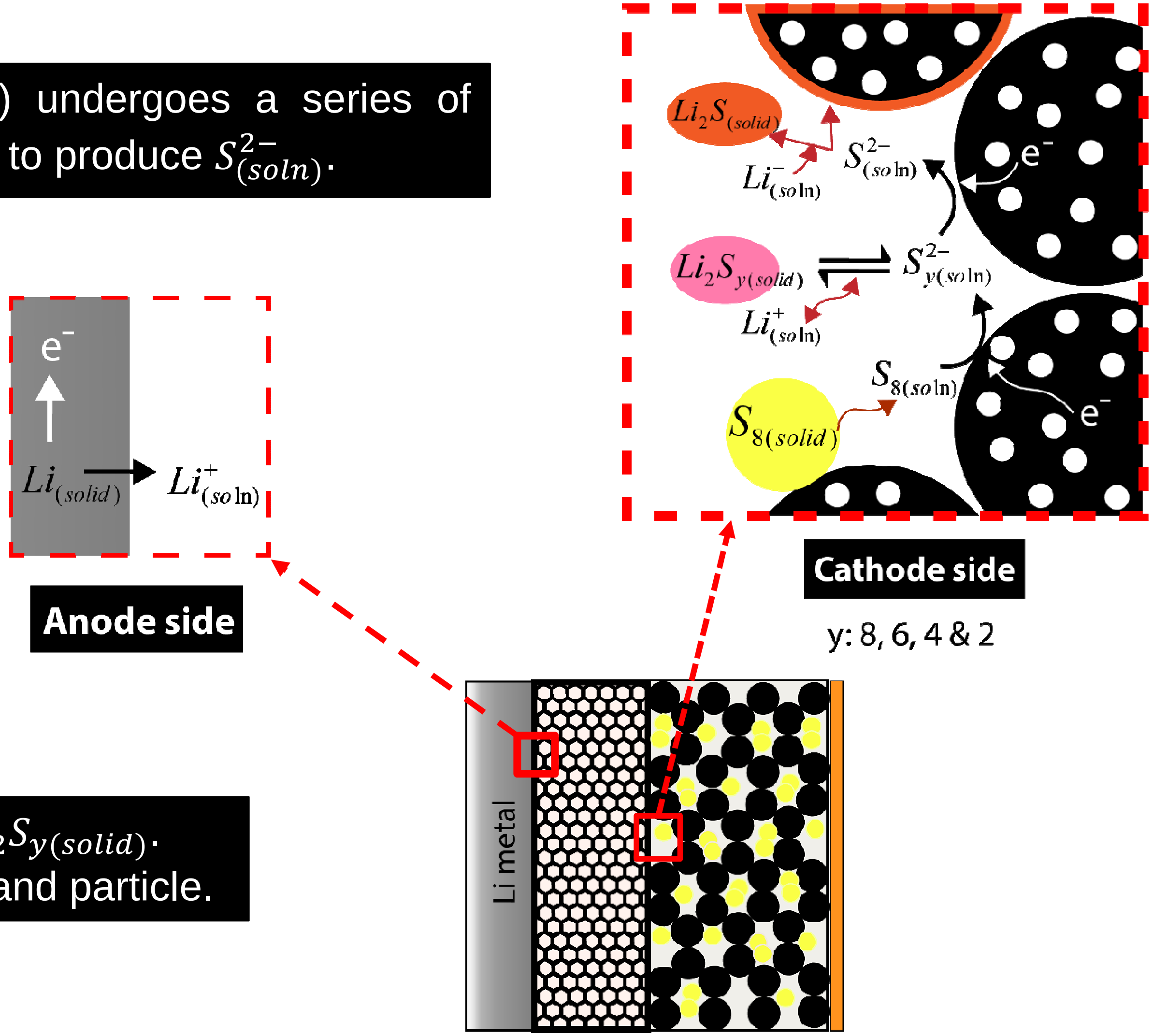
$$\frac{\mu}{\mu_0} = \frac{1+0.5\varphi}{(1-\varphi)^4}$$

$$\varphi = c_1\left(\mathrm{S}_8\right)\bar{V}_{\mathrm{S}_8} + c_1\left(\mathrm{S}_8^{2-}\right)\bar{V}_{\mathrm{S}_8^{2-}}$$

μ_0: Viscosity of the pure electrolyte.
φ: Volume fraction of long chain polysulfides.
$\overline{V_{S_8}}, \overline{V_{S_8^{2-}}}$: Partial molar volume of S_8 *and* S_8^{2-}

ELECTROCHEMICAL & PRECIPITATION REACTIONS

↳ The dissolved sulfur ($S_{8(soln)}$) undergoes a series of elementary reduction reactions to produce $S^{2-}_{(soln)}$.



↳ Precipitation/dissolution of $Li_2S_{y(solid)}$.
↳ Li_2S precipitates both as film and particle.

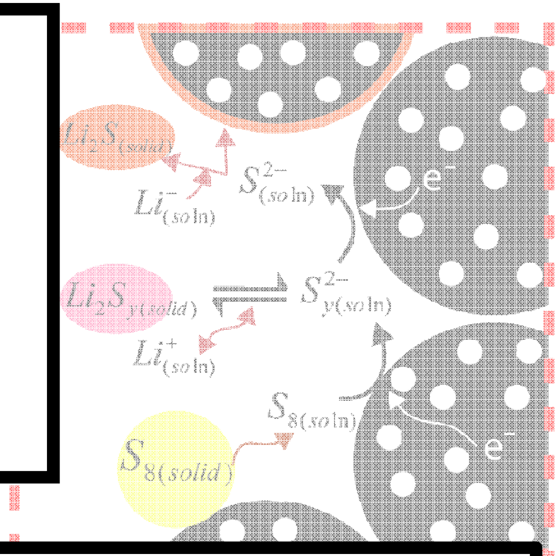
L

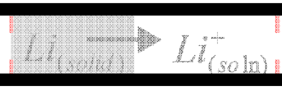
l : mesoscale or microscale.

ELECTROCHEMICAL & PRECIPITATION REACTIONS

↳ The dissolved sulfu
elementary reductior

$$\frac{\partial \varepsilon^l}{\partial t} \propto -\sum_k v_i^l$$

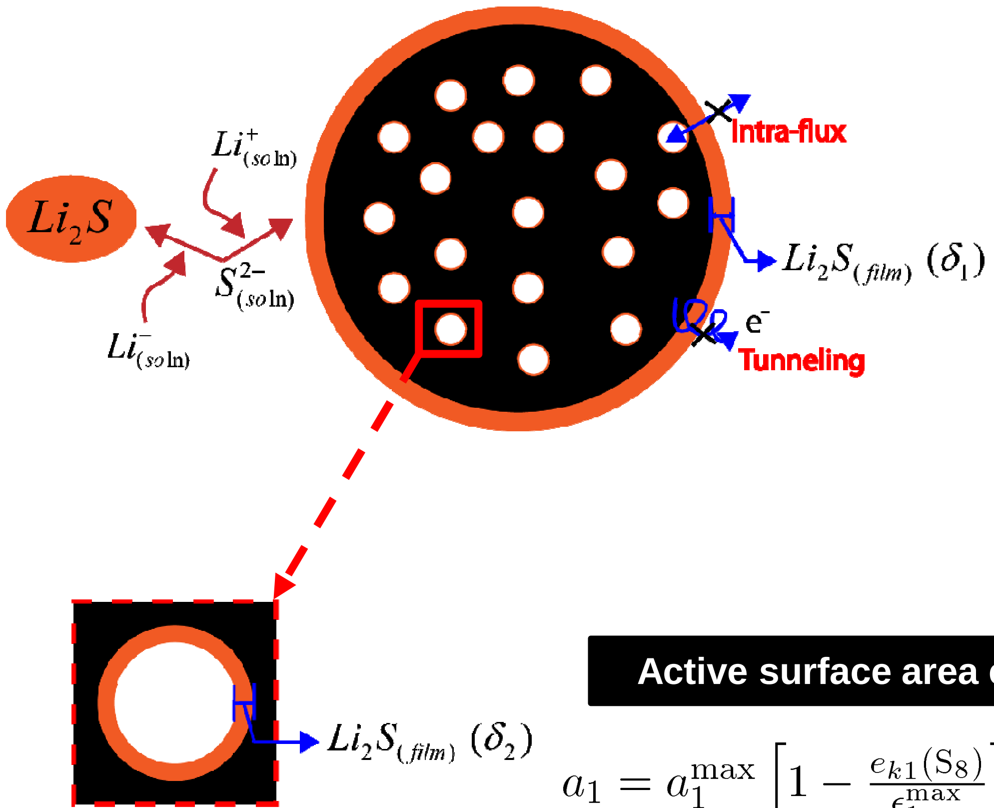


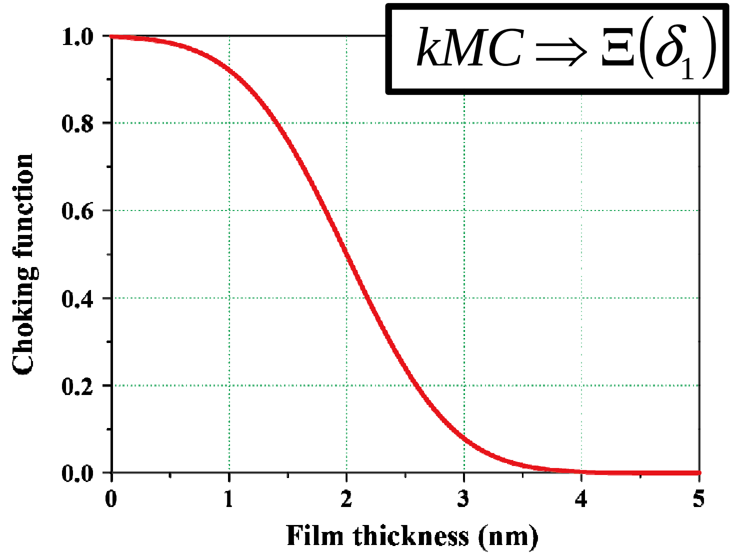


$$v_i^l \propto a^l(t)\left(k_i \prod_j C_j^l - k_{-i} \prod_{j'} C_{j'}^l\right)$$

l : mesoscale or microscale.

ACTIVE SURFACE AREA LOSS

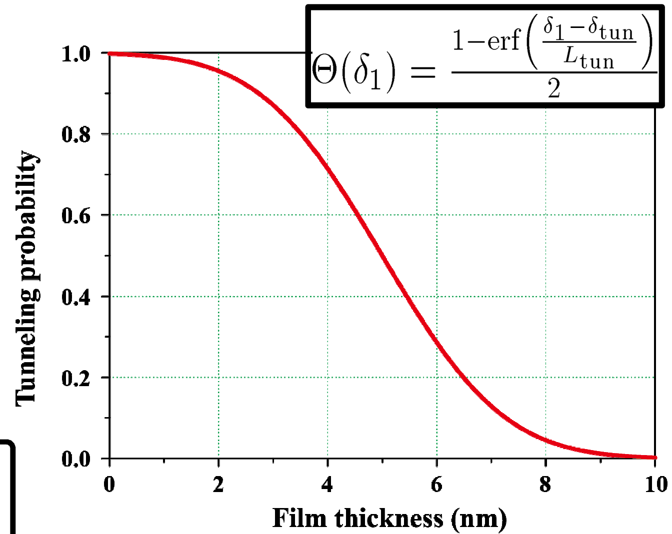




Active surface area evolution

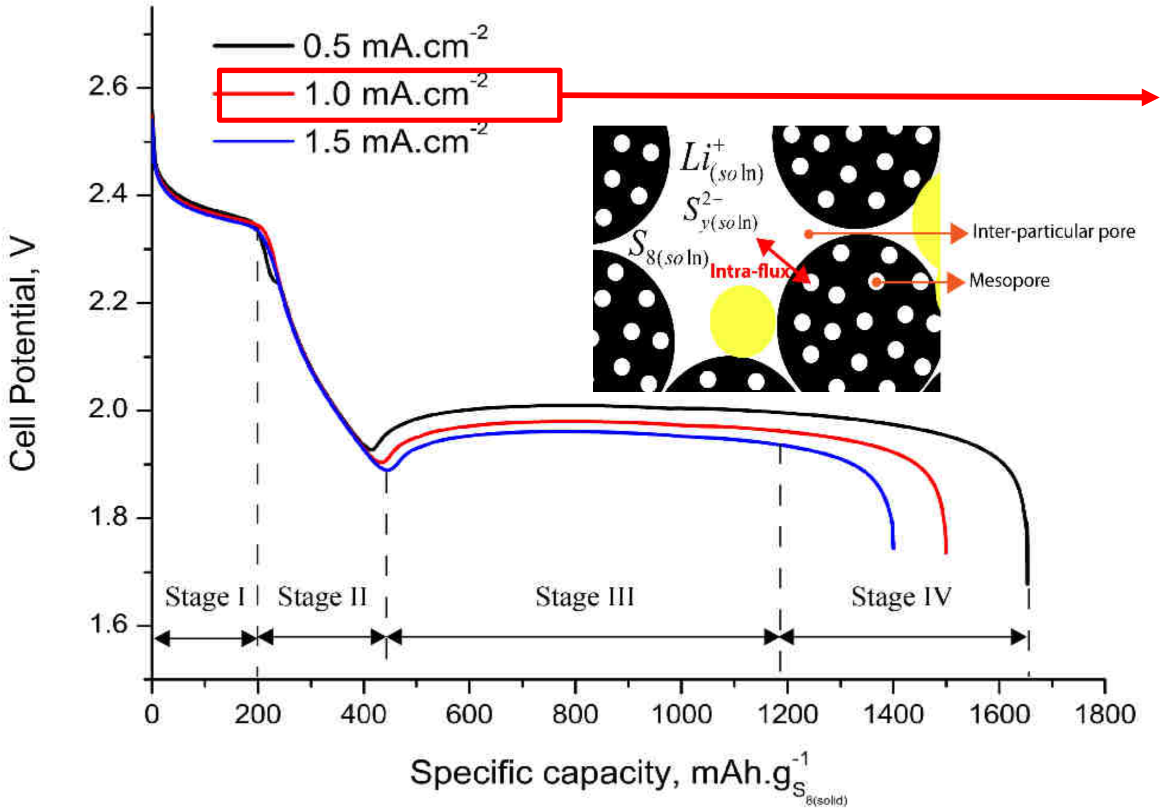
$$a_1 = a_1^{\max}\left[1 - \frac{e_{k1}(\mathrm{S}_8)}{\epsilon_1^{\max}}\right]^{1.5}\Theta(\delta_1)$$

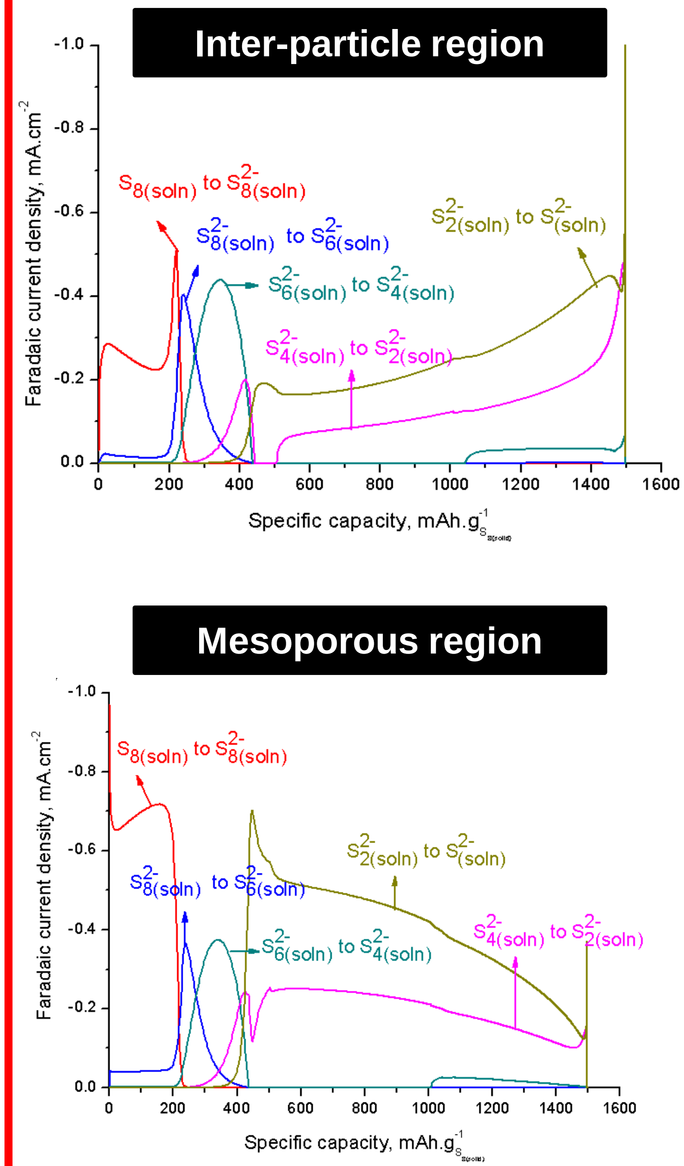
$$a_2 = a_2^{\max}\left(\frac{R_p - \delta_2}{R_p}\right)^2\Theta(\delta_2)\Xi(\delta_1)$$



δ_1, δ_2 : Li_2S thin film thickness over the surface of carbon
δ_{tun} : tunneling threshold

HETEROGENEITY OF REACTIONS AT MULTIPLE PORE SCALES



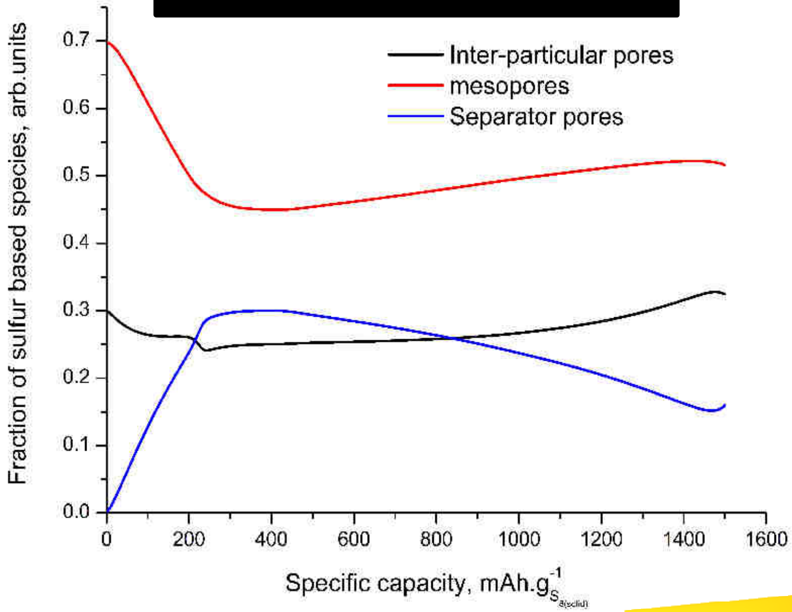


V. Thangavel, K.H. Xue, M. Quiroga, Y. Mammeri, C. Guery, A. Moustari, P. Johansson, M. Morcrette, A.A. Franco, **163** (13) (2016) A2817.

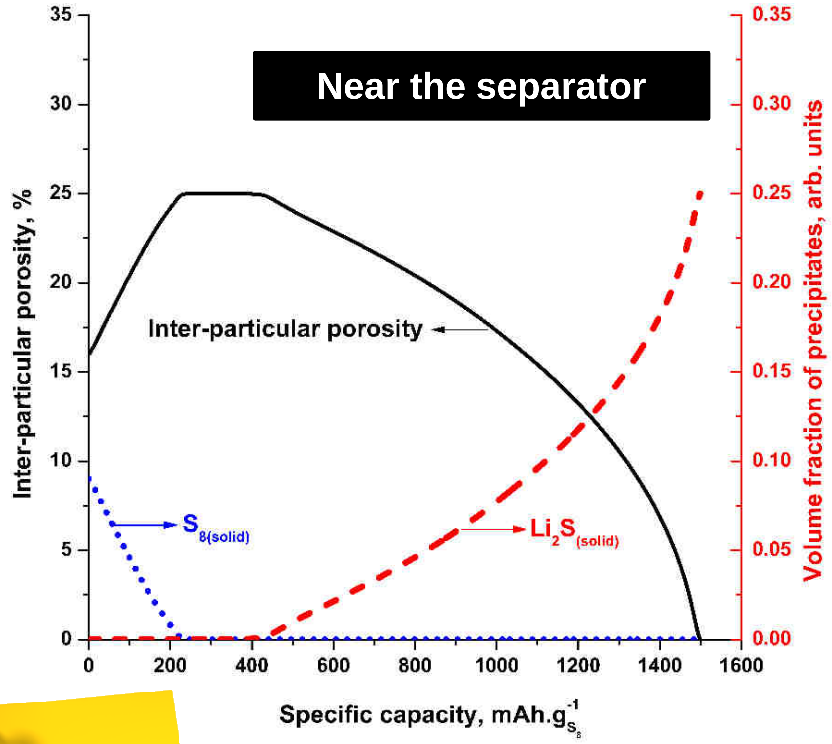
HETEROGENEITY OF REACTIONS ALONG THE CATHODE THICKNESS (1/2)

1.0 mA.cm^{-2}

Exchange of sulfur between various domains

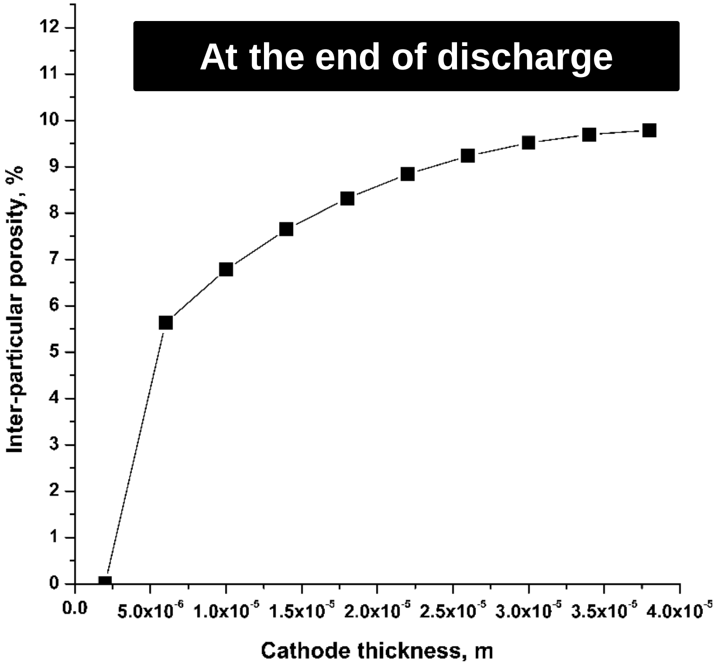


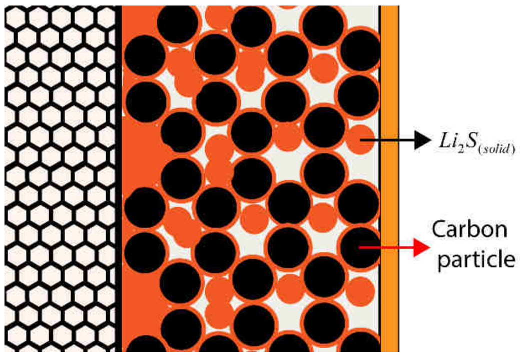
Near the separator



Still sulfur in separator at the end of discharge

HETEROGENEITY OF REACTIONS ALONG THE CATHODE THICKNESS (2/2)





↳ Discharge stops due to clogging of the inter-particle pores.

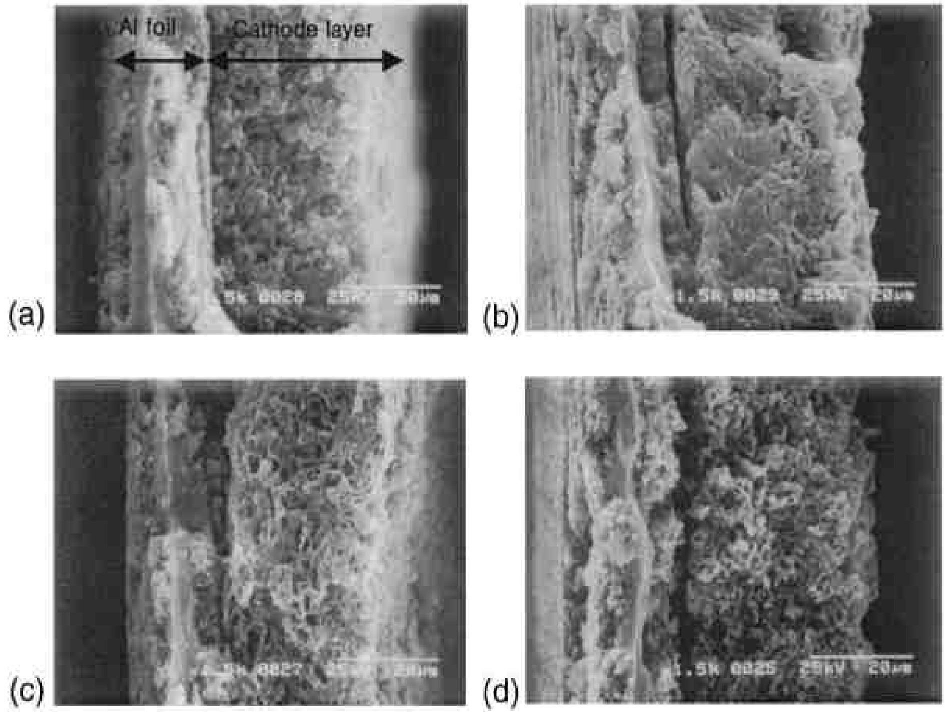
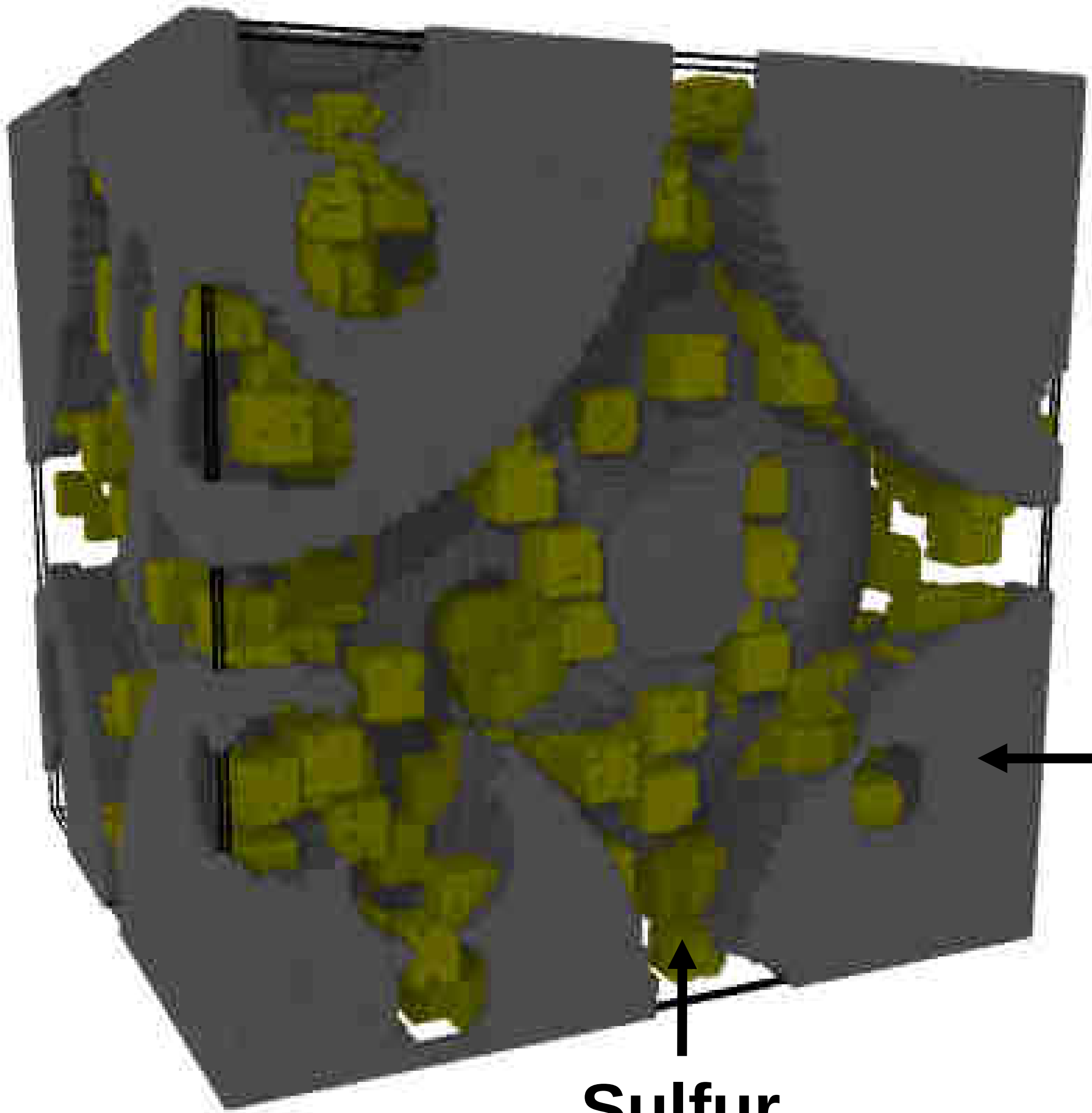


Figure 2. SEM micrographs of the cross section of the sulfur cathodes (a) before discharge, (b) after discharge to 1.5 V at 0.26 mA/cm^2, (c) after discharge to 1.5 V at 1.74 mA/cm^2, and (d) after discharge to 1.5 V at 3.00 mA/cm^2.

Cheon et al., J. Electrochem. Soc., **150** (2003) A800.



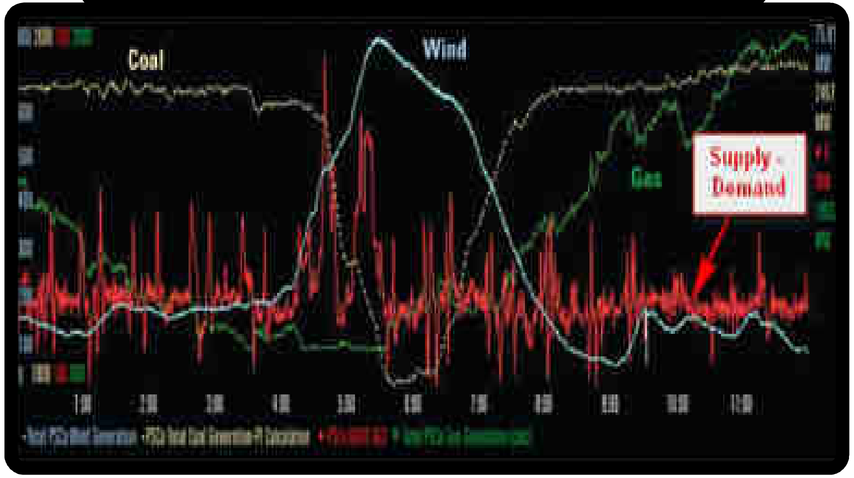
PRISTINE Li-S CATHODE…

3. REDOX FLOW BATTERIES

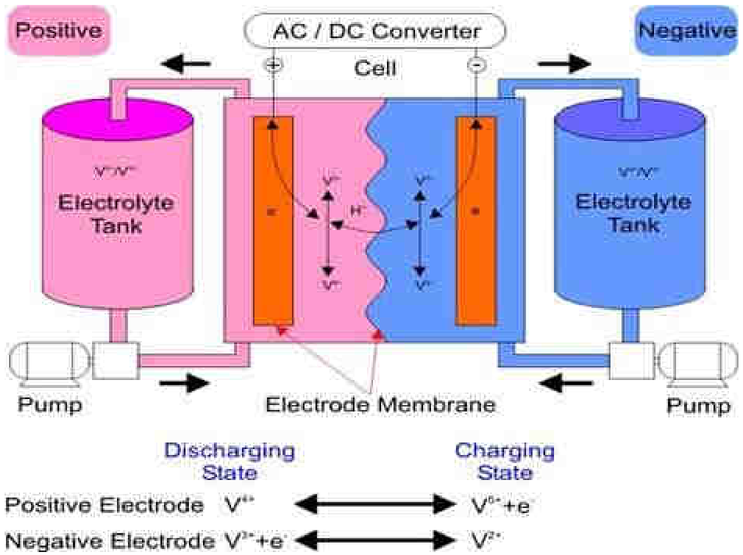
STORING ENERGY FROM RENEWABLE SOURCES

Intermittent renewable energies

Issues on grid management



Public Service Co. of Colorado (PSCo) (July 2, 2008).



A. Z. Weber et al., Journal of Applied Electrochemistry **41** (10) (2011) 1137.

Redox Flow Batteries

↳ High energy efficiency (85-90%)

↳ Unlimited theoretical capacity

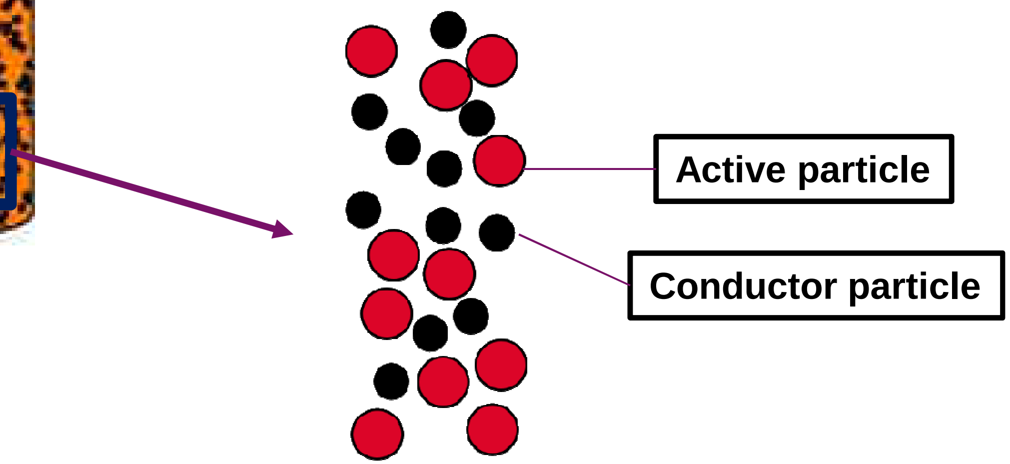
↳ Long lifetime

↳ Fast response time (milisecond)

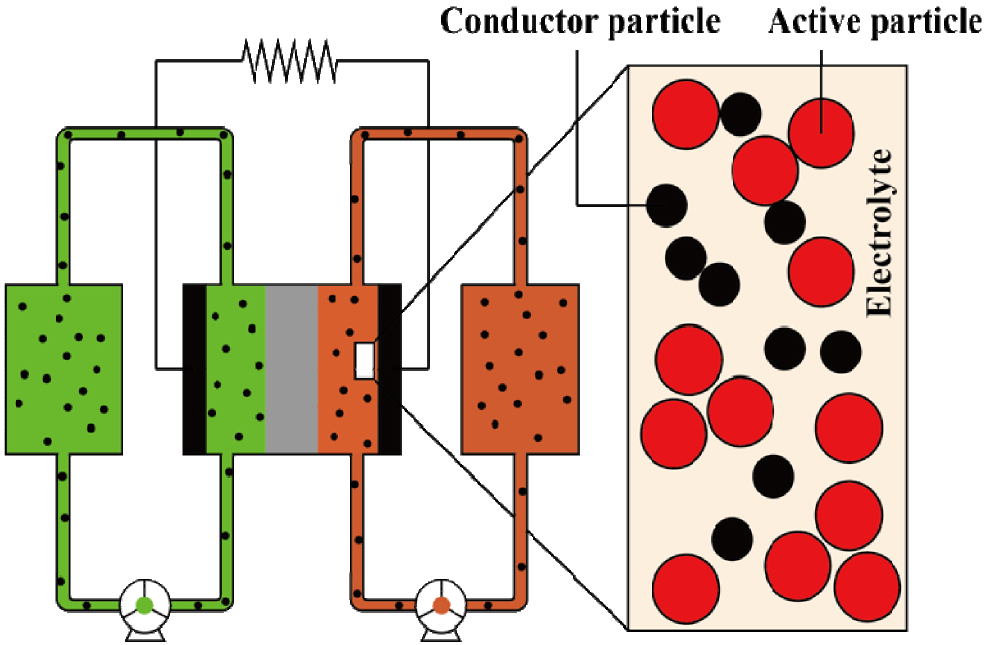
SLURRY-BASED REDOX FLOW BATTERIES (SRFB)

M. Duduta, B. Ho, V. C. Wood, P. Limthongkul, V. E. Brunini, W. C. Carter, Y.-M. Chiang, *Adv. Energy Mater.*, **1**, 511 (2011).

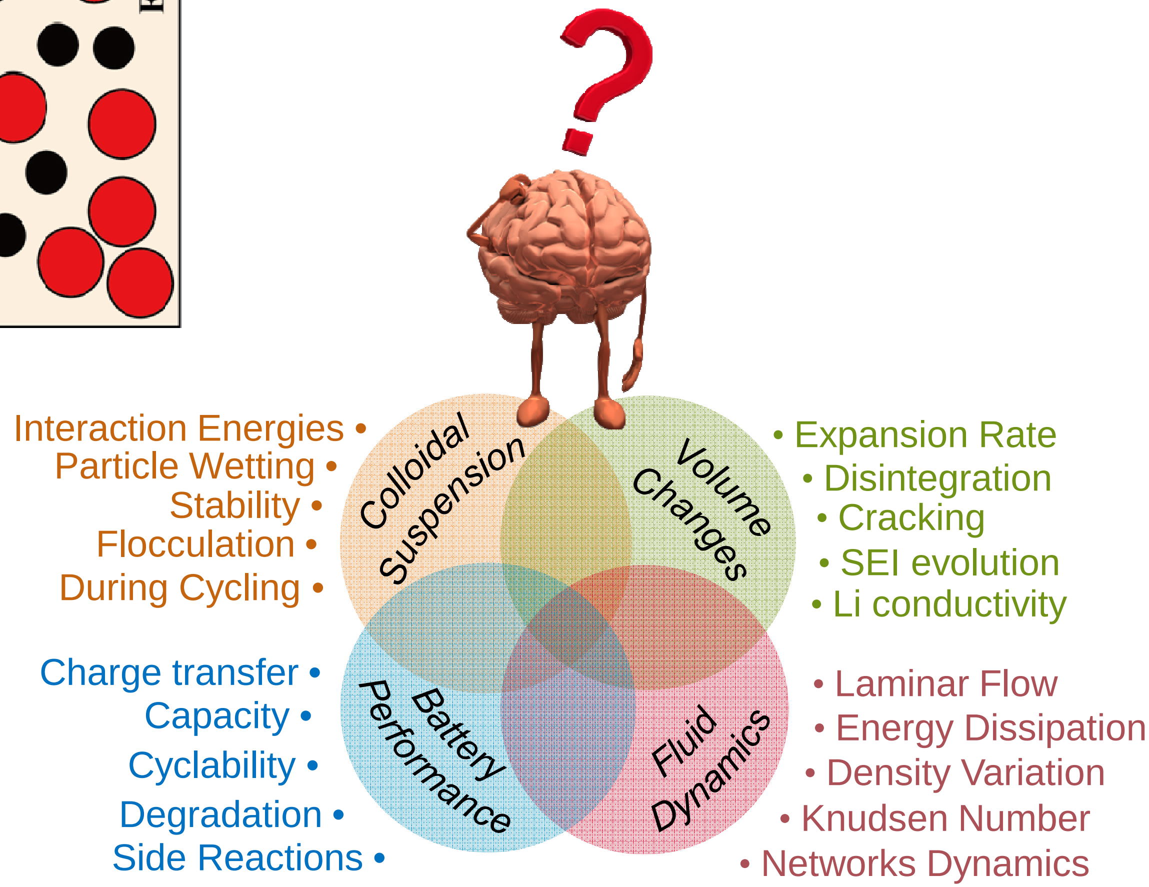
Flow battery fueled by semi-solid suspensions of **high-energy-density** lithium storage compounds that are electrically "wired" by dilute percolating networks of nanoscale conductor particles.

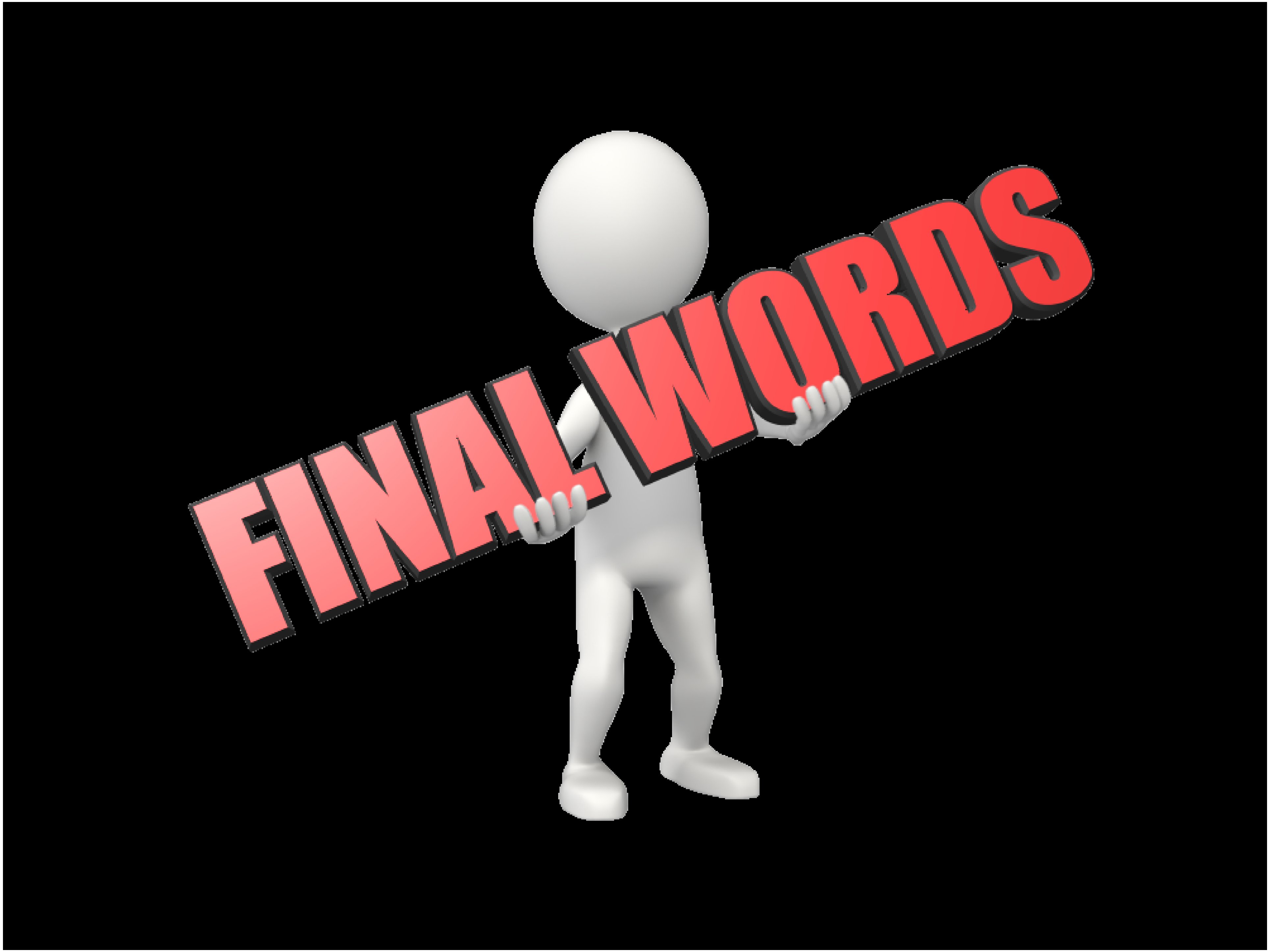


SRFB: FUNDAMENTAL CHALLENGES (1/2)

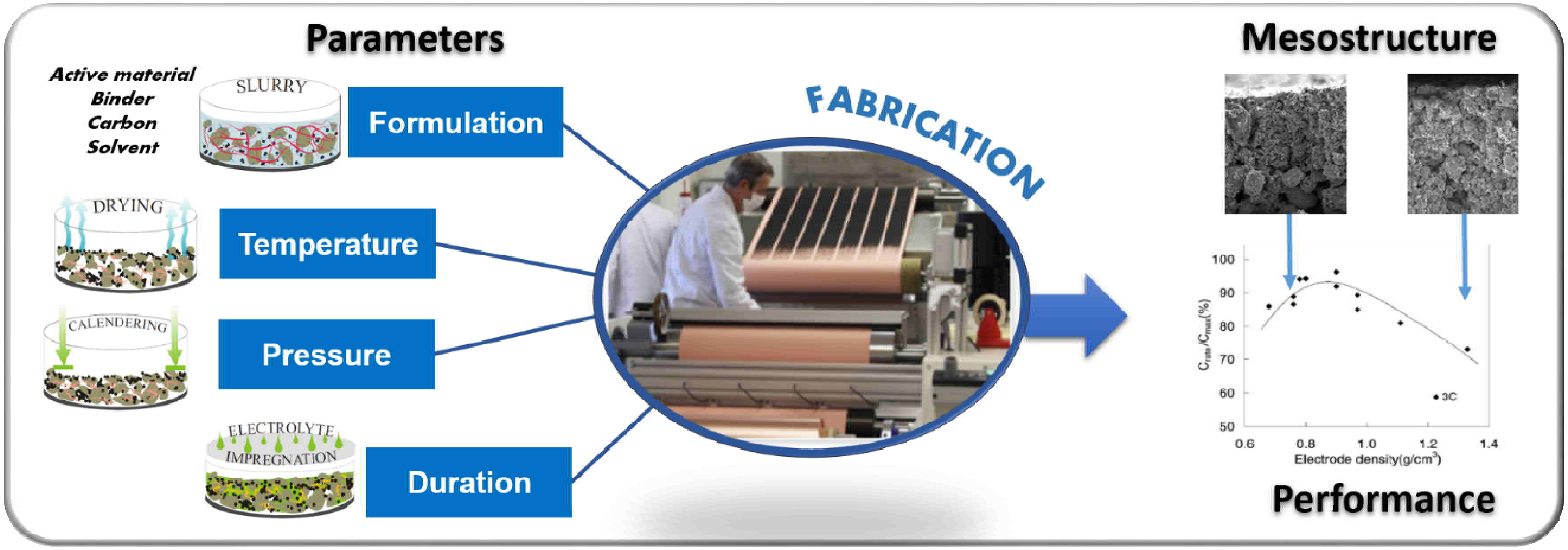


FUNDAMENTALS




FINAL WORDS

MODELING OF BATTERIES FABRICATION



institut
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de France

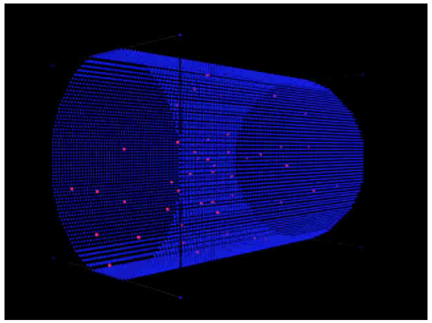
Project started in October 2016

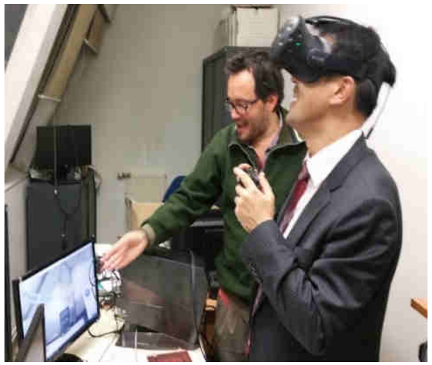
TEACHING: USING IMMERSIVE VIRTUAL REALITY (VR)

Interactive Virtual Reality-based tool for energy storage teaching and immersive data analysis.

Use in lectures within Master M.E.S.C.:

↳ Driving a Li-O_2-powered Electric Car
↳ Tool informed by Kinetic Monte Carlo databases.





A.A. Franco, Y. Yin, R. Zhao, R. Lelong, I. Thouvenin, *J. Chem. Education*, in preparation (2016).

Région Hauts-de-France

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REVIATECH heudiasyc

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From left to right: R. Zhao, Dr. M. Quiroga, A. Torayev, G. Shukla, Y. Yin, A. Geng, Prof. A..A Franco, M. Maiza, V. Thangavel, R. Andersson, C. Gaya, A. Shodiyev.

Amiens cathedral by night

THANK YOU

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