

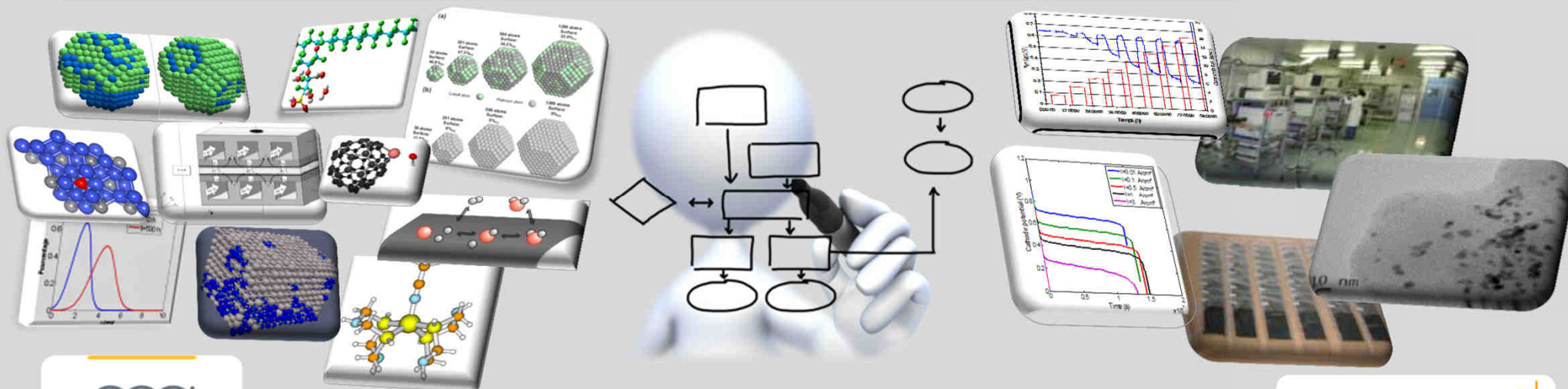
# A Multiscale Modeling Framework for the Transient Analysis of PEMFCs

**Dr. Alejandro A. Franco**

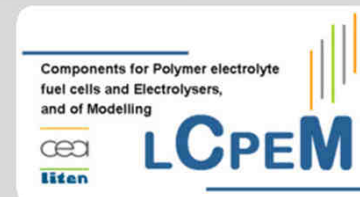
*Modeling Group Leader @*

**Atomic and Alternative Energies Commission of France (CEA)/LITEN/DEHT/**

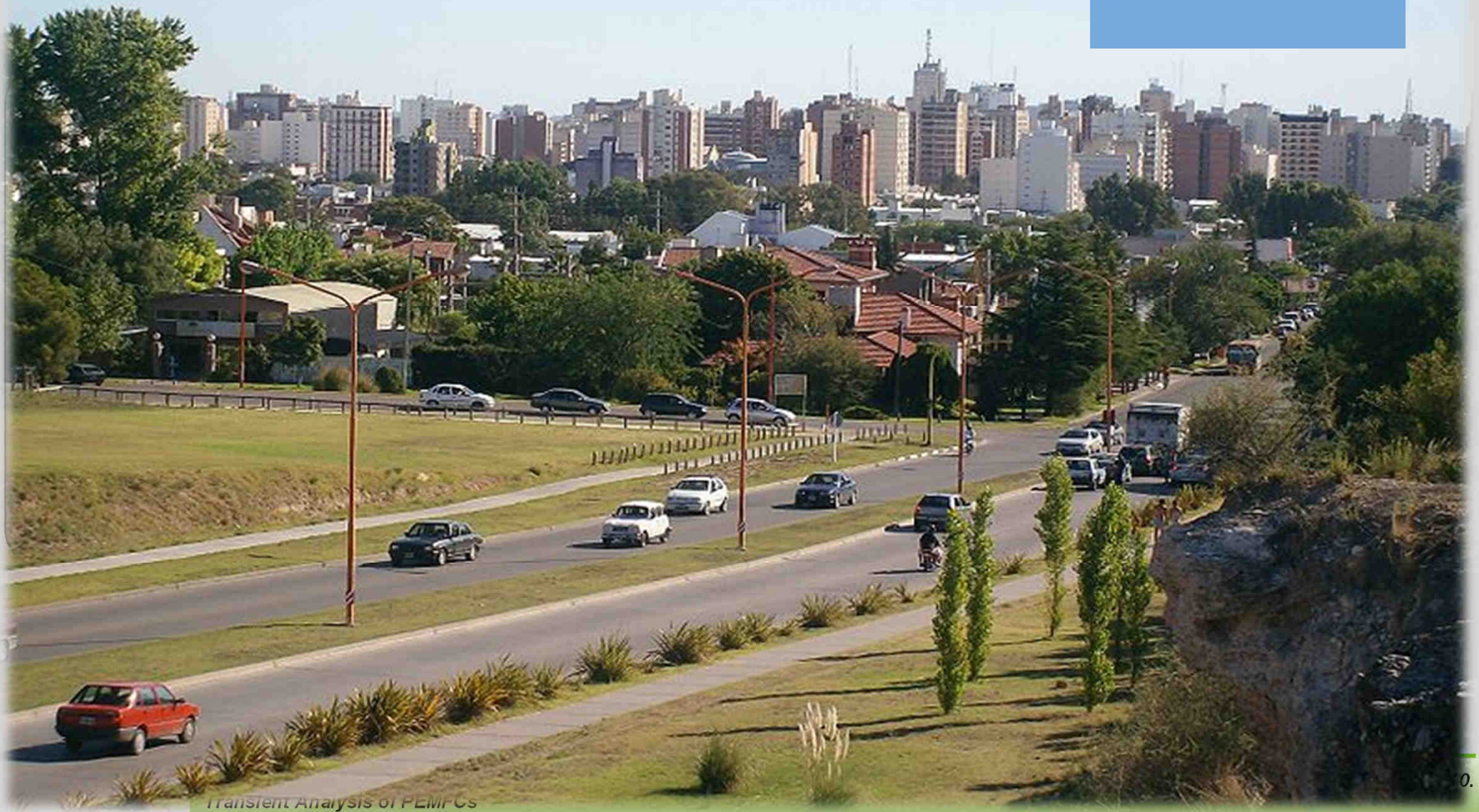
*Laboratory of Components for Fuel Cells and Electrolysers, and of Modeling (LCPEM), Grenoble*



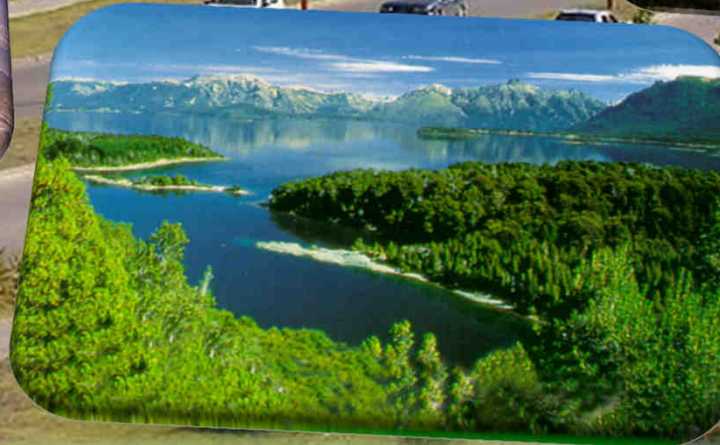
H.D.R. Defense – Grenoble, September 23<sup>rd</sup>, 2010



A December 10<sup>th</sup>, 1977...in Bahia Blanca...



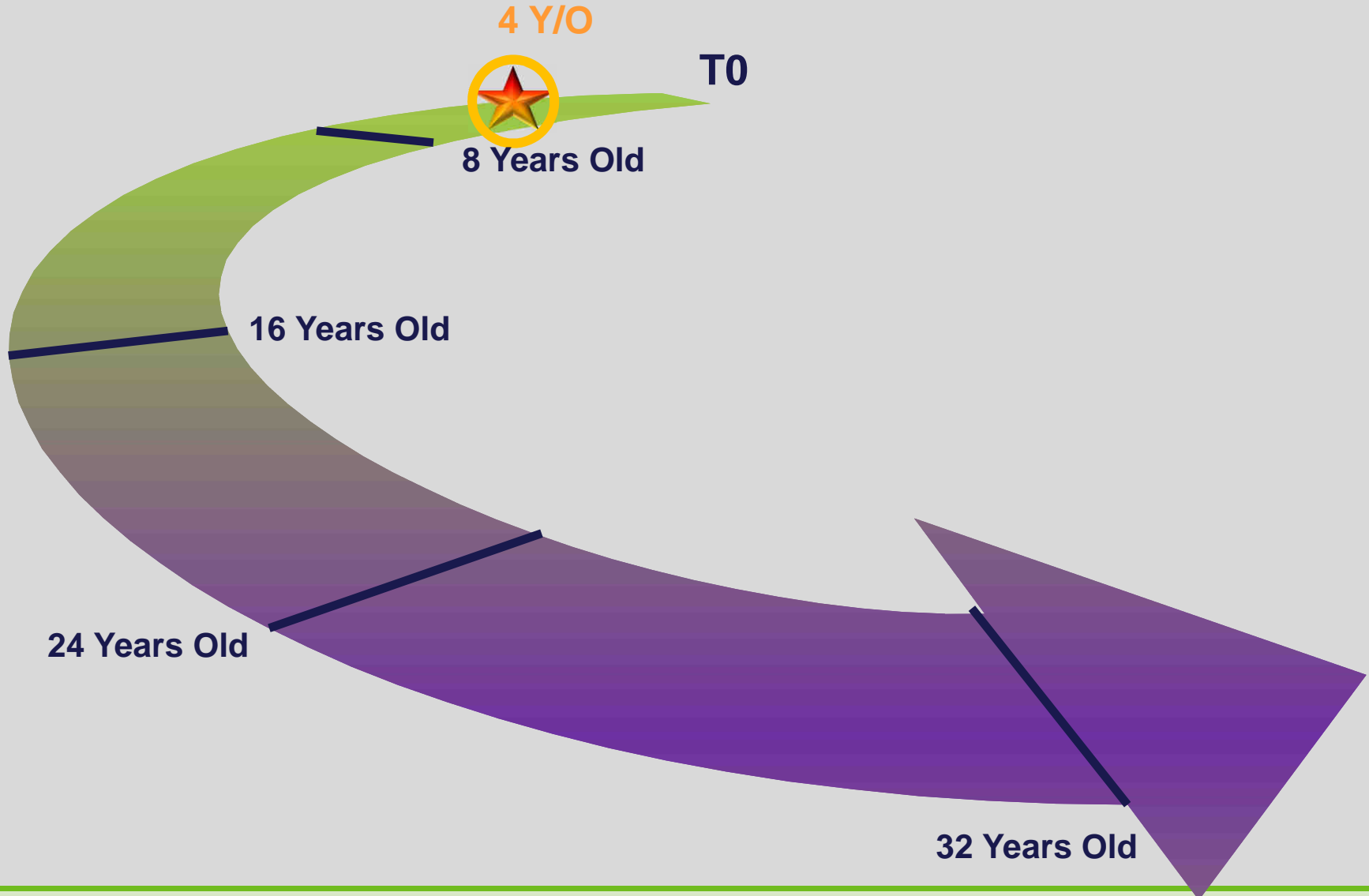
A December 10<sup>th</sup>, 1977...in Bahia Blanca...





# My becoming a scientist...

- Becoming a scientist
- Research motivations
- Research contribution
- Perspectives





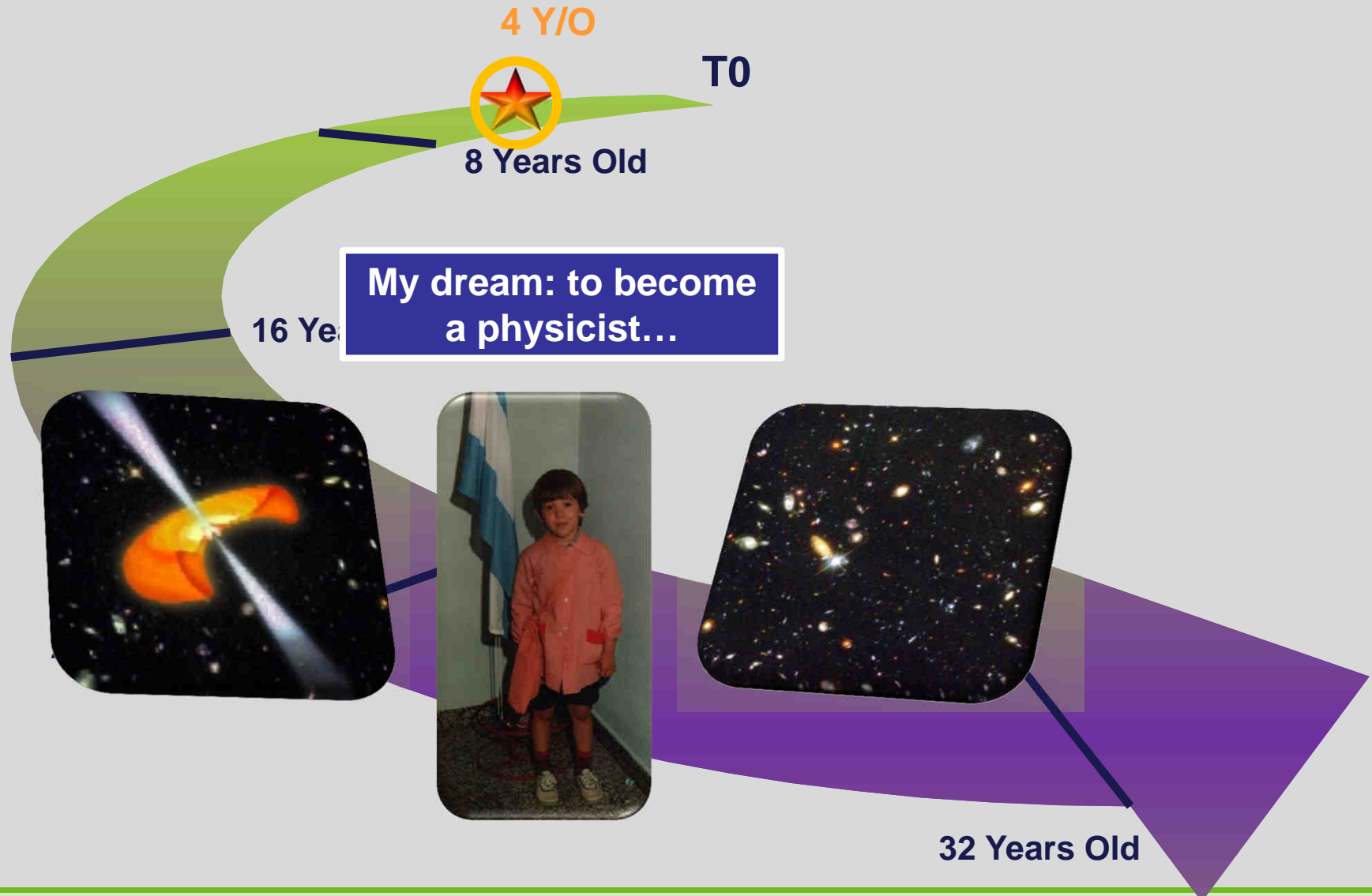
# My becoming a scientist...

Becoming a scientist

Research motivations

Research contribution

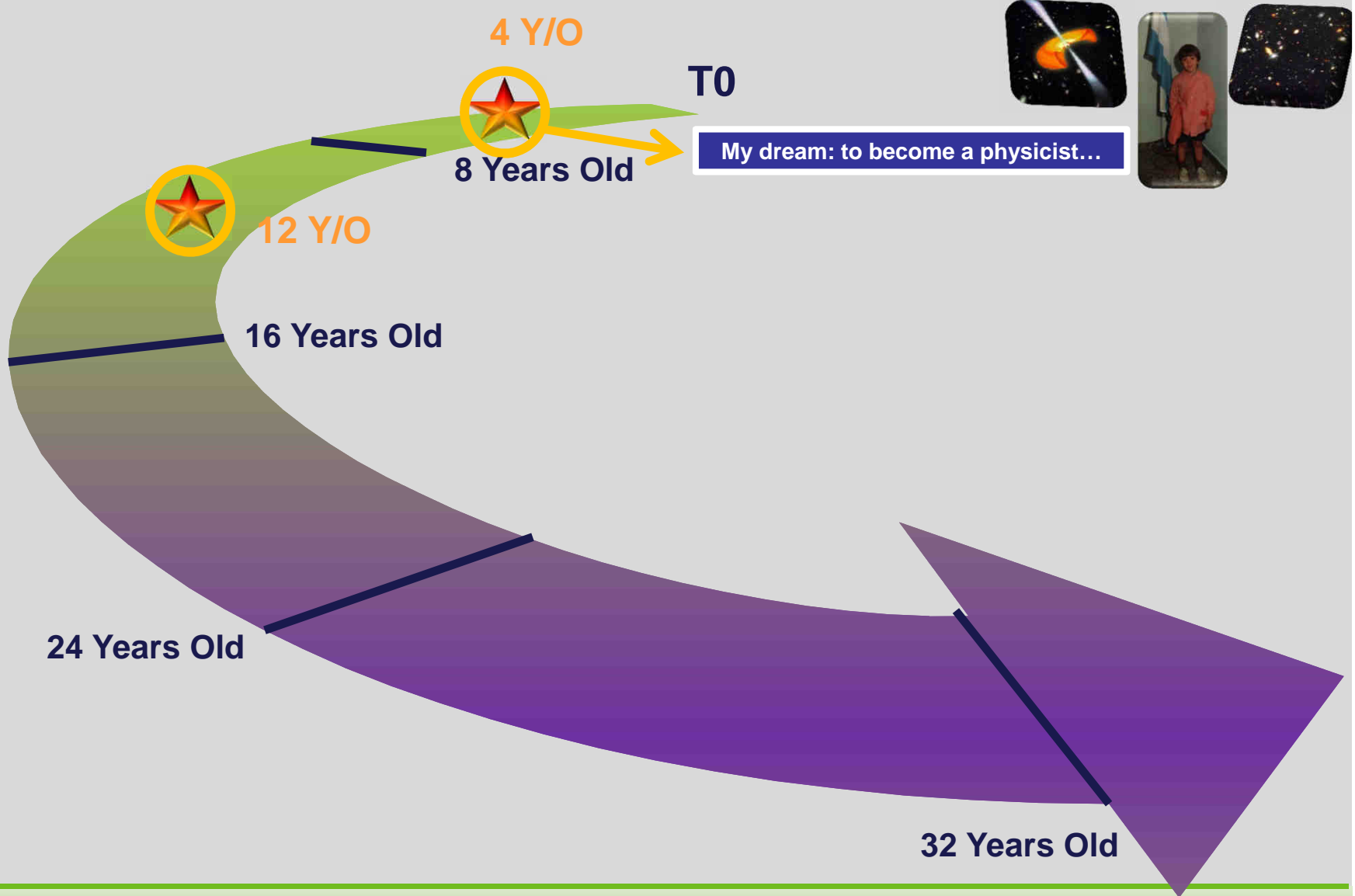
Perspectives





- Becoming a scientist
- Research motivations
- Research contribution
- Perspectives

# My becoming a scientist...





# My becoming a scientist...



4 Y/O



T0

My dream: to become a physicist...

8 Years Old



12 Y/O

My hydrogen machine (first patent)...

Becoming a scientist

Research motivation

Research contribution

Perspectives



FERIA LOCAL DE LAS CIENCIAS Y LA TECNOLOGIA ESCUELAS MEDIAS DE LA UNIVERSIDAD NACIONAL DEL SUR



AÑO 1993



32 Years Old



# My becoming a scientist...



My first hydrogen machine (first patent)...

4 Y/O



8 Years Old

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My dream: to become a physicist...



Becoming a scientist

Research motivations

Research contribution

Perspectives

12 Y/O



16 Years Old

19 Y/O



24 Years Old

32 Years Old





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My first hydrogen machine (first patent)...

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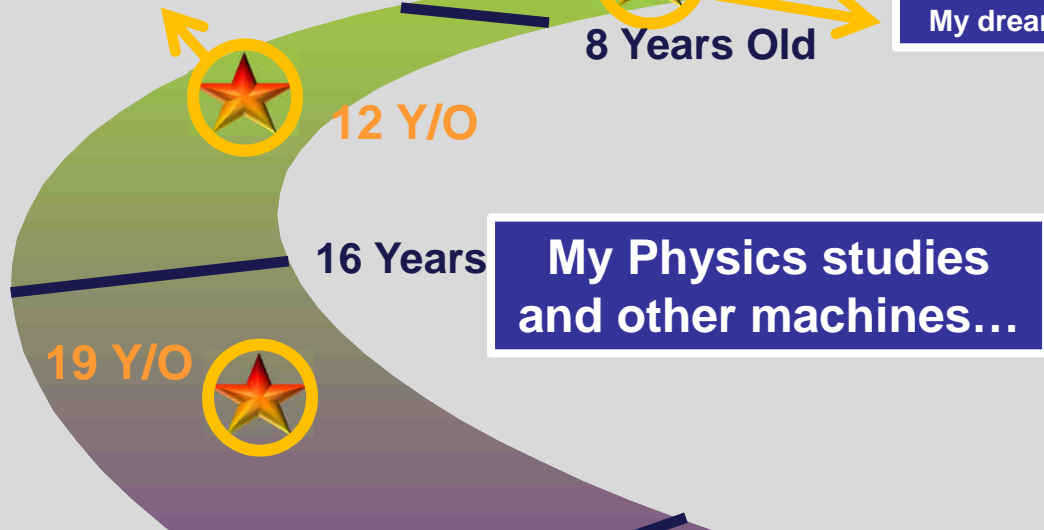


Becoming a scientist

Research motivations

Research contribution

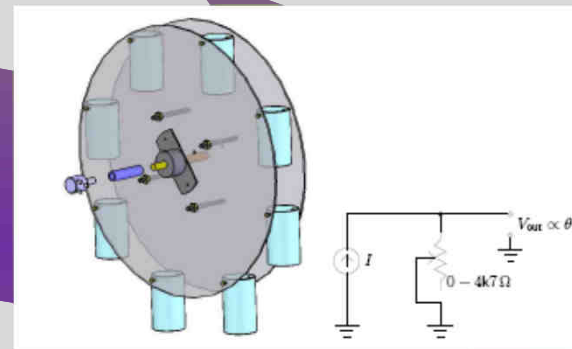
Perspectives



Universidad Nacional del Sur



Instituto Balseiro



32 Years Old



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My first hydrogen machine (first patent)...

4 Y/O



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Becoming a scientist

Research motivations

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Perspectives

12 Y/O



16 Years Old

My Physics studies and other machines...



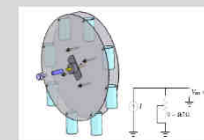
19 Y/O



24 Years Old



32 Years Old



cea

# My becoming a scientist...

liton

Components for Polymer electrolyte fuel cells and Electrolysers, and of Modelling  
LCPEM



My first hydrogen machine (first patent)...

4 Y/O



8 Years Old

T0

My dream: to become a physicist...



Becoming a scientist

Research motivations

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12 Y/O



16 Years Old

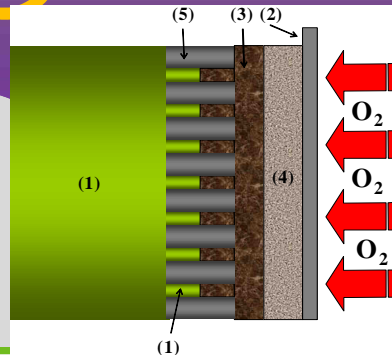
19 Y/O



24 Years Old



My arrival to France and 2002 stay at CEA...



### Références

- 1) Électrolyte
- 2) Plaque collectrice
- 3) Couche active
- 4) Couche de diffusion
- 5) Aimant permanent

DETAIL BARRE - AIMANT  
Couche protection anti-corrosion



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Dr. Alejandro A. Franco - H.D.R. Derense, Grenoble, Sep.23<sup>rd</sup>, 2010.



# My becoming a scientist...



My first hydrogen machine (first patent)...

4 Y/O



8 Years Old

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My dream: to become a physicist...



Becoming a scientist

Research motivations

Research contribution

Perspectives

12 Y/O



16 Years Old

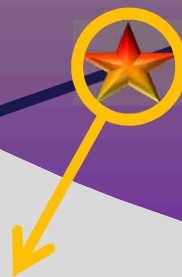
My Physics studies and other machines...



19 Y/O



24 Years Old



My arrival to France and 2002 stay at CEA...



32 Years Old



# My becoming a scientist...



My first hydrogen machine (first patent)...

4 Y/O



8 Years Old

T0

My dream: to become a physicist...



Becoming a scientist

Research motivations

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12 Y/O



16 Years Old

My Physics studies and other machines...

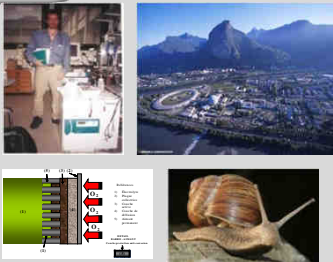


19 Y/O



24 Years Old

My arrival to France and 2002 stay at CEA...



My young scientist life

32 Years Old



# My becoming a scientist...

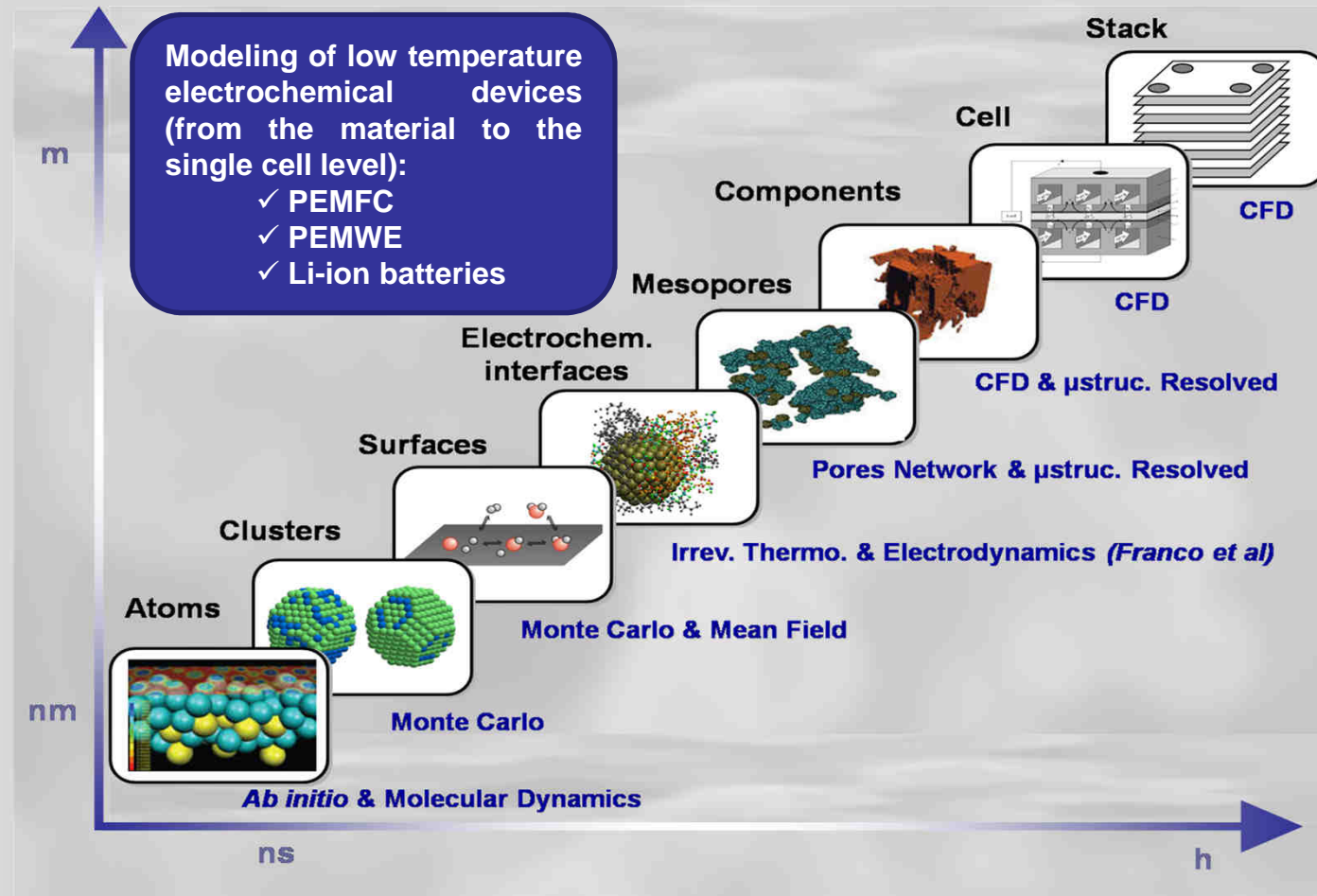
- Jan 2003 – Nov 2005: PhD student (CEA-UCBL LAGEP) → PEMFC multiscale modeling
- From Dec 2005: permanent researcher at CEA-LCPEM
- From Jan 2006: WP leader in 7 national and 4 international projects
- From Apr 2009: leader of the Modeling Group at CEA-LCPEM (4 permanents, 3 postdocs, 9 PhD students, 1 MSc. Student)

Becoming a scientist

Research motivations

Research contribution

Perspectives





# My becoming a scientist...

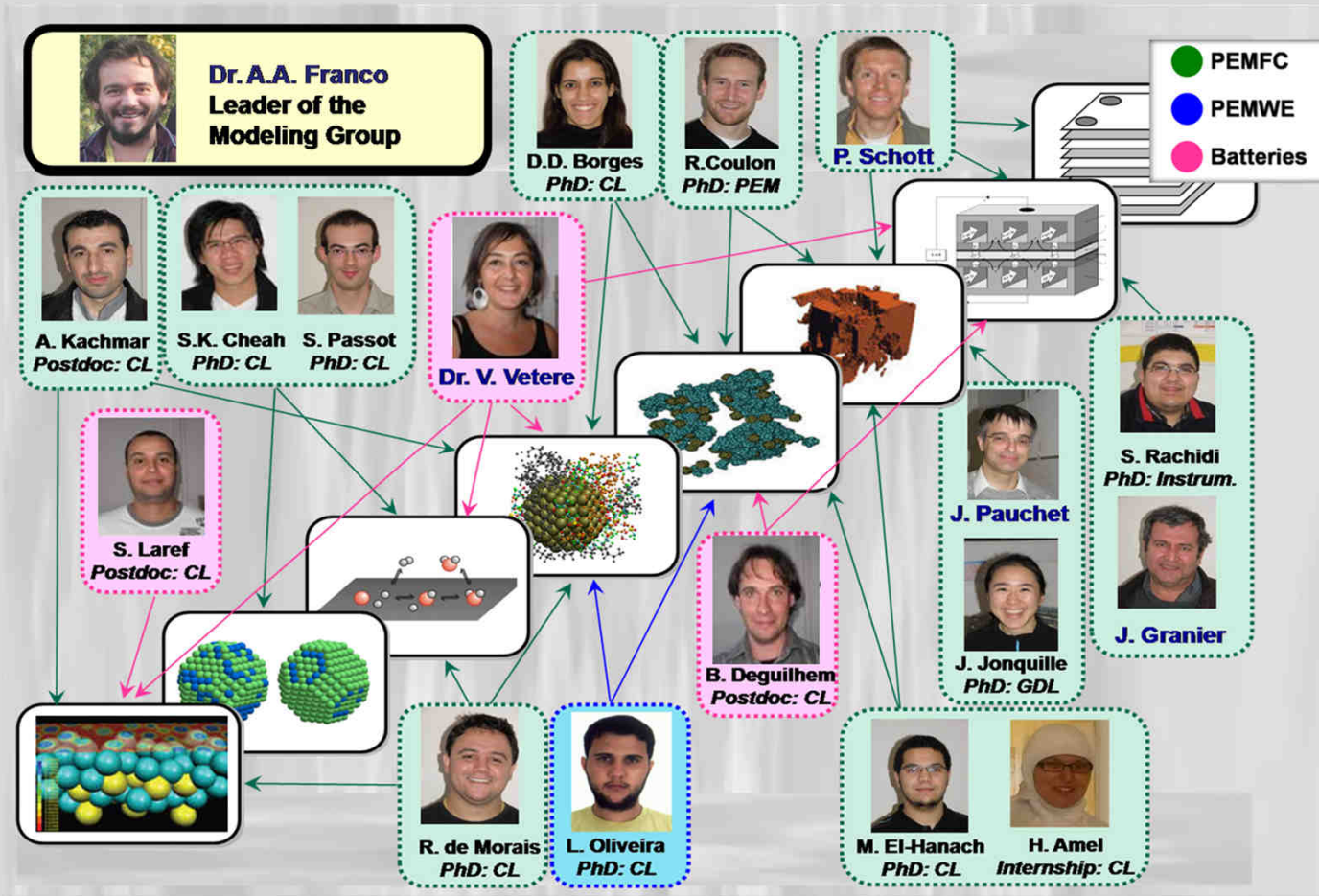
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Becoming a scientist

Research motivations

Research contribution

Perspectives





# My research motivations within PEM Fuel Cells

➤ **PEMFC:** electric generator by transformation of the energy “stored” in molecular hydrogen. *Concept:* 1838 (Sir Grove); *first PEMFC:* 1959 (Grubb & Niedrach); *first modern PEMFC:* 1991 (LANL).

### Some advantages:

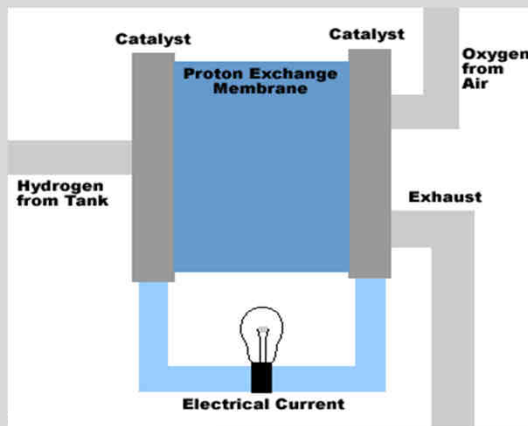
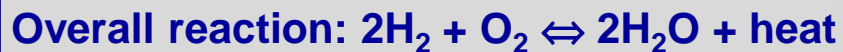
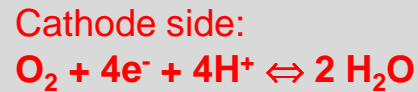
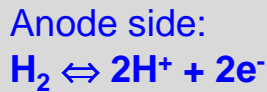
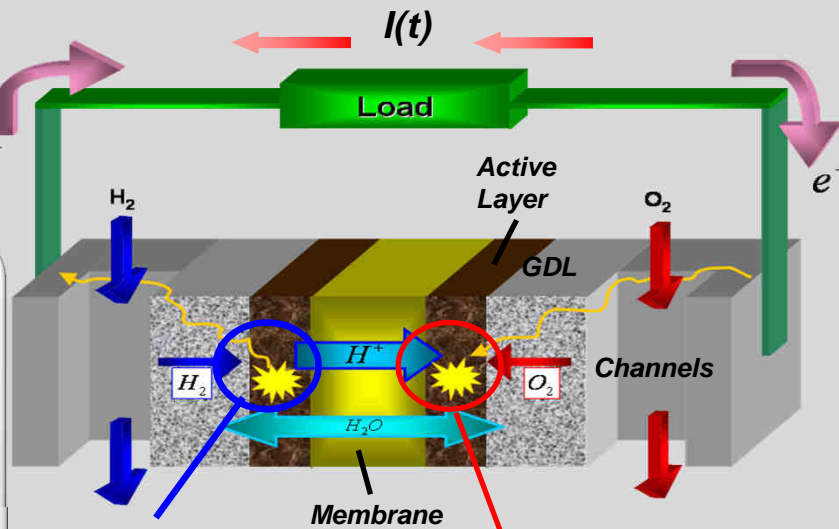
Fast start-up, dynamic operation with shutdown (low working temperature), compact units, lot of applications from portable electronics to vehicles  
⇒ Most important developments during the last ten years

Becoming a scientist

Research motivations

Research contribution

Perspectives







# My research motivations within PEM Fuel Cells

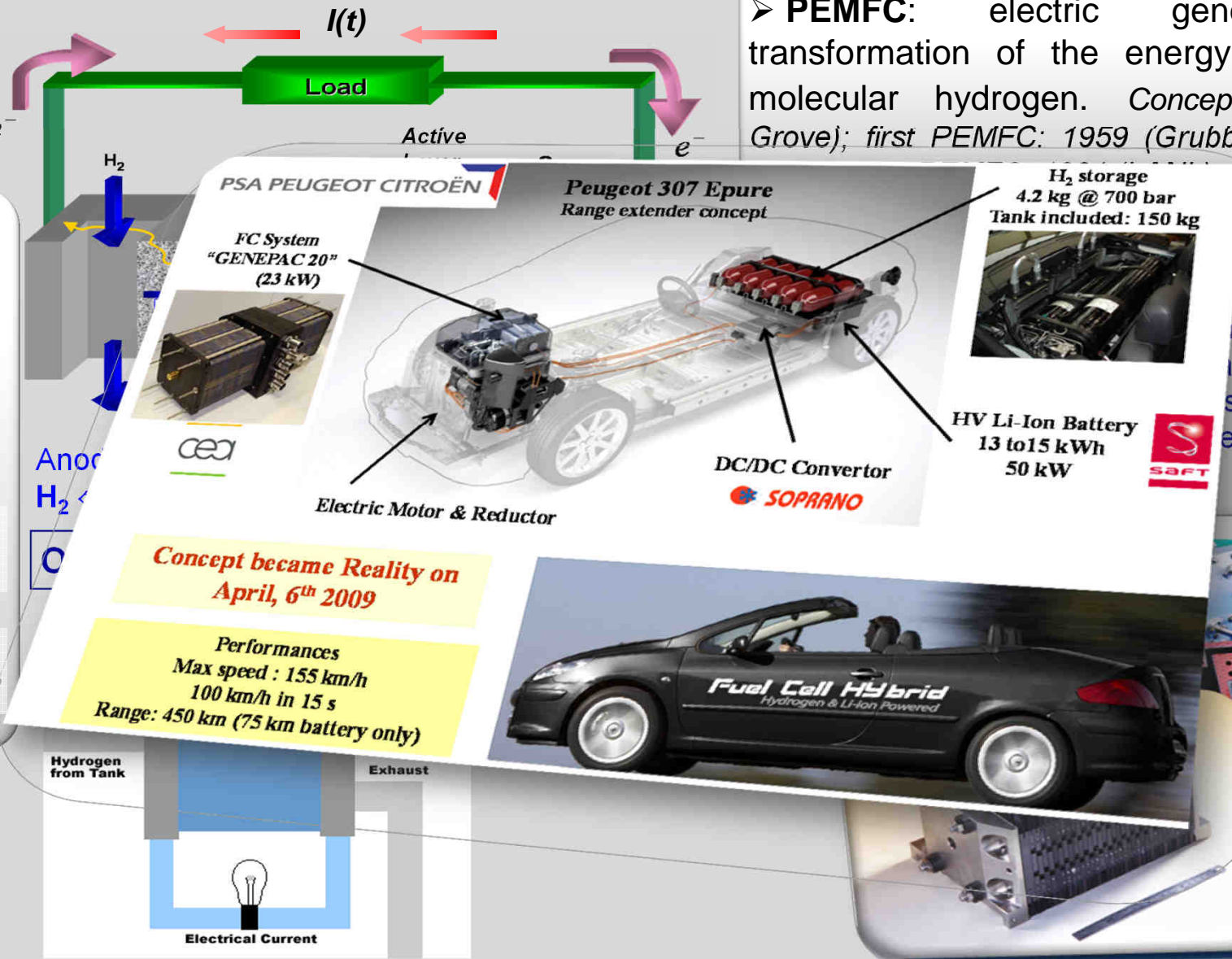
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Becoming a scientist

Research motivations

Research contribution

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# My research motivations within PEM Fuel Cells

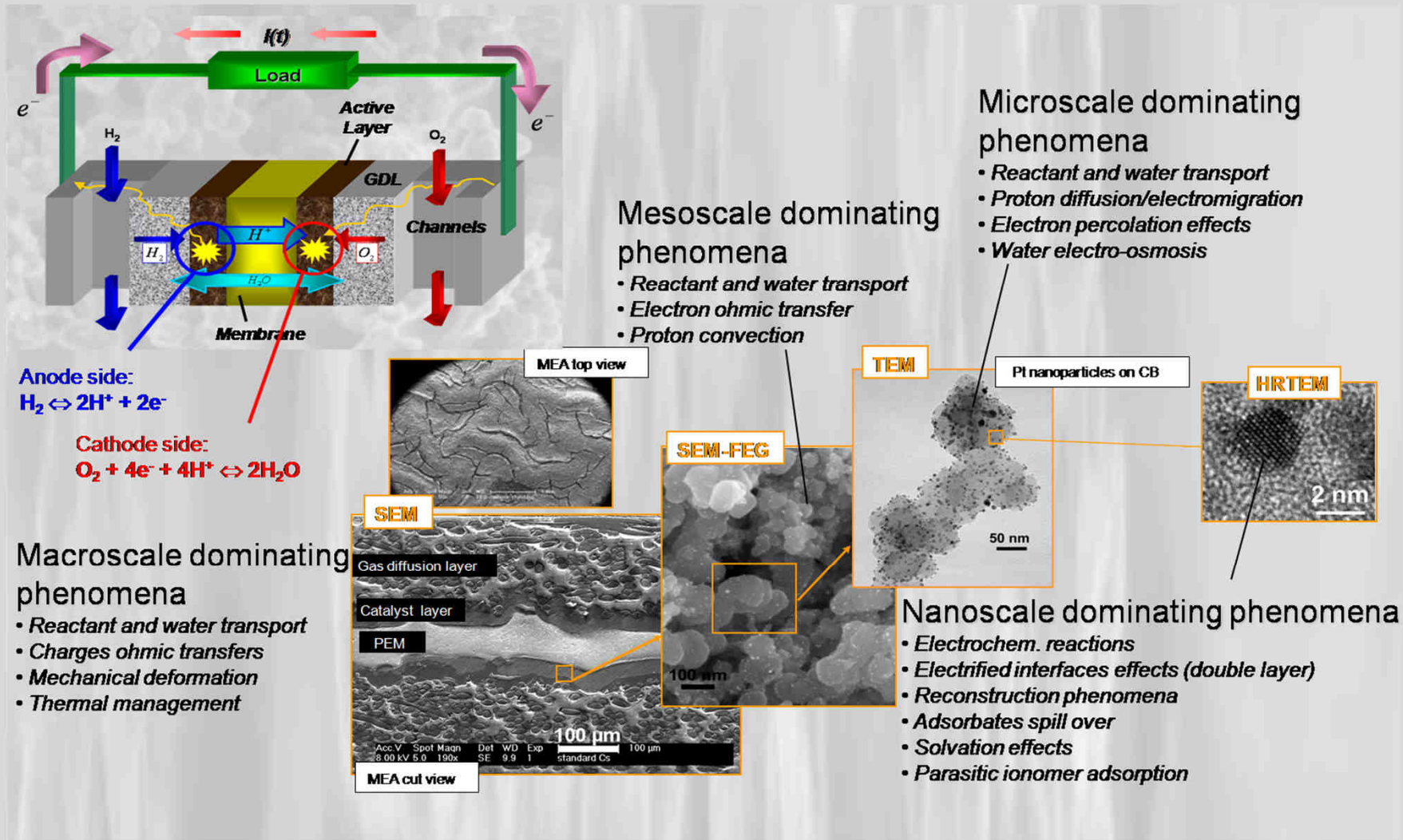
Becoming a scientist

Research motivations

Research contribution

Perspectives

□ PEMFC: strong coupling between physicochemical phenomena occurring at different spatiotemporal scales → complex multiphysics system





# My research motivations w

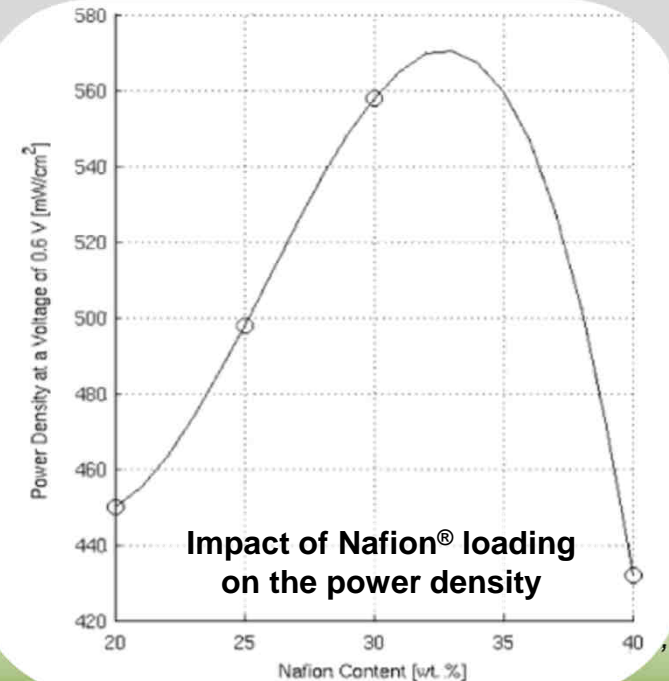
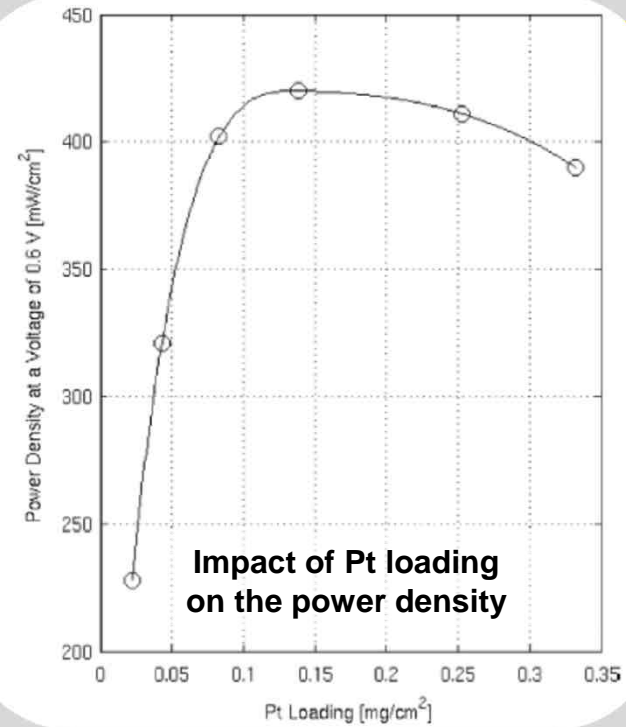
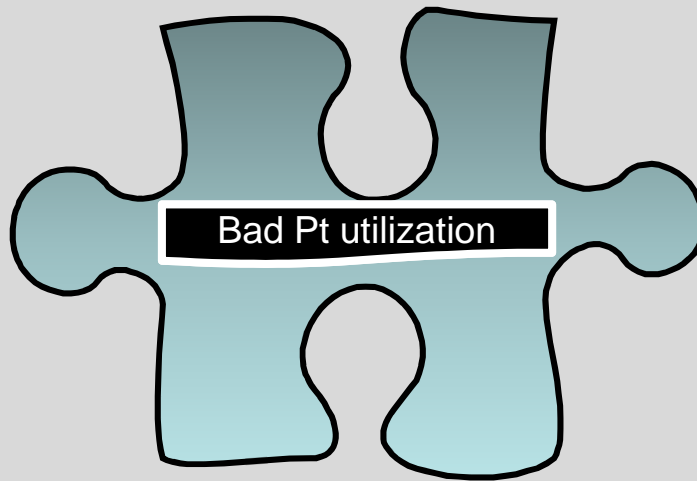
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Becoming a scientist

Research motivations

Research contribution

Perspectives

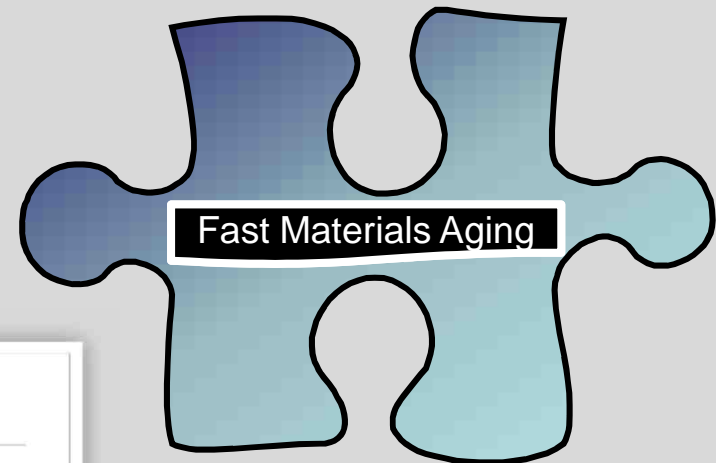
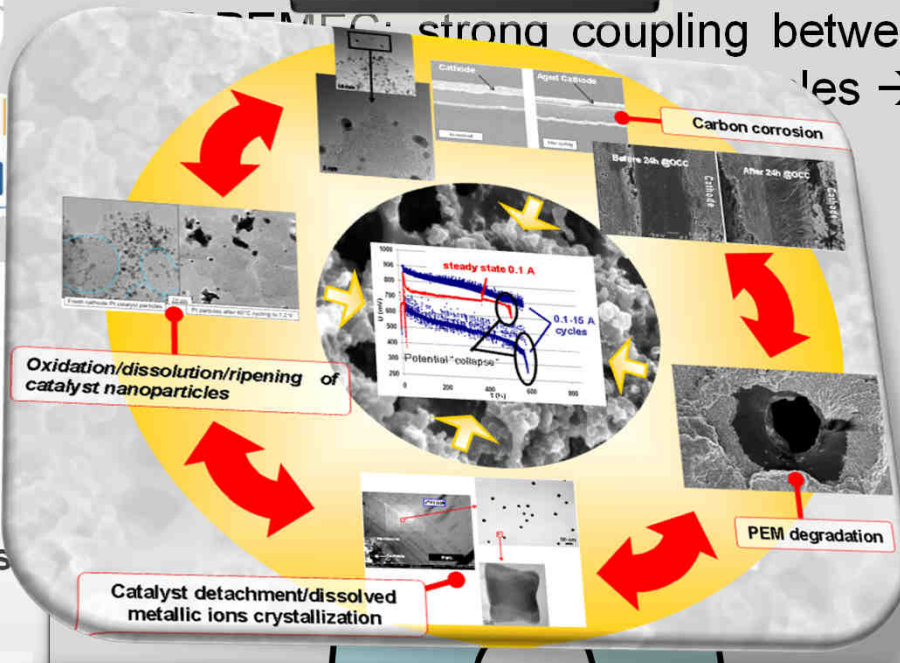


different

# My research motivations within PEM Fuel Cells

Degradation processes

strong coupling between physicochemical phenomena occurring at different scales → complex multiphysics system

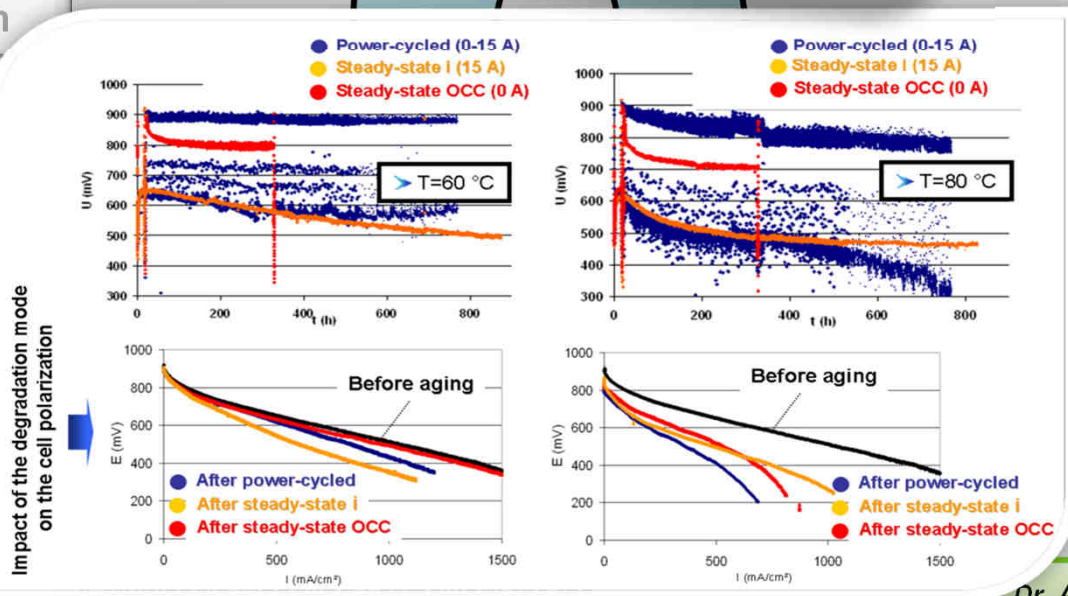


Becoming a scientist

Research motivations

Research contribution

Perspectives



Transient Analysis of PEMFCs



# My research motivations within PEM Fuel Cells



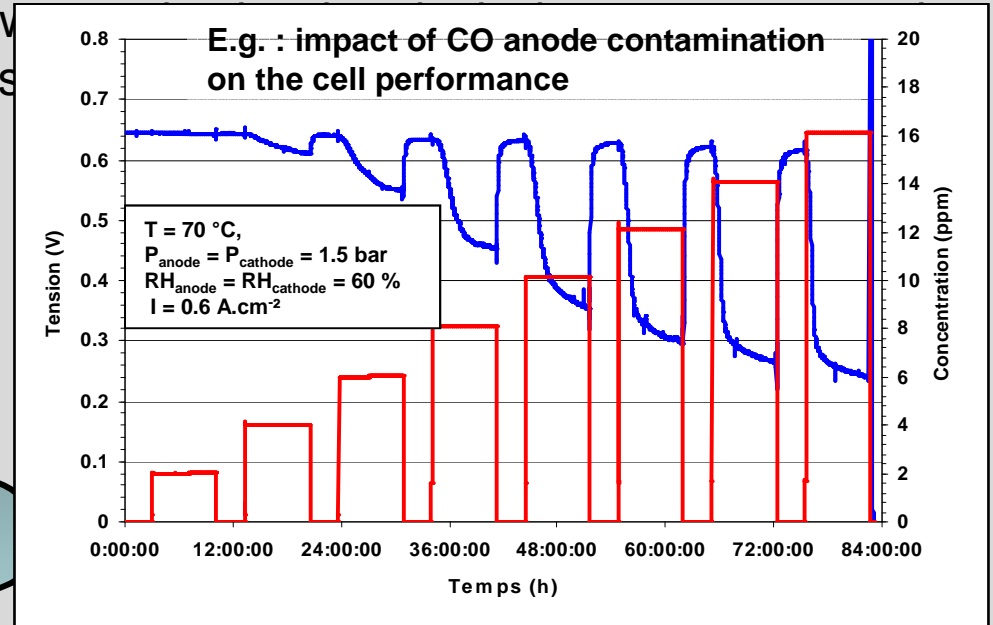
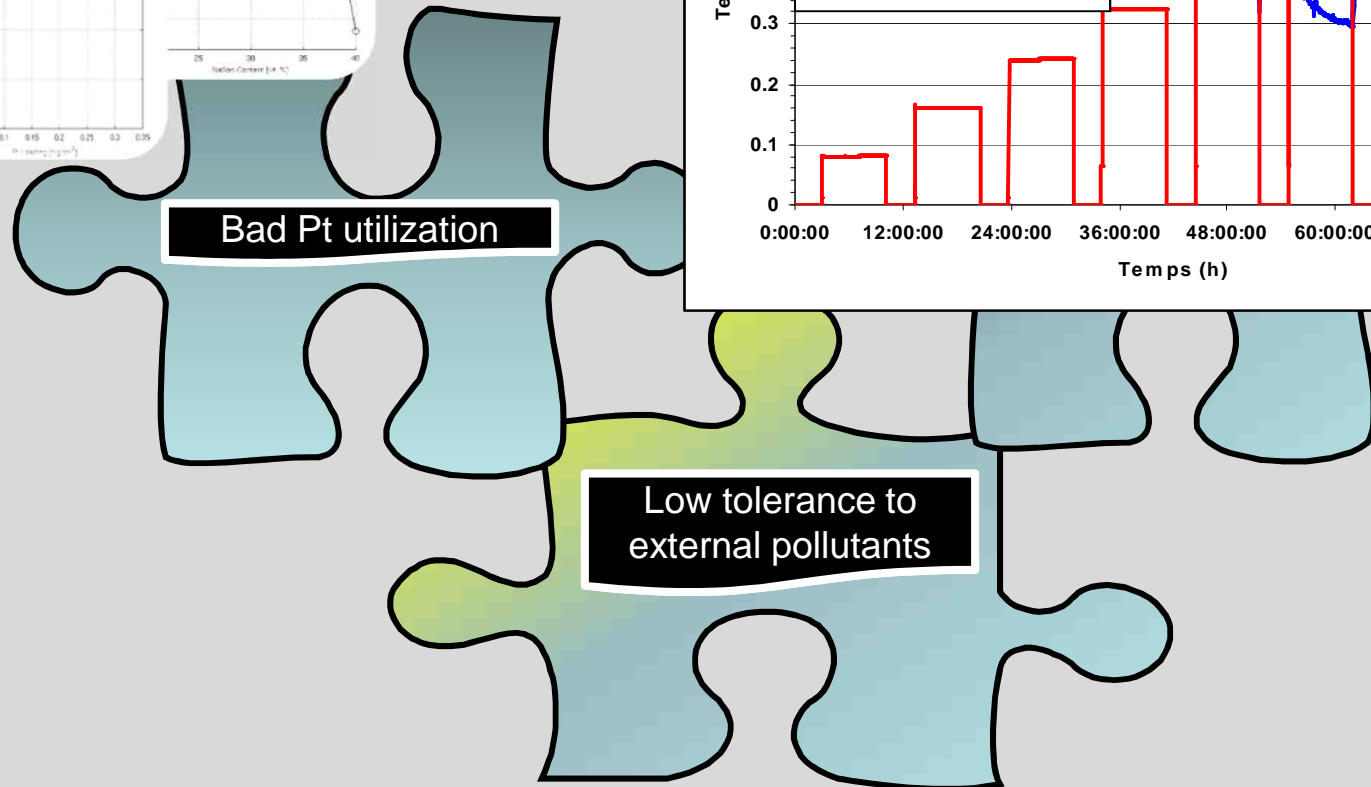
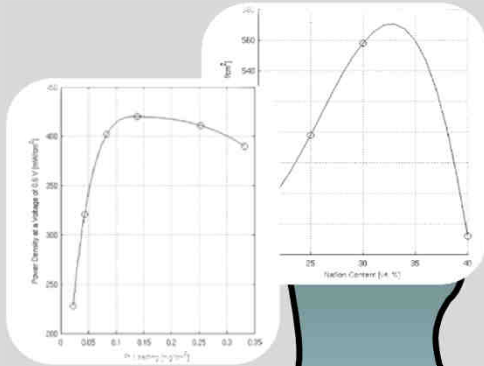
Becoming a scientist

Research motivations

Research contribution

Perspectives

□ PEMFC: strong coupling between different spatiotemporal scales





# My research motivations within PEM Fuel Cells

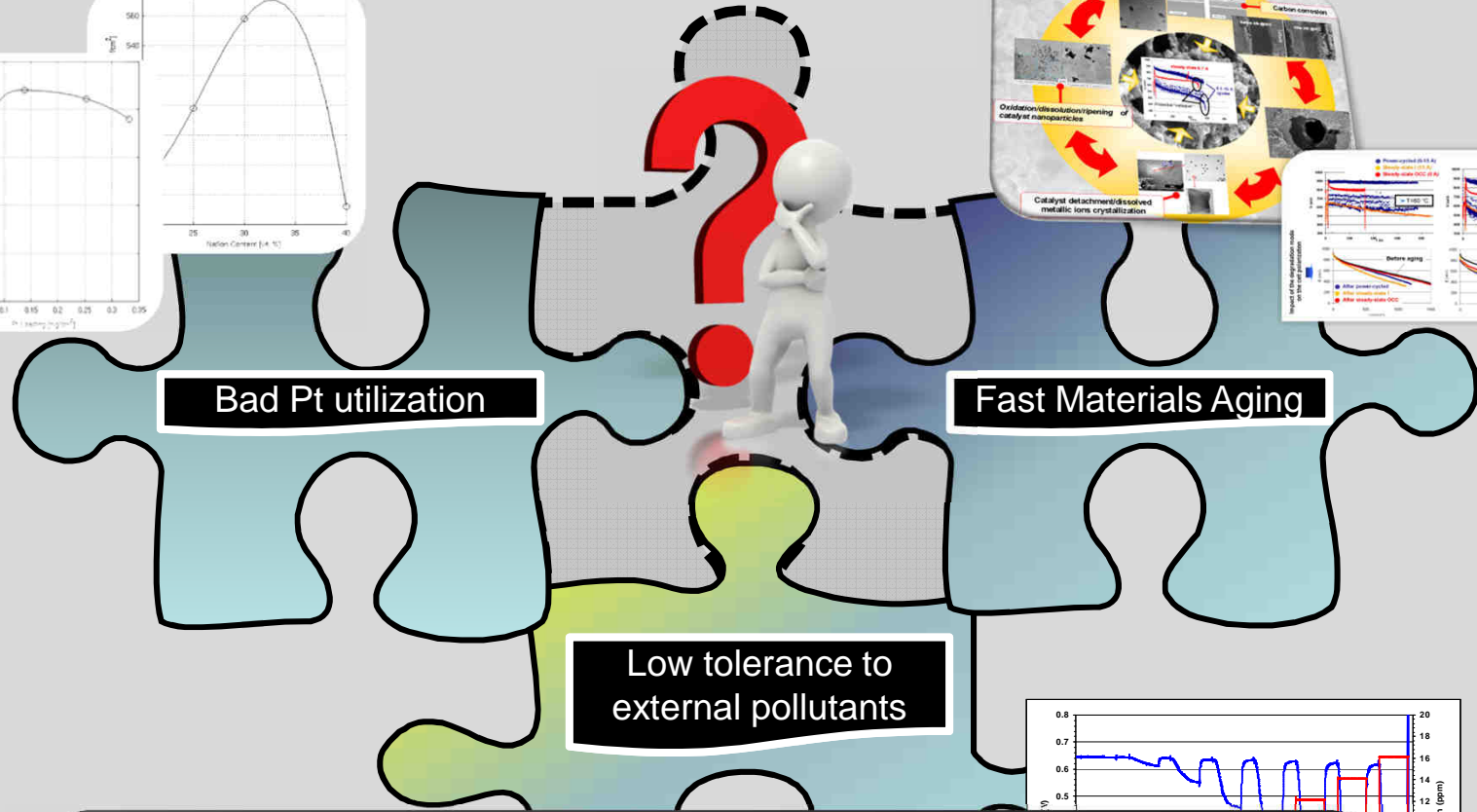
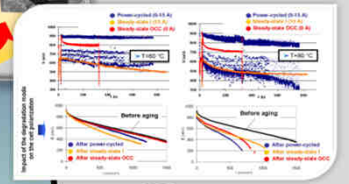
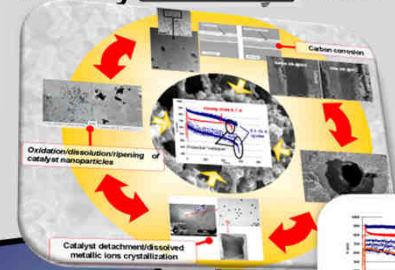
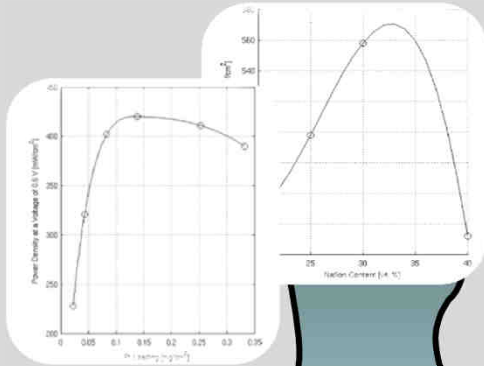
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Becoming a scientist

Research motivations

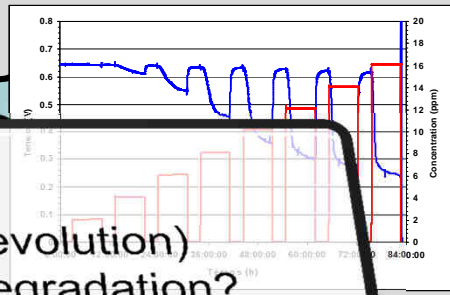
Research contribution

Perspectives



### Current questions in engineering practice:

- How predict MEA durability? (cell-potential evolution)
- Operation modes mitigating cell potential degradation?
- How design accelerated test representative of long-term aging mechanism(s) effect?





# Physical modeling in engineering practice



Becoming a scientist

Research motivations

Research contribution

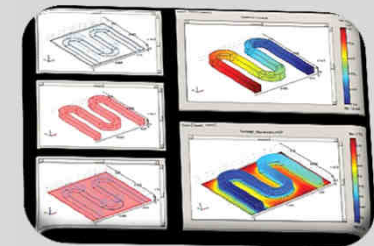
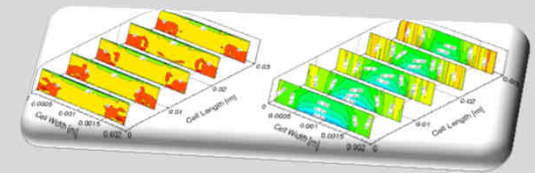
Perspectives

Some available modeling approaches of PEMFC performance:

→ CFD (detailed description of thermofluidics, charge transport phenomena, simplified electrochemistry -Butler Volmer theory-): e.g. C.Y. Wang.

→ Analytical, model reduction: e.g. M. Eikerling, A. Kulikovskiy.

→ PEMFC as a complex physical system constituted by several sub-systems in interaction (Bond Graphs): e.g. my PhD thesis (2003-2005).

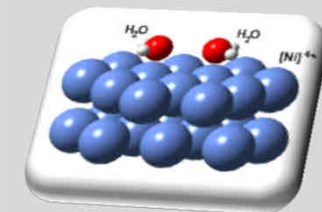
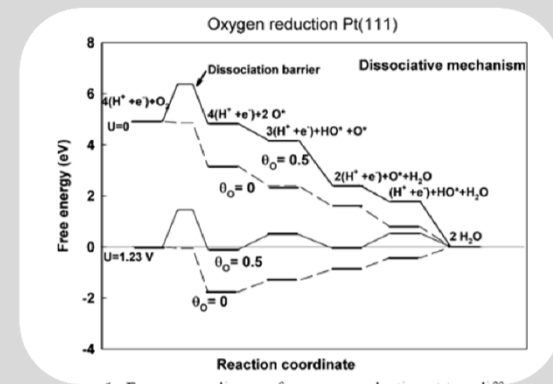


Some available modeling approaches of PEMFC materials:

→ DFT (e.g. detailed description of electrochemical reactions), challenges: e.g. T. Jacob, J. Nørskov (challenges:  $T > 0$  K, solvent + ionomer, electric field, scaling up into kinetic models)

→ MD (detailed description of transport processes): e.g. E. Spohr, S. Paddisson,

→ CGMD (mesoscale MD, prediction of CLs self-organization): e.g. K. Malek, M. Eikerling.



# Modeling of degradation phenomena: review and challenges

Becoming a scientist

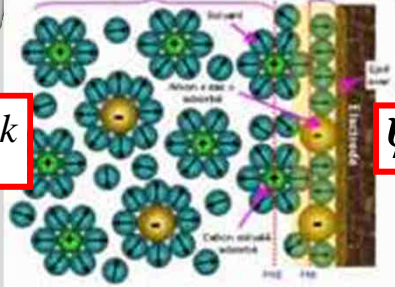
Research motivations

Research contribution

Perspectives

Mechanism	Example
Pt/C-ionomer interface delamination	
C corrosion	<p>Rong <i>et al.</i>: Model region for the contact between ionomer and catalyst powder; purple domain represents the C/Pt agglomerate and the cyan domain represents ionomer [217].</p> <p><math>O_2 + 4H^+ + 4e^- \leftrightarrow 2H_2O</math>      <math>C + 2H_2O \rightarrow CO_2 + 4H^+ + 4e^-</math></p> <p>Fuller <i>et al.</i>: Impact of hydrogen concentration heterogeneities on cathode C corrosion [189].</p>
PEM degradation	<p>Shah <i>et al.</i>: A schematic of the MEA and definitions of the positions along the thickness coordinate <math>y</math>. A schematic of the peroxide/radical formation, backbone unzipping, and side-chain cleavage is also shown [213].</p>

Mechanism	Example
Pt oxidation	<p>Jacob: Bulk-unitcells of the three most stable Pt-oxides: <math>\alpha</math>-PtO<sub>2</sub>, <math>\beta</math>-PtO<sub>2</sub>, PtO. Dark spheres indicate Pt atoms, while bright ones are oxygens [22].</p>
Pt coarsening	<p>Chen <i>et al.</i>: Two clusters with 50 Pt atoms during aggregation (left: before, right: after 2 ns) [247].</p>
Bimetallic nanoparticles reconstruction	<p>Zhu <i>et al.</i>: Impact of the environment on the nanoparticle reconstruction Structures of Rh<sub>5</sub>Pt<sub>5</sub> clusters at 304 K predicted by MD simulations (a) in the absence of hydrogen and (b) in the presence of hydrogen. Pt atoms are white, Rh atoms are grey, and H atoms are black [224].</p>
Bimetallic nanoparticles electrochemical dissolution	<p>Greeley and Norskov: impact of bimetallic catalysts composition on their stability (dissolution potential) [225].</p>



Electrochemical double layer

$$\phi^{bulk}$$

$$W \propto \exp\left(\frac{\alpha e_0 E}{k_B T}\right) = \exp\left(\frac{\alpha e_0 (\psi - \phi^{bulk})}{k_B T}\right)$$

$$\theta_O = 1 - \theta_{Pt}$$



# Modeling of degradation phenomena: review and challenges

Mechanism	Example
Use of Butler-Volmer approach (frequently potentiostatic conditions) and lack of connection with <i>ab initio</i> data.	
No account for feedback between performance and degradation: U(t) and MEA structure evolution not captured.	$O_2 + 4H^+ + 4e^- \leftrightarrow 2H_2O$ $C + 2H_2O \rightarrow CO_2 + 4H^+ + 4e^-$
Aging phenomena addressed in a separated way	
Electrochemical double layer	$W \propto \exp\left(\frac{\alpha e_0 E}{k_B T}\right) = \exp\left(\frac{\alpha e_0 (\psi - \phi^{bulk})}{k_B T}\right)$ $\theta_O = 1 - \theta_{Pt}$

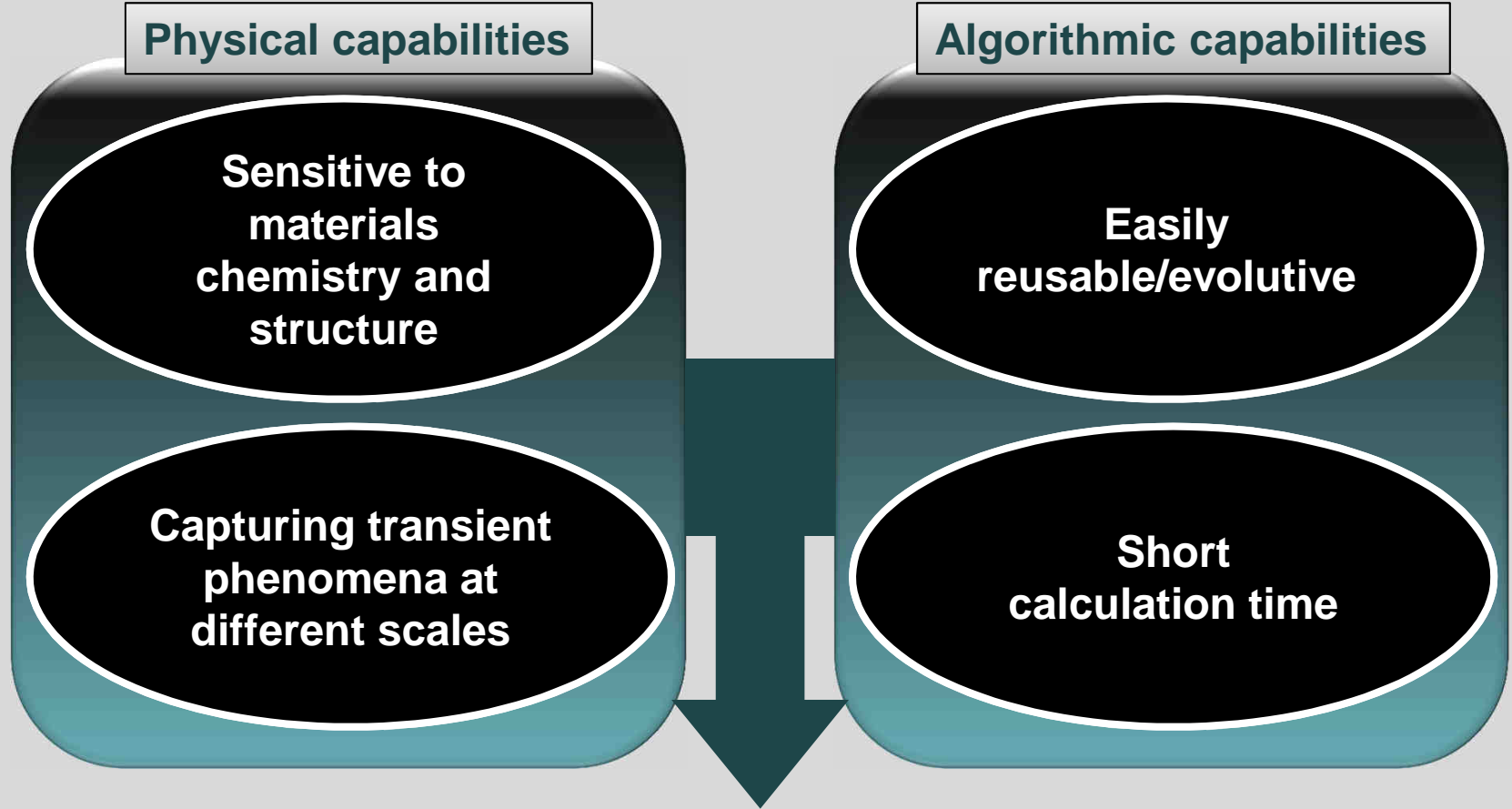
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Lack of connection with microkinetics	Chen et al.: Two clusters with 50 Pt atoms during aggregation (left: before, right: after 2 ns) [24].
Bimetallic nanoparticles reconstruction	Zhu et al.: Impact of the environment on the nanoparticle reconstruction Structures of Rh <sub>25</sub> Pt <sub>25</sub> clusters at 304 K predicted by MD simulations (a) in the absence of hydrogen and (b) in the presence of hydrogen. Pt atoms are white, Rh atoms are grey, and H atoms are black [23].
Bimetallic nanoparticles electrochemical dissolution	Greeley and Norskov: impact of bimetallic catalysts composition on their stability (dissolution potential) [235].



- Becoming a scientist
- Research motivations
- Research contribution
- Perspectives

# “Ideal model”: needs from an industrial viewpoint

☐ “Time is money”: typical cost of a single cell 500 h durability test = 1000 euros (+ test line=95000 euros) → need of *in silico* experiments to speed up the PEMFC development.



Interpretation of experiments, design of operation modes-materials for improved performance and durability in conditions as close as possible to the end-user application



# My multiscale model of PEMFC: MEMEPhys<sup>®</sup>

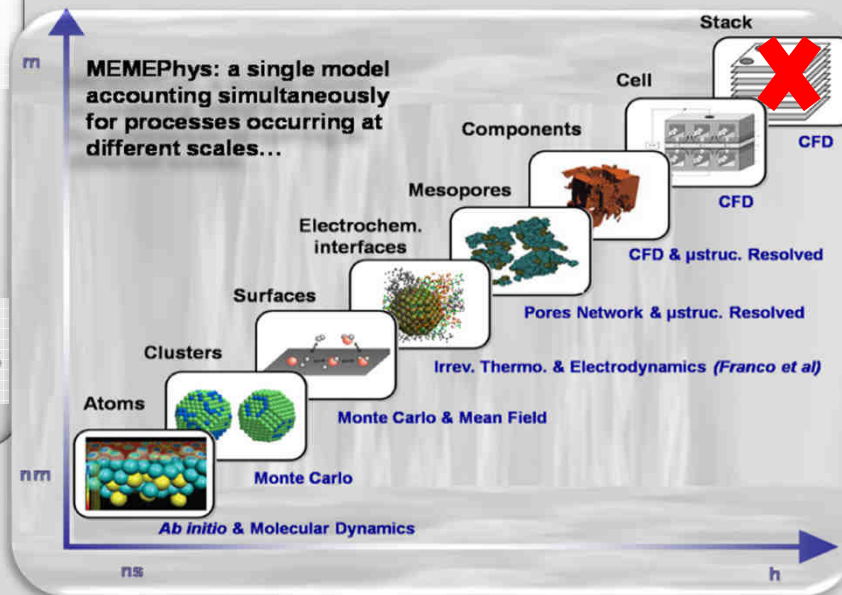
- MEMEPhys<sup>®</sup> (9 years of development by myself): multiscale mechanistic model of the electrochemical processes, scaling up *ab initio* concepts into an irreversible thermodynamics framework, accounting, within a *continuum* framework, for:
  - the MEA physicochemistry at spatial nano, micro and mesoscales, GDL and channels at the macroscale
  - the intrinsic MEA nanomaterials degradation and couplings between aging mechanisms

Becoming a scientist

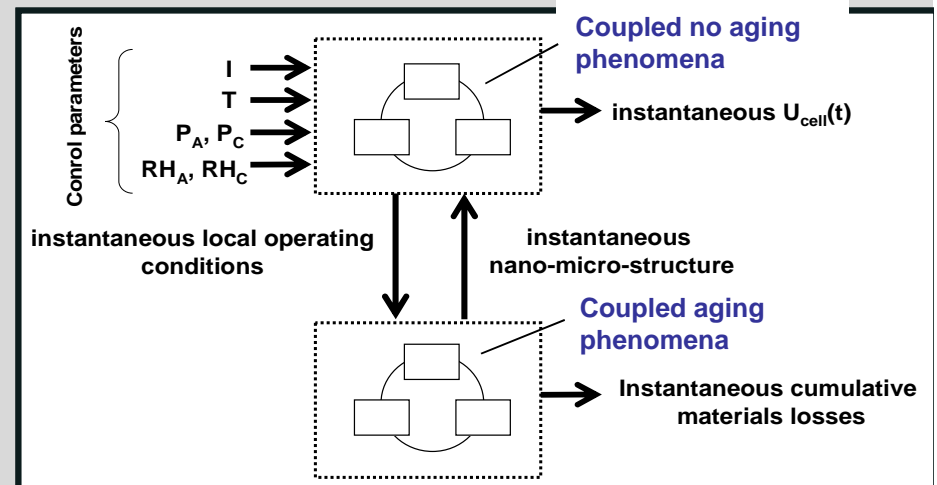
Research motivations

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**Description of the feedback between performance and aging: DURABILITY PREDICTION (unique in literature)**



**A Multiscale Modeling Framework for the Transient Analysis of PEMFCs**

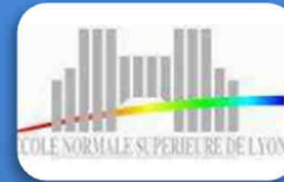
A.A. Franco et al., *J. Electrochem. Soc.* **153** (6) A1053 (2006).  
 A.A. Franco et al., *J. Electrochem. Soc.*, **154** (7) B712 (2007).  
 A.A. Franco et al., *Fuel Cells*, **7** (2) 99 (2007).  
 A.A. Franco et al., *J. Electrochem. Soc.*, **155** (4) B367 (2008).



# My multiscale model of PEMFC: MEMEPhys<sup>®</sup>

MEMEPhys<sup>®</sup> (9 years of development by myself): multiscale mechanistic model of the PEMFC into an irreversible framework, for:

Some partnerships (ANR/EU projects, bilateral projects, PhD thesis...)



Becoming a scientist

Research motivations

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feedback  
aging: DURABILITY  
in literature)

Coupled no aging  
phenomena

→ instantaneous  $U_{cell}(t)$

instantaneous  
micro-structure

Coupled aging  
phenomena

→ Instantaneous cumulative  
materials losses



- Becoming a scientist
- Research motivations
- Research contribution
- Perspectives

# MEMEPhys<sup>®</sup> capabilities

## Physical capabilities

**Sensitive to materials chemistry and structure**

**Capturing transient phenomena at different scales**

## Algorithmic capabilities

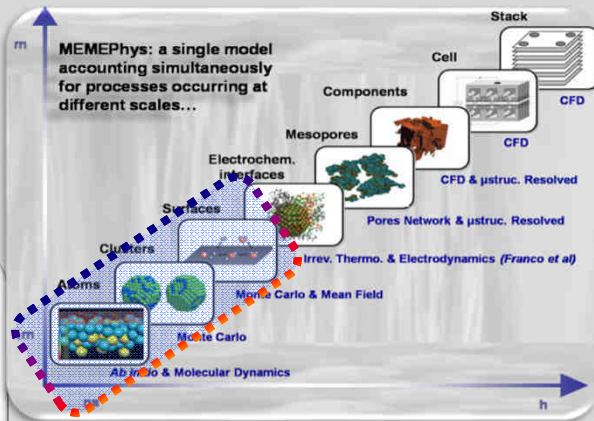
**Easily reusable/evolutive**

**Short calculation time**

**Interpretation of experiments, design of operation modes-materials for improved performance and durability in conditions as close as possible to the end-user application**



# Ab initio-based elementary kinetics @ MEMEPhys<sup>®</sup>



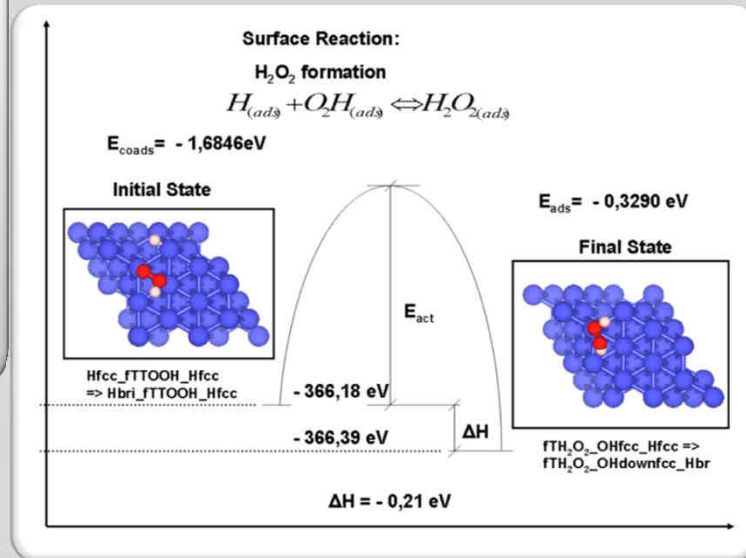
- ❑ No global reactions! No Butler-Volmer equations!
- ❑ DFT-generated database of adsorption and reactivity properties of Pt, Pt-free, Pt-M materials (surface PBC calculations -VASP-, for Pt and bimetallics 5/6-layer slab without solvent; or NPBC ADF).
- ❑ Databases of Pt, Pt-M, C and ionomer stability properties.
- ❑ Identification of most favorable reaction steps and pathways using NEB and integration in MEMEPhys<sup>®</sup> (DFT-based kinetic parameters: **initial guess values**).
- ❑ Captures nanostructural and chemistry properties of the materials.

Becoming a scientist

Research motivations

Research contribution

Perspectives



Step	Barrier in eV
O <sub>2</sub> dissociation	0.35
OH formation	0.95
H <sub>2</sub> O formation	0.20
OOH formation	0.35

$$k_i = \kappa \frac{k_B T}{h} \exp\left(-\frac{1}{RT} [\Delta G_r(t) + f_1(\eta_F(t)) + f_2(\theta_i(t))]\right)$$

current TS for the O<sub>2</sub> dissociation

current TS for the OH formation

current TS for the water formation

current TS for the OOH formation

$$v_1 = v_1(\tilde{\mu}_H, \mu_R, \theta_i, \eta_F)$$

$$v_2 = v_2(\tilde{\mu}_H, \mu_K, \theta_i, \eta_F)$$

...

$$v_N = v_N(\tilde{\mu}_H, \mu_O, \theta_j, \eta_F)$$

$$\tilde{K}_1 \frac{d\theta_1}{dt} = \sum_i v_i - \sum_j v_j'$$

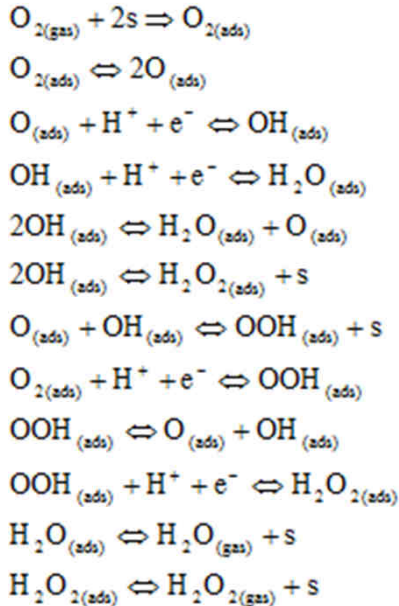
$$\tilde{K}_2 \frac{d\theta_2}{dt} = \sum_i v_i'' - \sum_j v_j'''$$

...

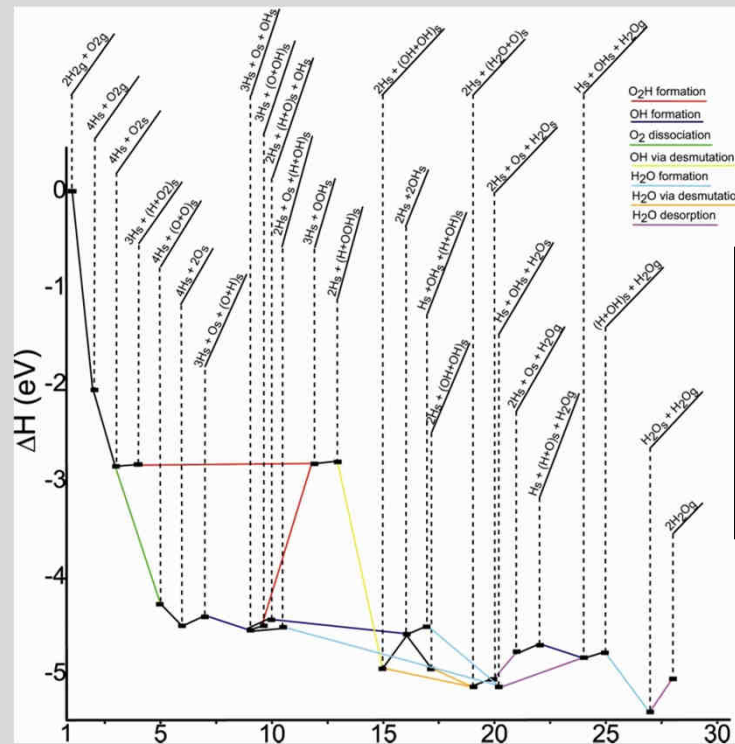
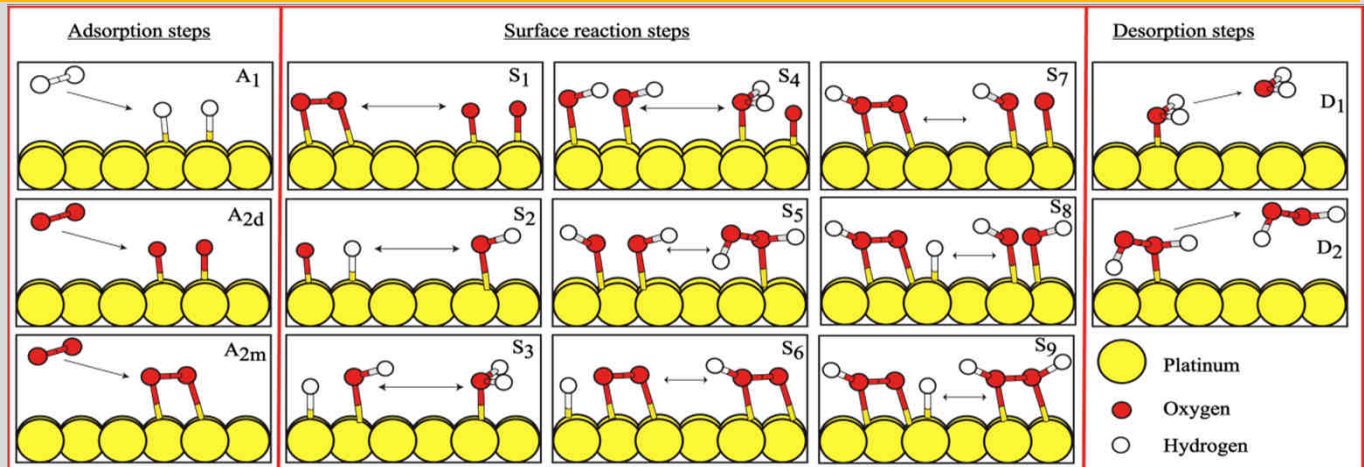
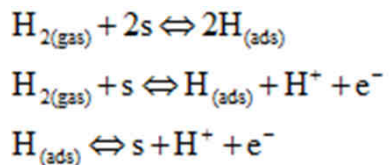
$$\tilde{K}_3 \frac{d\theta_3}{dt} = \sum_i v_i'''' - \sum_j v_j'''''$$

# Ab initio-based elementary kinetics @ MEMEPhys<sup>®</sup>

## ORR

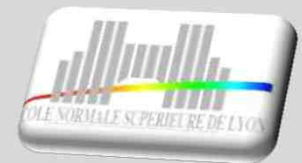


## HOR



Selected reaction mechanism for oxidation of hydrogen and the reduction of oxygen.

Low coverage thermodynamic profile of water formation through all the competitive elementary steps.





# Ab initio-based elementary kinetics @ MEMEPhys®

Becoming a scientist

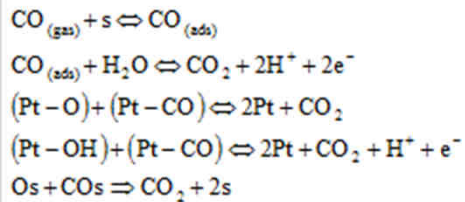
Research motivations

Research contribution

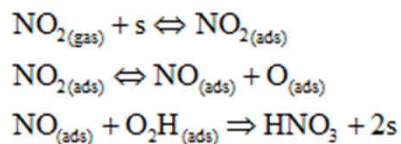
Perspectives

## Contamination reactions

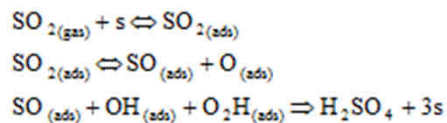
### CO poisoning



### NO<sub>2</sub> poisoning

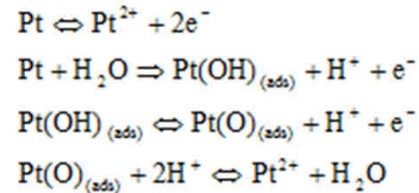


### SO<sub>2</sub> poisoning

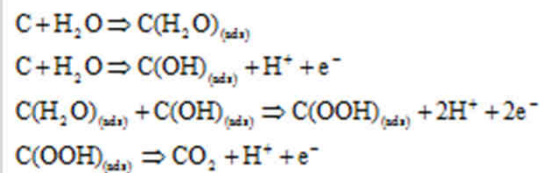


## Materials degradation

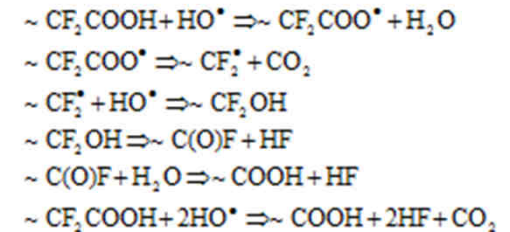
### Pt oxidation/dissolution



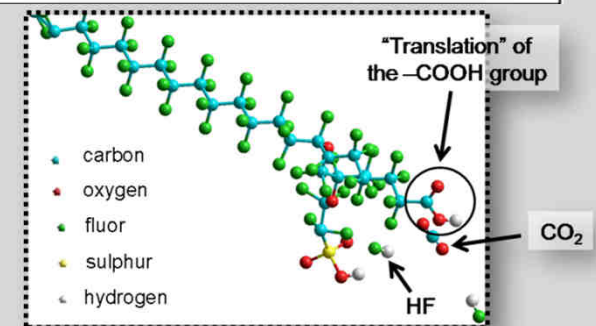
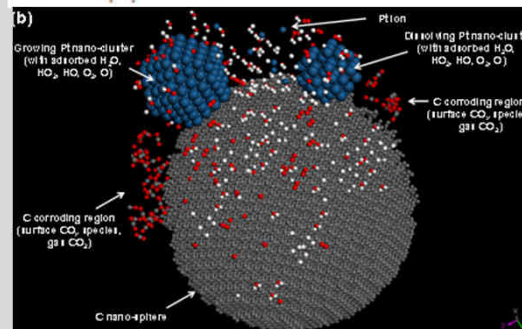
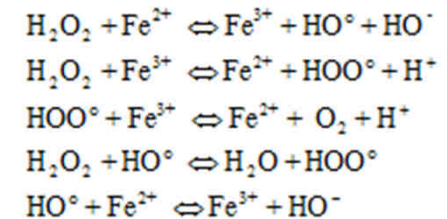
### C corrosion



### PFSA-side chain degradation



### Fenton's reactions

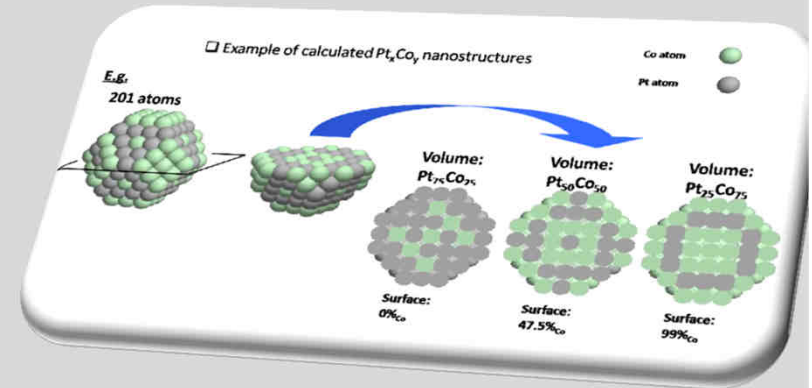






# Nanostructural data @ MEMEPhys®

- Aging of bimetallic nanoparticles: feedback between MEMEPhys® and MC-generated nanostructural databases.



Becoming a scientist

Research motivations

$$S_{Pt_xM_y} = f_a(m_{Pt_xM_y})$$

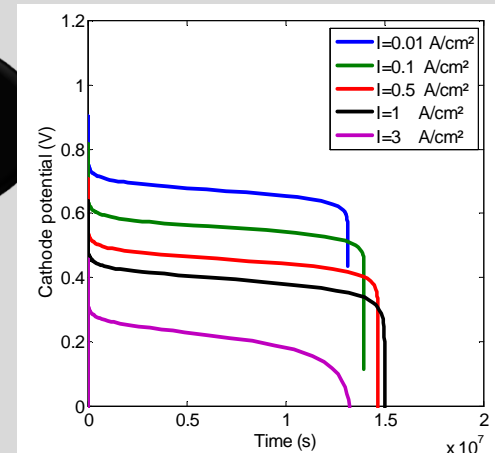
Research contribution

$$\Delta G_i = f_b(m_{Pt_xM_y})$$

Perspectives

## MEMEPhys®

Prediction of temporal evolution of experimental observables



$$U_{cell}(t) = \psi_{Cathode}(t) - \psi_{Anode}(t)$$

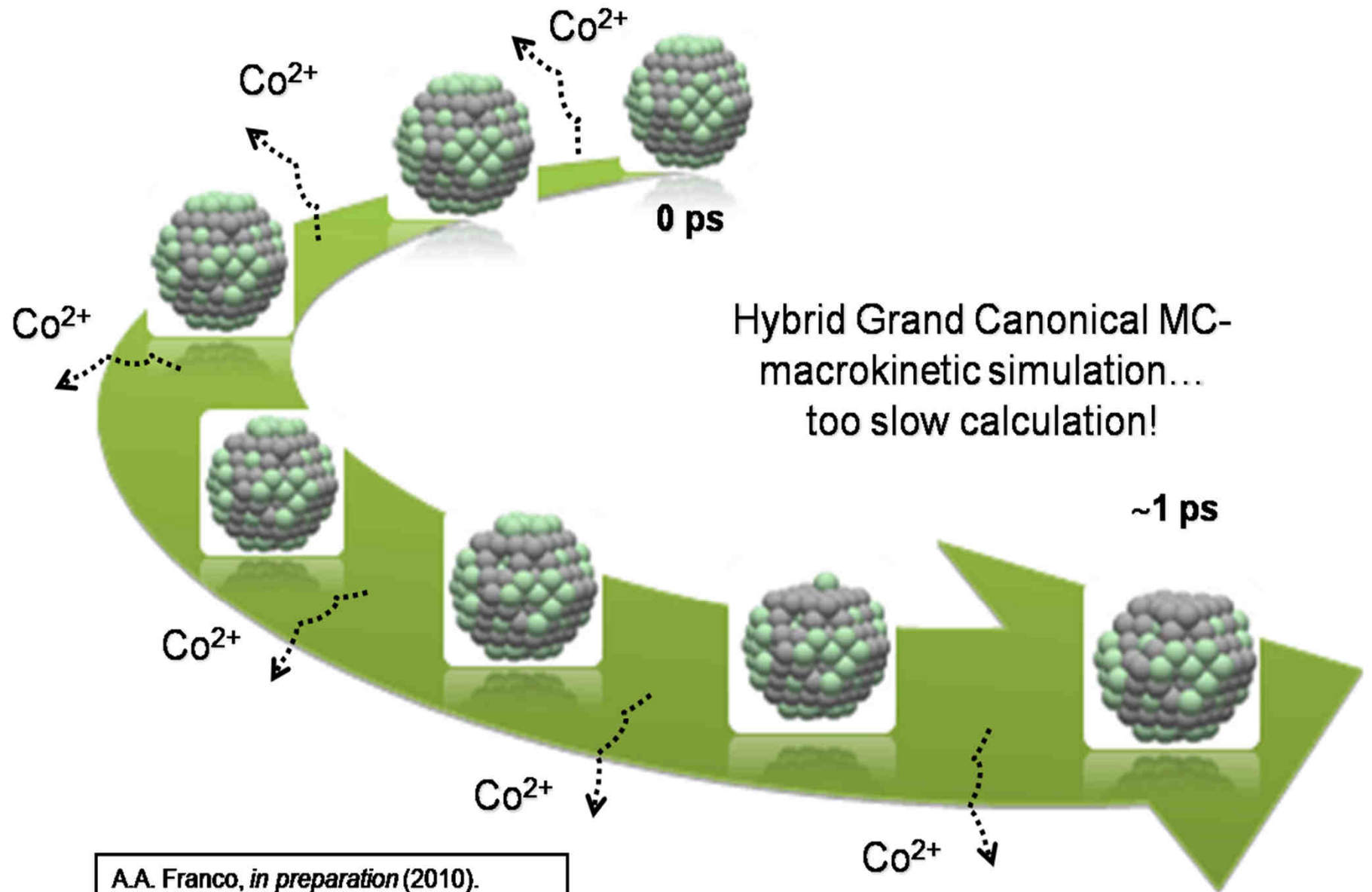
A.A. Franco et al., *J. Electrochem. Soc.*, **154** (7) B712 (2007).  
 A.A. Franco et al, *ECS Trans.*, (2009).  
 A.A. Franco et al., *J. Electrochem. Soc.*, **156** (3) B410 (2009).

Becoming  
a scientist

Research  
motivations

Research  
contribution

Perspective





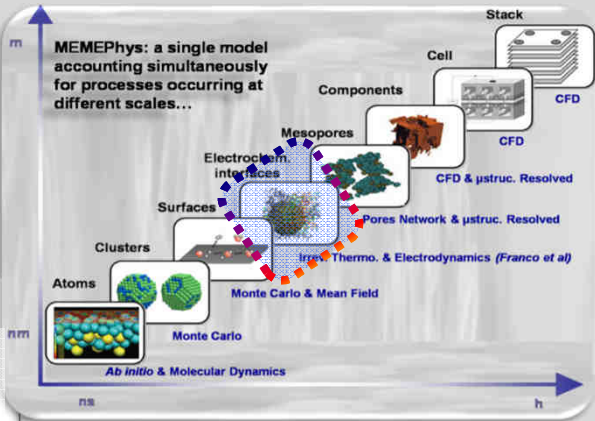
Becoming a scientist

Research motivations

Research contribution

Perspectives

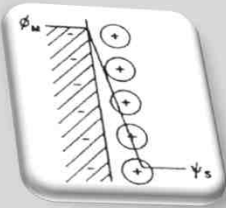
# Electrochemical interface @ MEMEPhys<sup>®</sup>



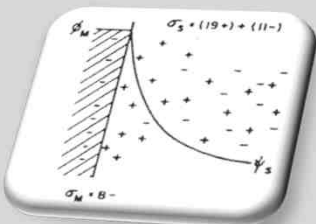
Which electrochemical interface?

Classical electrochemical double layer models (equilibrium conditions)

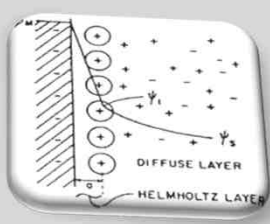
Helmholtz model



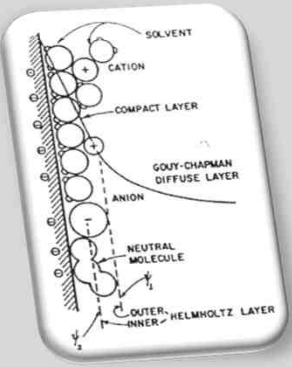
Gouy and Chapman model



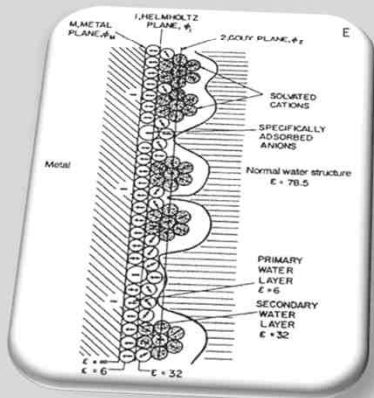
Stern model



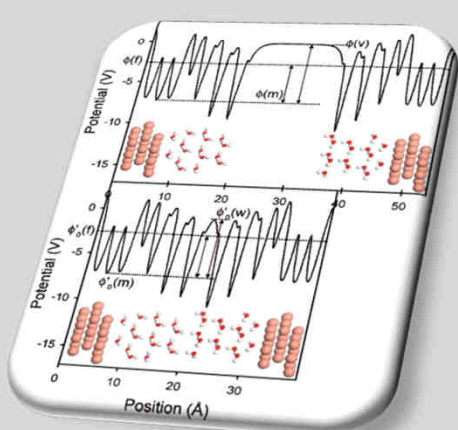
Grahame model



Bockris, Devanathan and Muller model



Neurock model





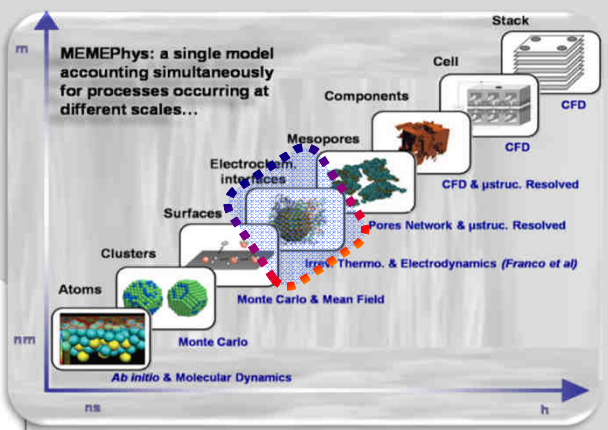
# Electrochemical interface @ MEMEPhys<sup>®</sup>

Becoming a scientist

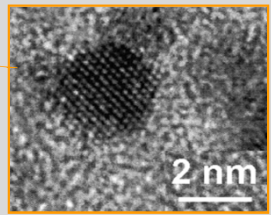
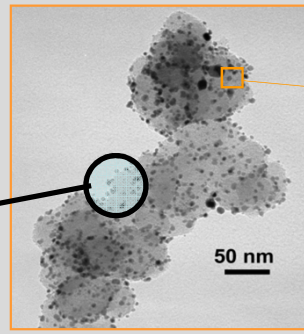
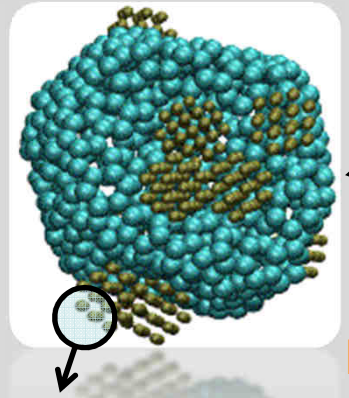
Research motivations

Research contribution

Perspectives

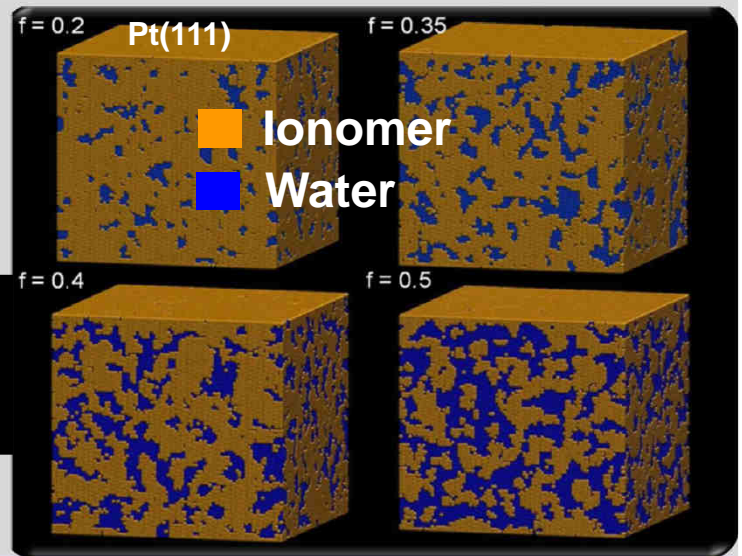
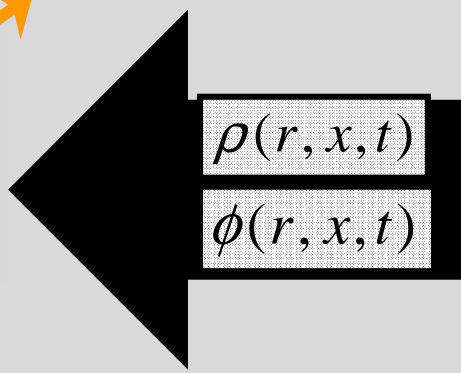
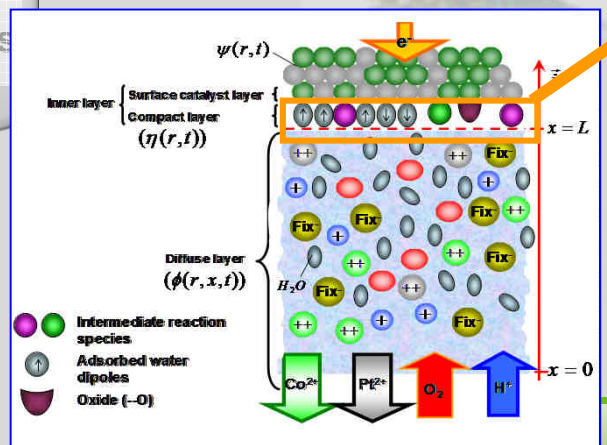


- Nanoscale model describing the interface structure during the electrochemical processes (including degradation): **non-equilibrium model**.
- Diffuse layer: PNP or grand canonical Monte Carlo calculation of interfacial charge distribution (protons, parasitic ions, sulfonate groups). Inner layer: elementary kinetics + parasitic H<sub>2</sub>O adsorption.



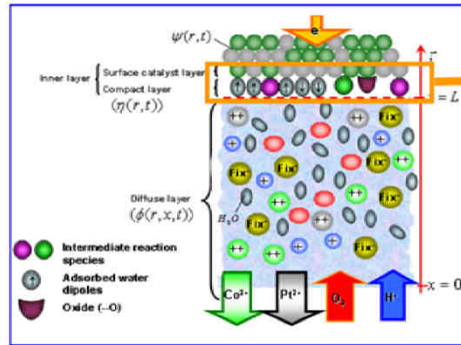
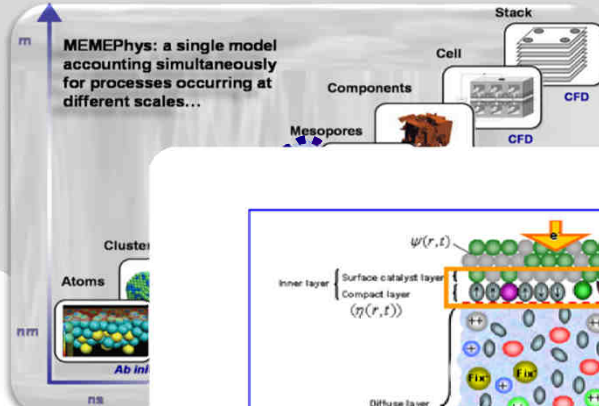
Charge distribution as function of the local water content (primary pores)

Elementary kinetics



# Electrochemical interface @ MEMEPhys<sup>®</sup>

- Nanoscale model describing the interface structure during the electrochemical processes (including degradation): **non-equilibrium model**.



Elementary steps with time-dependent rates

$$k_i = \kappa \frac{k_B T}{h} \exp\left(-\frac{1}{RT} [\Delta G_r(t) + f_1(\eta_F(t)) + f_2(\theta_i(t))]\right)$$

Compositional effect (reconstruction)

Interfacial electric field effect

Adsorbates effect

$$\Delta G_r = \xi(x_{Co}(t)) \Delta G_r^o$$

$$f_1(\eta^F) = \mp \ln \left[ \frac{\int_{-E_F}^{\Phi} \frac{1}{\sqrt{4\pi\epsilon_s k_B T}} e^{-\frac{(e+E_s-e\eta^F)^2}{(4E_s k_B T)}} \frac{1}{1+e^{-\frac{-e}{k_B T}}} d\epsilon}{\int_{-E_F}^{\Phi} \frac{1}{\sqrt{4\pi\epsilon_s k_B T}} e^{-\frac{(e+E_s)^2}{(4E_s k_B T)}} \frac{1}{1+e^{-\frac{-e}{k_B T}}} d\epsilon} \right] \pm f\eta^F$$

Compact layer thickness effect

Compact layer dipolar density effect

Ion solvation effect

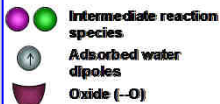
$$\eta_F(t) = -\frac{\sigma \cdot d}{\epsilon_{CC}} \frac{(x_{Co}^s(t) \cdot a_{Co} \cdot \theta^{Co} + (1-x_{Co}^s(t)) a_{Pt} \cdot \theta^{Pt}) n^{\max} \cdot \Theta_{H_2O} \cdot \mu \cdot \sinh[X(\sigma, \theta_i)]}{\epsilon_{CD}} + \frac{\mu N_A}{3\epsilon_{DL}} [\alpha_+ r_s^+ C_{r^+}(x=L,t)] + g(\sigma)$$

Inner layer: Surface (Surr), Compact (Com), Electrolyte ( $\eta$ )

INPUT: nanoscale current density

OUTPUT: local electrode potential

$$\frac{i(y,z,t)}{\gamma_{Pt} V_{agg}} = J(y,z,t) = F \sum_i v_i^{Far} \pm \frac{\partial \sigma}{\partial t} \rightarrow \psi(y,z,t) = \eta^F(y,z,t) + \phi(x=L,y,z,t)$$



A.A. Franco et al., *J. Electrochem. Soc.* **153** (6) A1053 (2006).  
 A.A. Franco et al., *ECS Trans.*, **13** (17), 29 (2008).  
 A.A. Franco et al., *J. Electrochem. Soc.*, **156** (3) B410 (2009).

Carlo  
protons,  
layer:

tribution as  
local water  
ary pores)



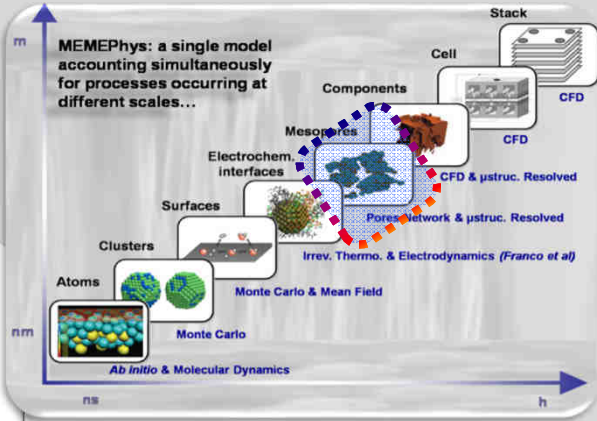
Becoming a scientist

Research motivations

Research contribution

Perspectives

# Mesostructural resolution @ MEMEPhys<sup>®</sup>

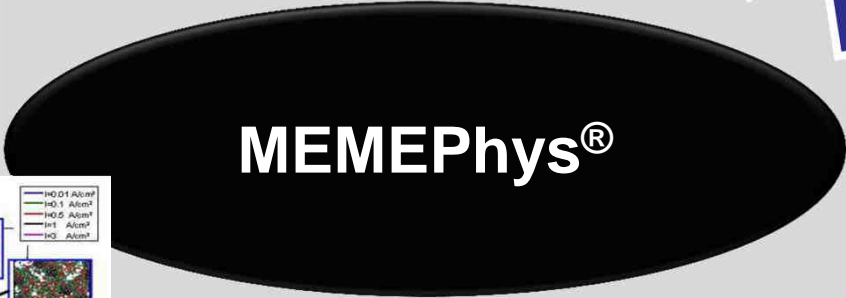


□ Aging of electrodes: feedback between MEMEPhys<sup>®</sup> and mesostructural databases.



$$m_C(t = t^*)$$

$$m_{ionomer}(t = t^*)$$



$$\theta_{Nafion}^{Pt} = f_1(m_C)$$

$$\theta_{H_2O}^{Pt} = f_2(m_C)$$

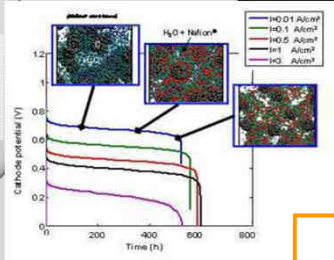
$$\theta_{Nafion}^C = f_3(m_C)$$

$$\theta_{H_2O}^C = f_4(m_C)$$

$$g_{e^-}^C = f_5(m_C)$$

$$D_i^{eff} = f_6(m_C)$$

$$S_C = f_7(m_C)$$



Prediction of temporal evolution of experimental observables

$$U_{cell}(t) = \psi_{Cathode}(t) - \psi_{Anode}(t)$$

A.A. Franco et al., *J. Electrochem. Soc.*, **154** (7) B712 (2007).  
 A.A. Franco et al, *ECS Trans.*, (2009).  
 A.A. Franco et al., *J. Electrochem. Soc.*, **156** (3) B410 (2009).



# Mesostructural resolution @ MEMEPhys®

Example: ionomer mesostructure impact on C corrosion kinetics.

K. Malek, A.A. Franco *in preparation* (2010).



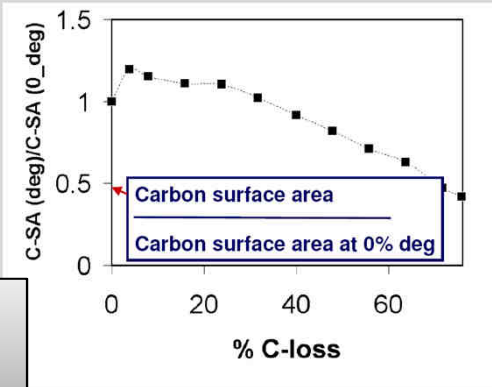
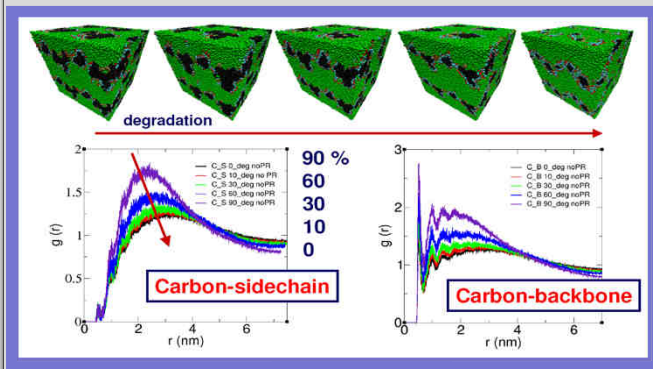
Becoming a scientist

Research motivations

Research contribution

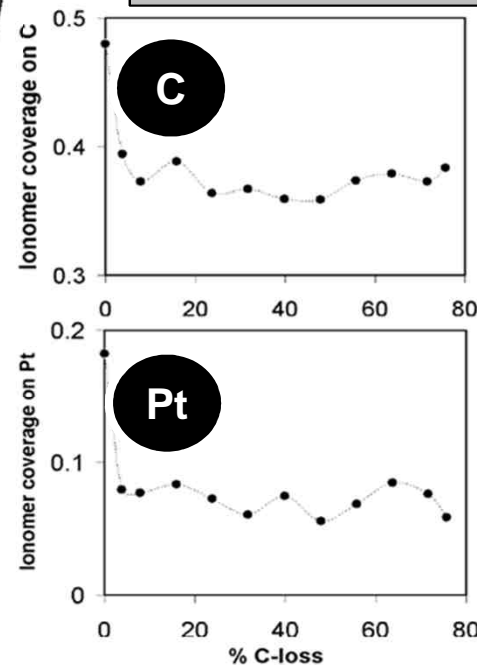
Perspectives

## CGMD-predicted mesostructure evolution

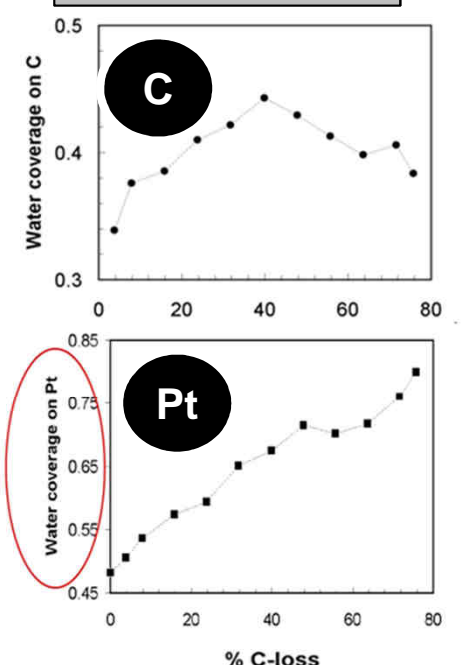


## CGMD-predicted C surface area

## CGMD-predicted ionomer coverage



## CGMD-predicted water coverage



- ✓ Case study: I/C ratio = 0.9.
- ✓ Cathode C corrosion induces high re-organization of the catalyst and the ionomer inside the electrode.
- ✓ Strong impact on Pt catalytic properties and electrode transport properties.



- Becoming a scientist
- Research motivations
- Research contribution
- Perspectives

# MEMEPhys<sup>®</sup> capabilities

## Physical capabilities

Sensitive to materials chemistry and structure

Capturing transient phenomena at different scales

## Algorithmic capabilities

Easily reusable/evolutive

Short calculation time

Interpretation of experiments, design of operation modes-materials for improved performance and durability in conditions as close as possible to the end-user application





# Multiscale character @ MEMEPhys<sup>®</sup>

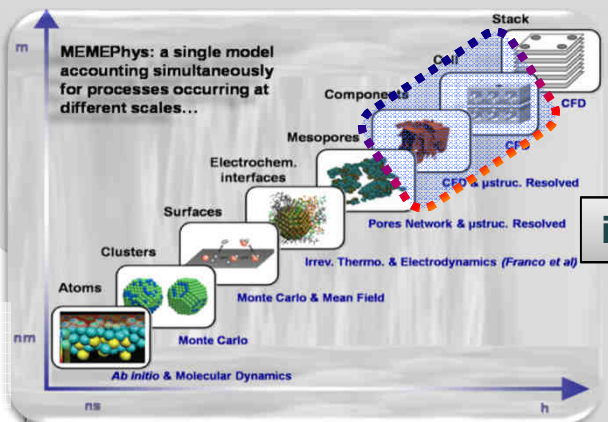


Becoming a scientist

Research motivations

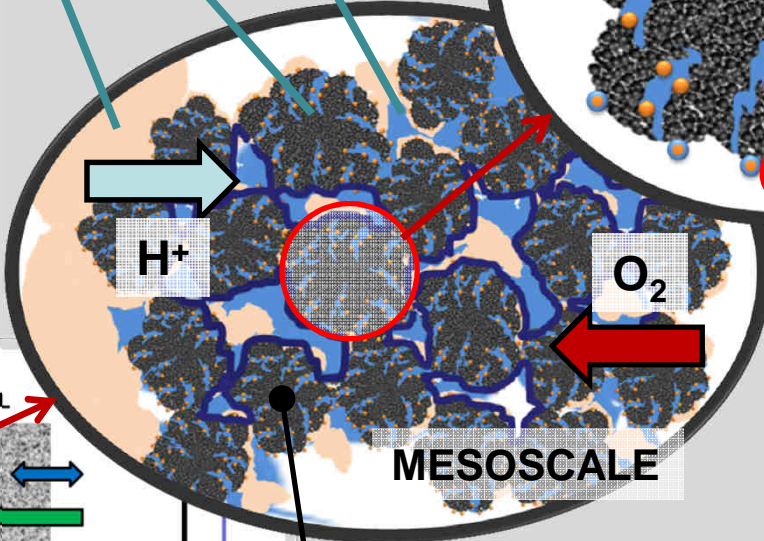
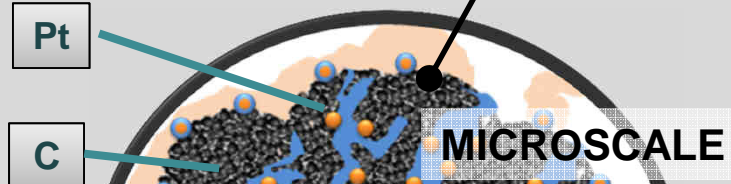
Research contribution

Perspectives

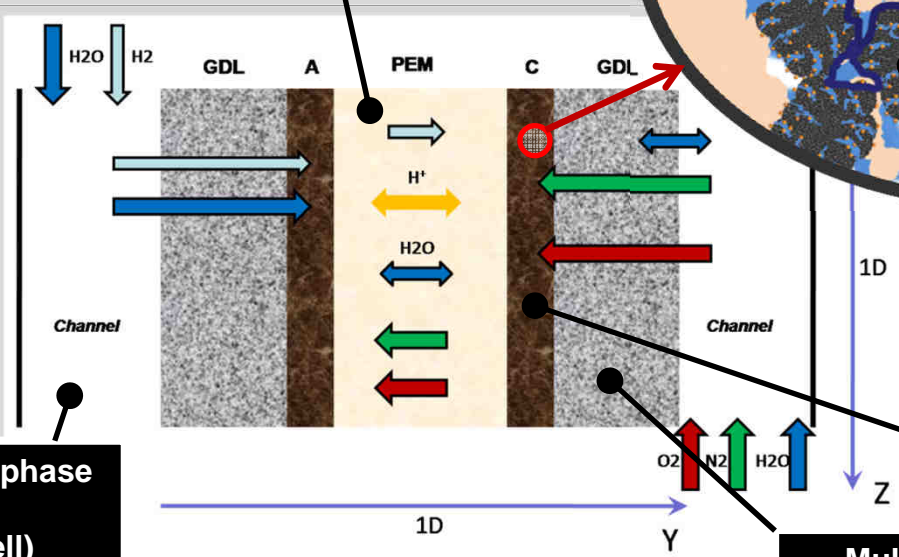


ionomer Pt/C Water

Reactants transport



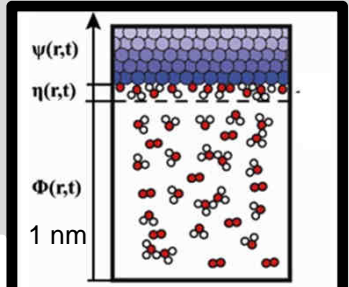
Water (electro-osmosis + diffusion) + charge transport + crossover (O<sub>2</sub>+H<sub>2</sub>+N<sub>2</sub>)



Charges transport and elementary kinetics

Structural-resolved water+reactants+charge transport

Multispecies/multiphase transport (Stefan-Maxwell + Knudsen)



R. Defense, *Chemical Engineering Progress*, 2010.

A Multiscale Modeling Framework for the Transient Analysis of PEMFCs

Multispecies/multiphase transport (Stefan-Maxwell)

# Couplings between scales

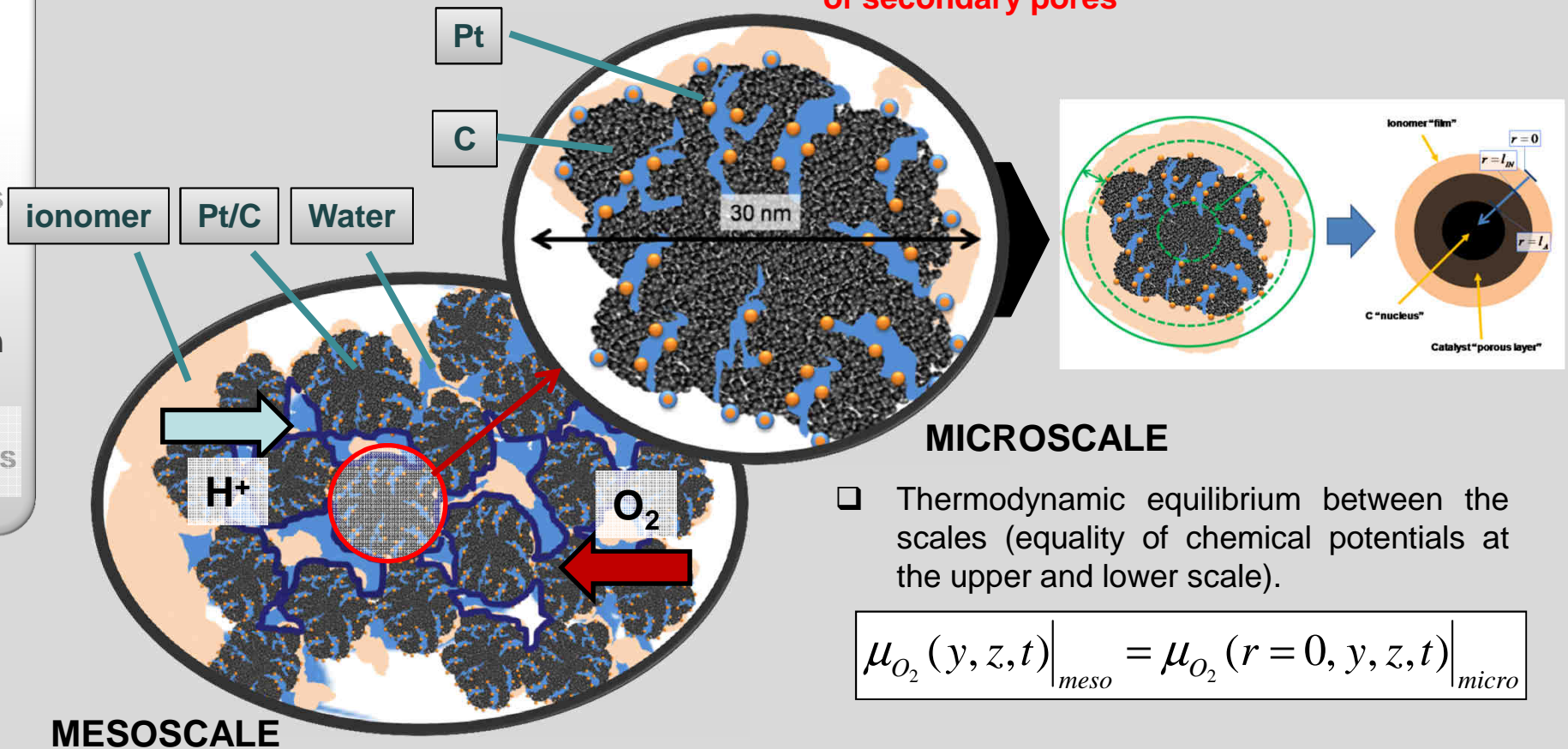
□ Example: pure O<sub>2</sub> transport through the electrode.

At the  
**MESOSCALE**  
level

$$\frac{\partial C_{O_2}}{\partial t} + \nabla_y \cdot J_{O_2} = S_{O_2}(y, z, t) = \underbrace{\gamma_{SP}(y, z, t)}_{\text{Specific surface area of secondary pores}} \times J_{O_2}(r=0, y, z, t)$$

Specific surface area  
of secondary pores

Becoming a scientist  
Research motivations  
Research contribution  
Perspectives



□ Thermodynamic equilibrium between the scales (equality of chemical potentials at the upper and lower scale).

$$\mu_{O_2}(y, z, t) \Big|_{meso} = \mu_{O_2}(r=0, y, z, t) \Big|_{micro}$$



- Becoming a scientist
- Research motivations
- Research contribution
- Perspectives

# MEMEPhys<sup>®</sup> capabilities

## Physical capabilities

Sensitive to materials chemistry and structure

Capturing transient phenomena at different scales

## Algorithmic capabilities

Easily reusable/evolutive

Short calculation time

Interpretation of experiments, design of operation modes-materials for improved performance and durability in conditions as close as possible to the end-user application



# Bond Graph: modular structure



□ Network modeling: the overall system is decomposed into subsystems interconnected to each other through pairs of conjugated variables (product = power exchanged between the subsystems)

□ Advantages:

- ✓ reusability of subsystem models (libraries),
- ✓ flexibility (coarse models of subsystems may be replaced by more refined ones leaving the rest of the system modeling untouched),
- ✓ hierarchical modeling,
- ✓ acausality,
- ✓ useful for the systematic modeling of multi-physics systems, where the subsystems belong to different physical domains (mechanical, electrical, hydraulic, etc.).

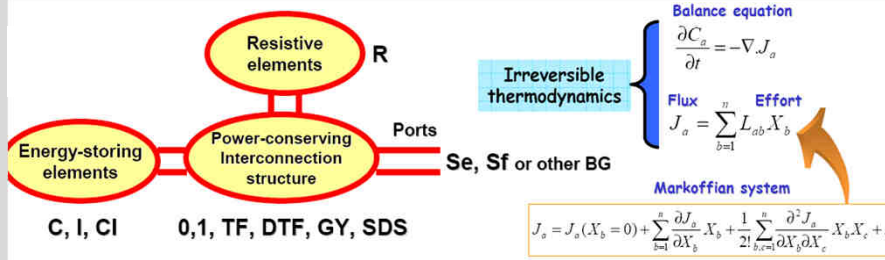


Becoming a scientist

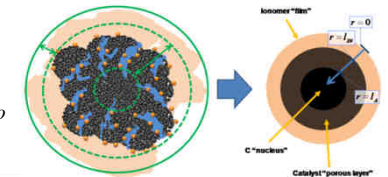
Research motivations

Research contribution

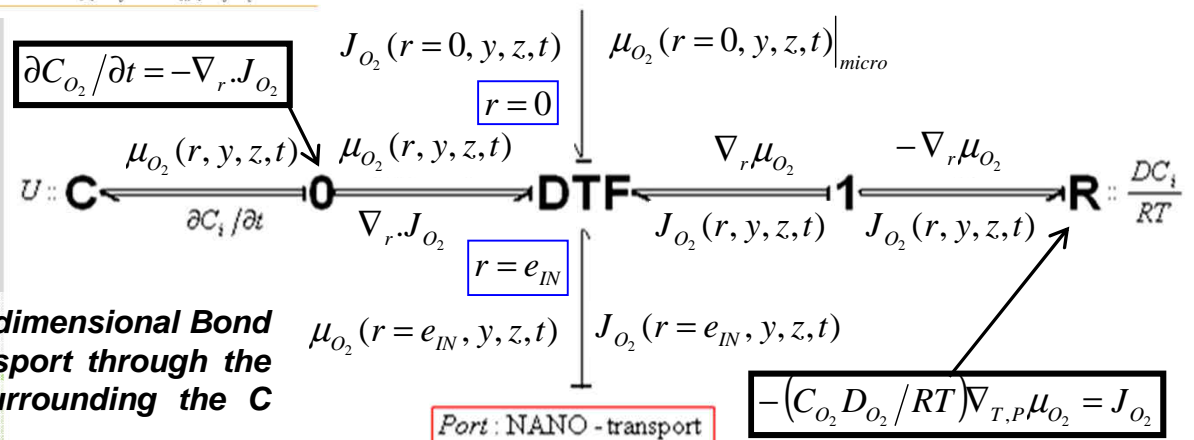
Perspectives



$$S_{O_2}(y, z, t) \quad \mu_{O_2}(y, z, t)|_{meso}$$



coupling



A.A. Franco et al., in *Proc. 5th Mathmod Conference*, Vienna (2006) P103.  
A.A. Franco, PhD thesis (2005).

**Example: infinite-dimensional Bond Graph of O<sub>2</sub> transport through the ionomer layer surrounding the C aggregate.**

A Multiscale Modeling Framework for the Transient Analysis of PE



# MEMEPhys<sup>®</sup> capabilities

- Becoming a scientist
- Research motivations
- Research contribution
- Perspectives

## Physical capabilities

- Sensitive to materials chemistry and structure
- Capturing transient phenomena at different scales

## Algorithmic capabilities

- Easily reusable/evolvable
- Short calculation time

Interpretation of experiments, design of operation modes-materials for improved performance and durability in conditions as close as possible to the end-user application



Becoming a scientist

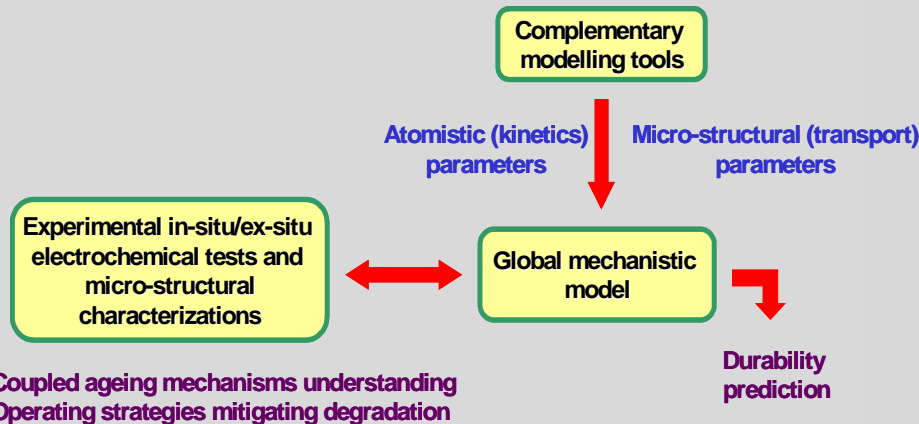
Research motivations

Research contribution

Perspectives

# Algorithm within MEMEPhys<sup>®</sup>

- ❑ Modular interface: constitutive and conservation equations kept separately → easy to change physical assumptions (constitutive relationships) and geometries / **flexible environment**.
- ❑ Integration of aging-induced parameters evolution through libraries or through fractal evolution “laws”.
- ❑ Variable-step solver to manage fast (e.g. chemical reaction with  $\tau \approx 10^{-6}$  s) and slow processes (e.g. transport with  $\tau \approx 10^{-1}$  s).
- ❑ In-house code combining C + Matlab<sup>®</sup>/Simulink<sup>®</sup> + Comsol Multiphysics<sup>®</sup>.
- ❑ Electrode macro-spatial meshing along the thickness and along the channels.
- ❑ Possibility of implementing both uniform and non-uniform 1D + 1D meshing.



- Coupled ageing mechanisms understanding
- Operating strategies mitigating degradation

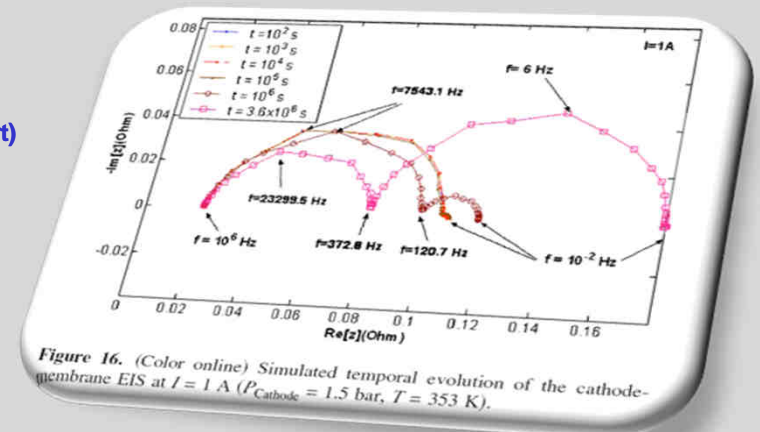


Figure 16. (Color online) Simulated temporal evolution of the cathode-membrane EIS at  $I = 1$  A ( $P_{\text{Cathode}} = 1.5$  bar,  $T = 353$  K).

Example: simulation of cathode EIS evolution during catalyst degradation

- Order of magnitude calculation time: dynamic polarisation curve  $\approx 1$  minute,  $U(t)$  (1000 h) for case accounting for Pt degradation  $< 5$  minutes
- Interfaces for parameter estimation toolboxes integrated
- To be commercialized



# Algorithm within MEMEPhys<sup>®</sup>

- *Snapshots of one of the multiple available versions...*
- *To be adapted for electrolyzers and batteries...*

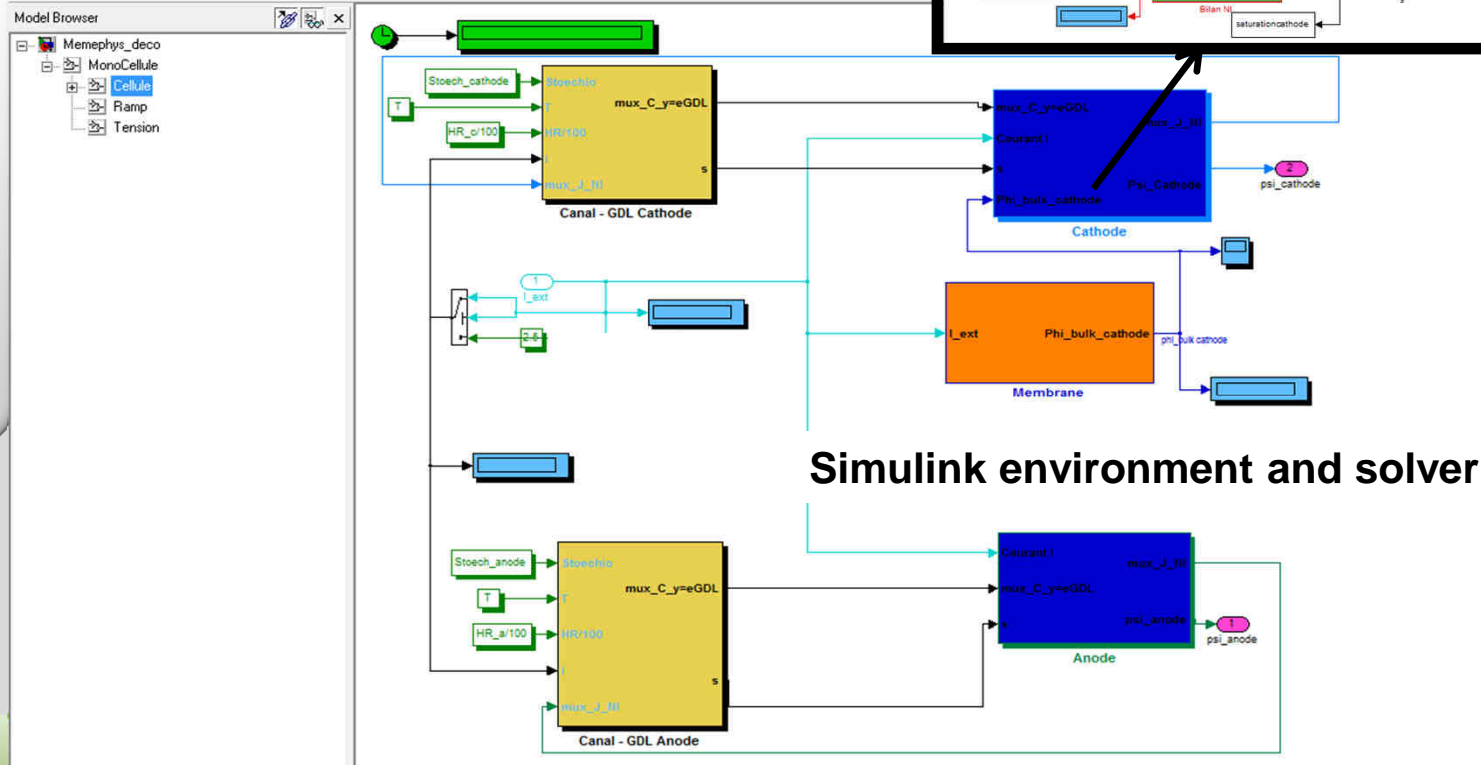
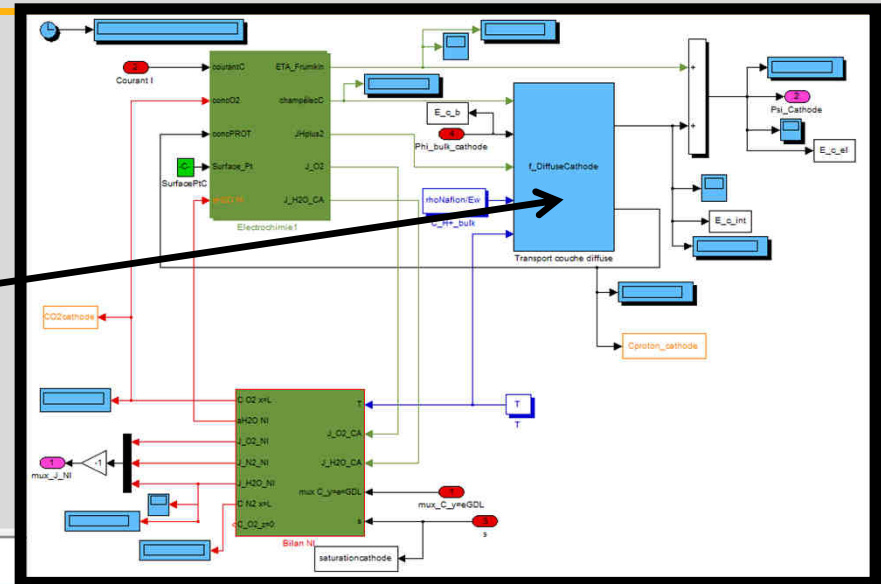
Becoming a scientist

Research motivations

Research contribution

Perspectives

C routines





- Becoming a scientist
- Research motivations
- Research contribution
- Perspectives

# MEMEPhys<sup>®</sup> capabilities

## Physical capabilities

Sensitive to materials chemistry and structure

Capturing transient phenomena at different scales

## Algorithmic capabilities

Easily reusable/evolvable

Short calculation time

Interpretation of experiments, design of operation modes-materials for improved performance and durability in conditions as close as possible to the end-user application





# MEMEPhys<sup>®</sup> capabilities



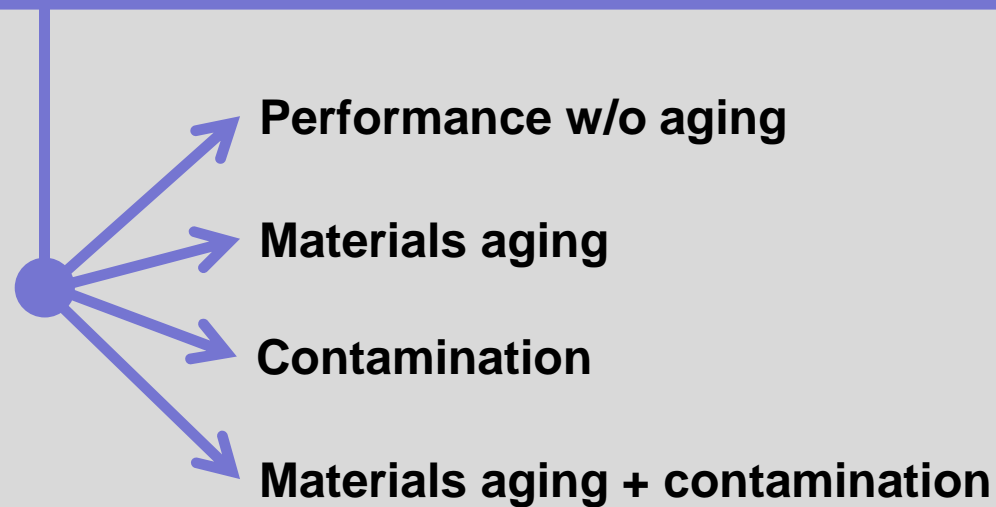
Interpretation of experiments, design of operation modes-materials for improved performance and durability in conditions as close as possible to the end-user application

Becoming a scientist

Research motivations

Research contribution

Perspectives





# Example #1: i-V characteristics



Becoming a scientist

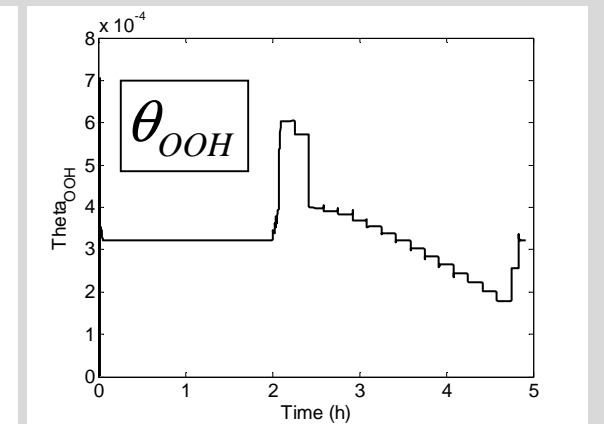
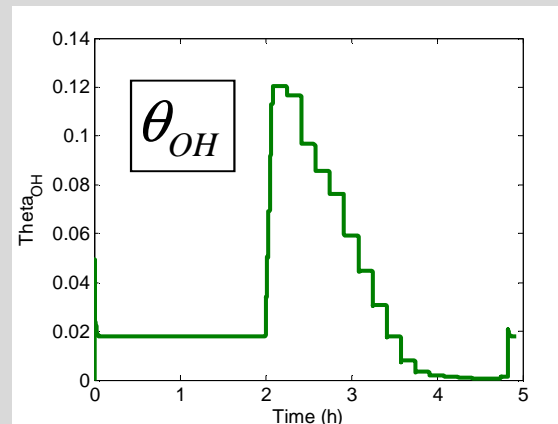
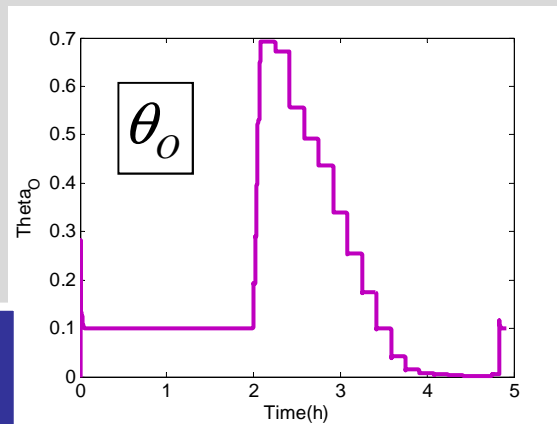
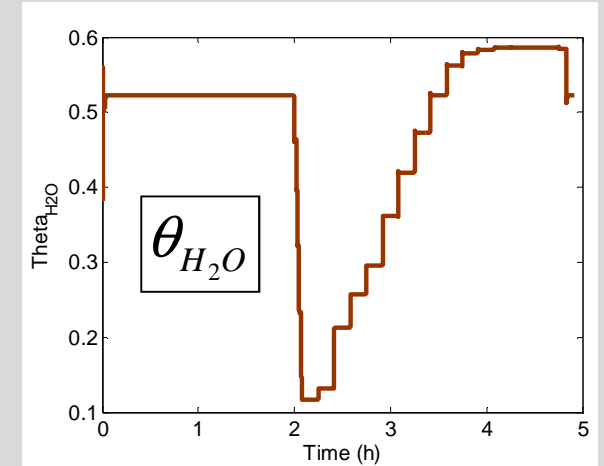
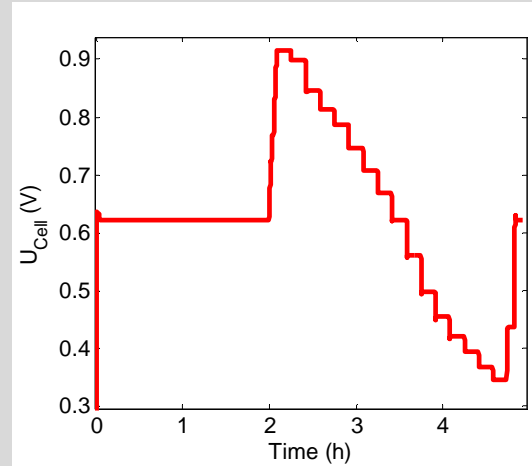
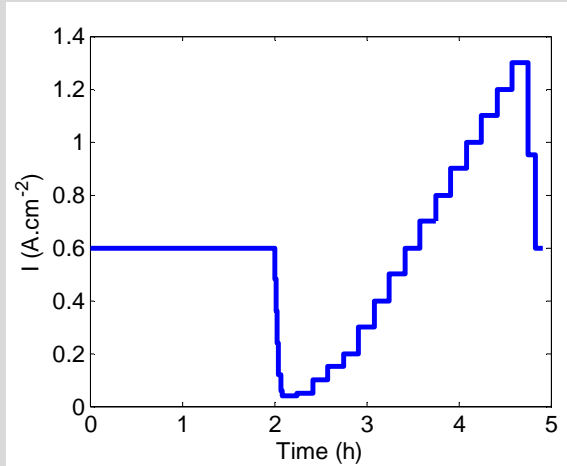
Research motivations

Research contribution

Perspectives

$T = 343 \text{ K}$   
 $P_A = P_C = 1.5 \text{ bar}$   
 $St_A = 1.2, St_C = 1.2$   
 $RH_A = RH_C = 50\%$   
 $S_{\text{electrode}} = 25 \text{ cm}^2$

- ❑ Powerful tool to capture behaviors at different scales.
- ❑ E.g.: cathode Pt coverage w/o materials aging (stepped i-V curve).





Becoming a scientist

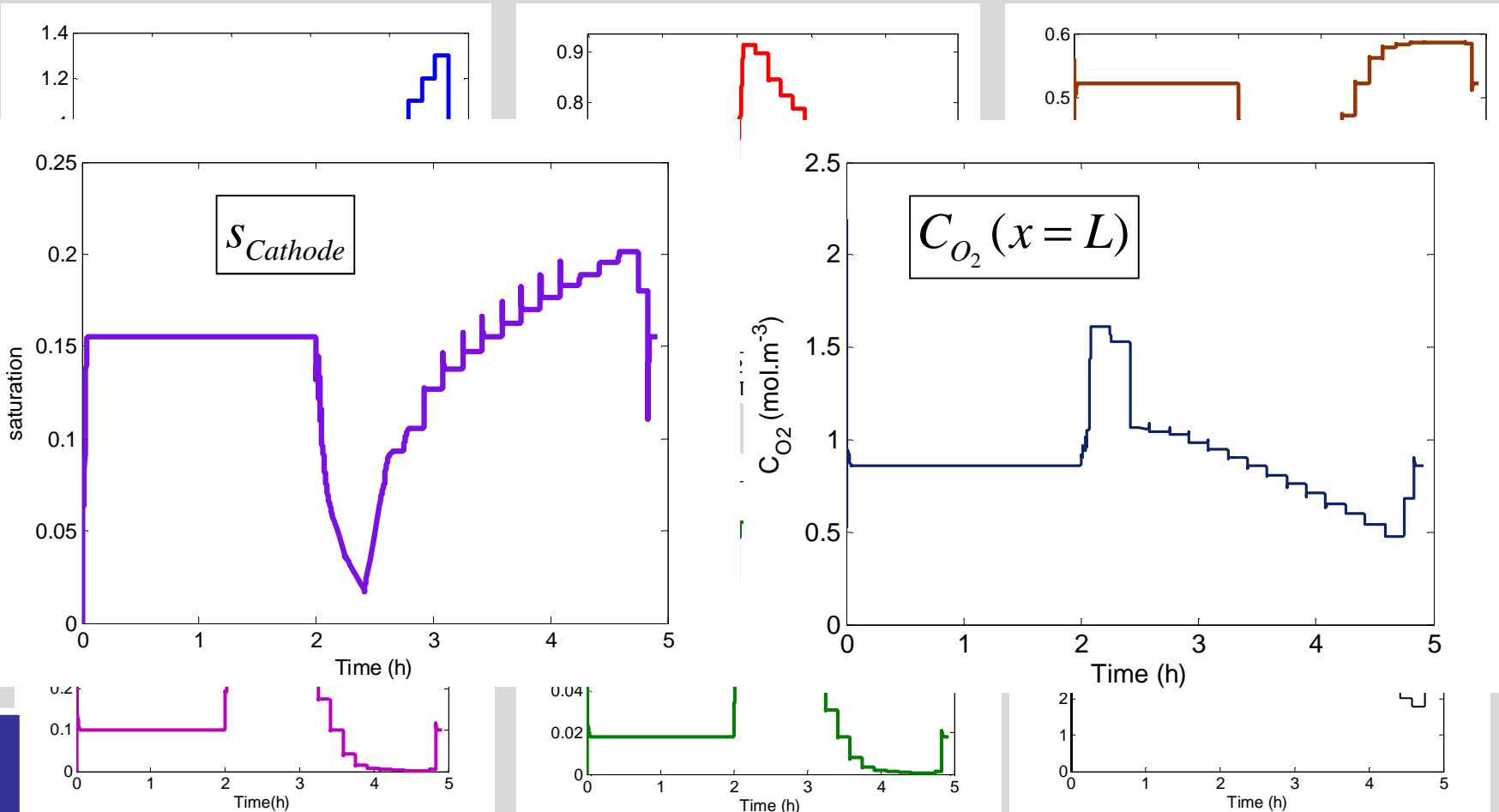
Research motivations

Research contribution

Perspectives

# Example #1: i-V characteristics

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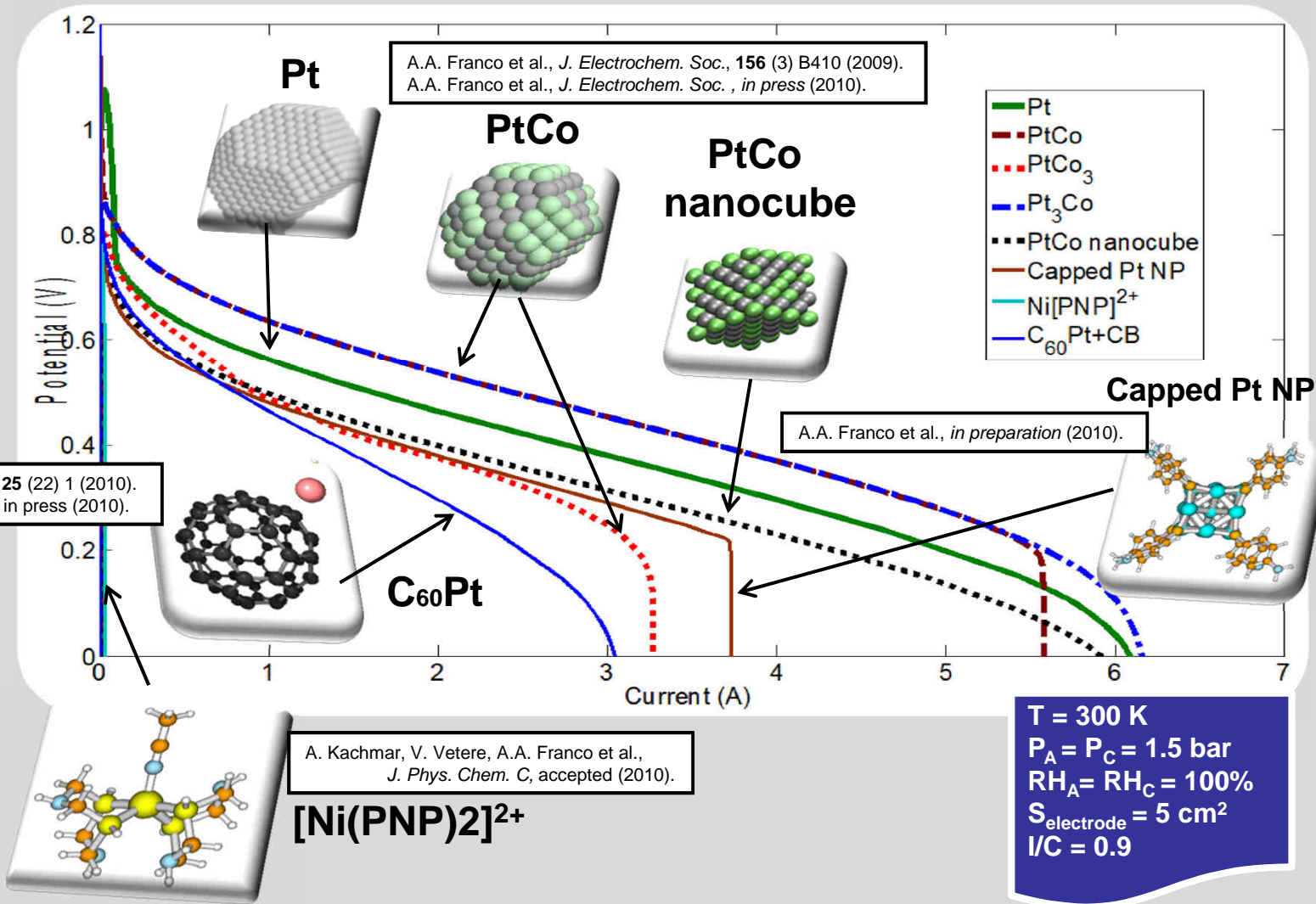


# Example #2: catalyst activity “benchmarking” (1/2)

Very flexible modeling tool to predict catalysts activities, stabilities and tolerances to external pollutants (“benchmarking”).



- Becoming a scientist
- Research motivations
- Research contribution
- Perspectives





Becoming a scientist

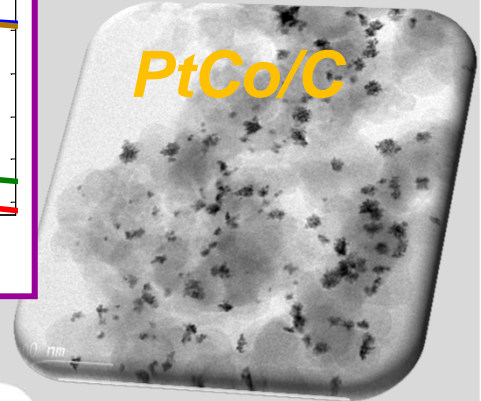
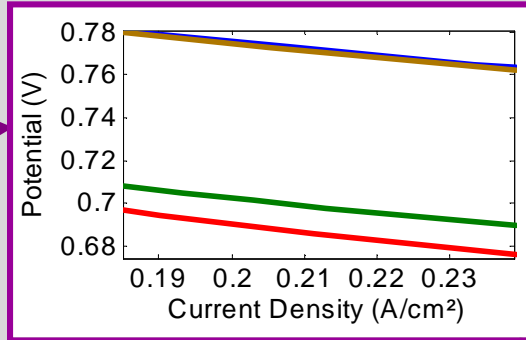
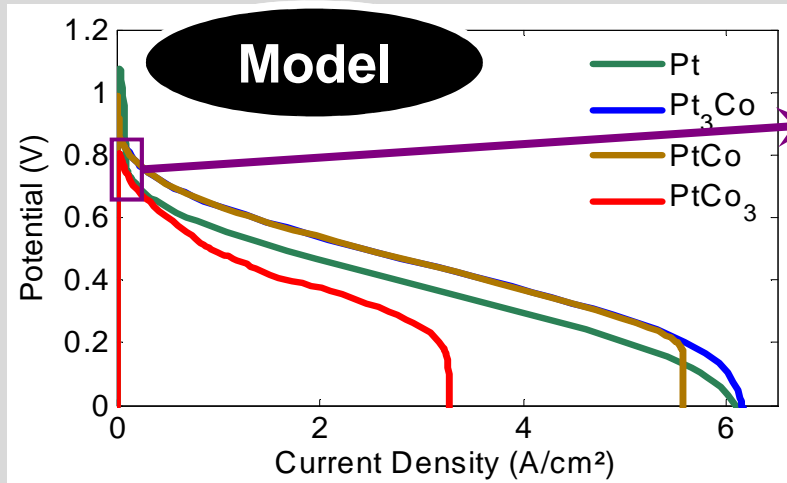
Research motivations

Research contribution

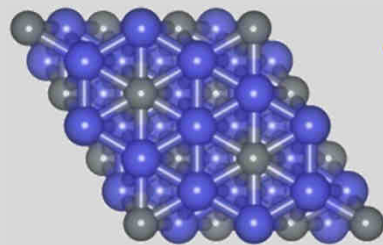
Perspectives

# Example #2: catalyst activity "benchmarking" (2/2)

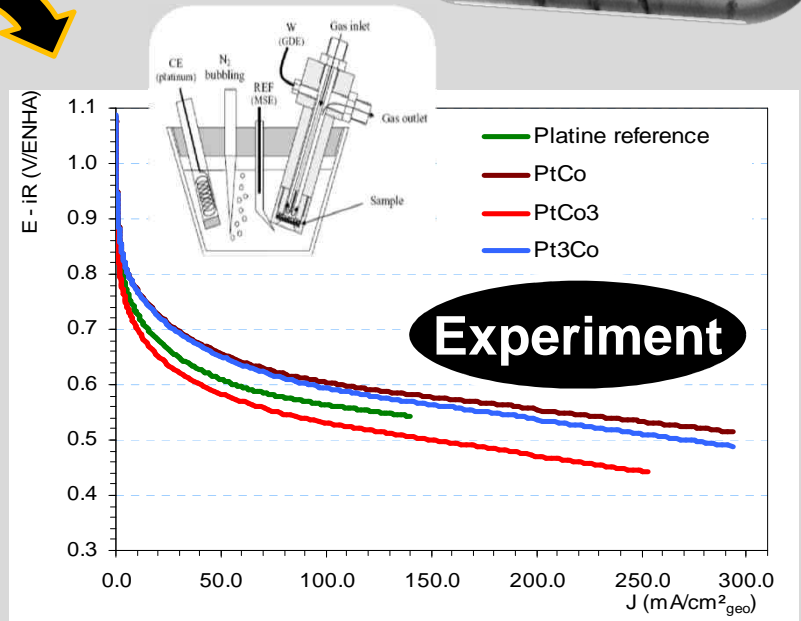
- ❑ Bulk-truncated  $Pt_xCo_y$  particles: composition impact on i-V.
- ❑ Predicted trends in good agreement with half-cell experimental results.



$T = 353 \text{ K}$   
 $P_A = P_C = 1.5 \text{ bar}$   
 $RH_A = RH_C = 100\%$   
 $S_{\text{electrode}} = 5 \text{ cm}^2$   
 $I/C = 0.9$



$$x_{Co}^{\text{Surface}}(t) = x_{Co}^{\text{Volume}}(t)$$

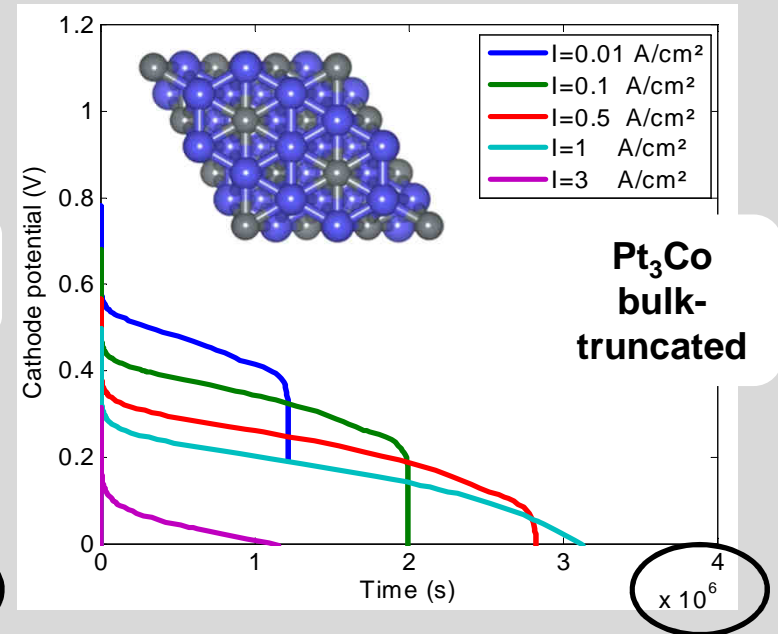
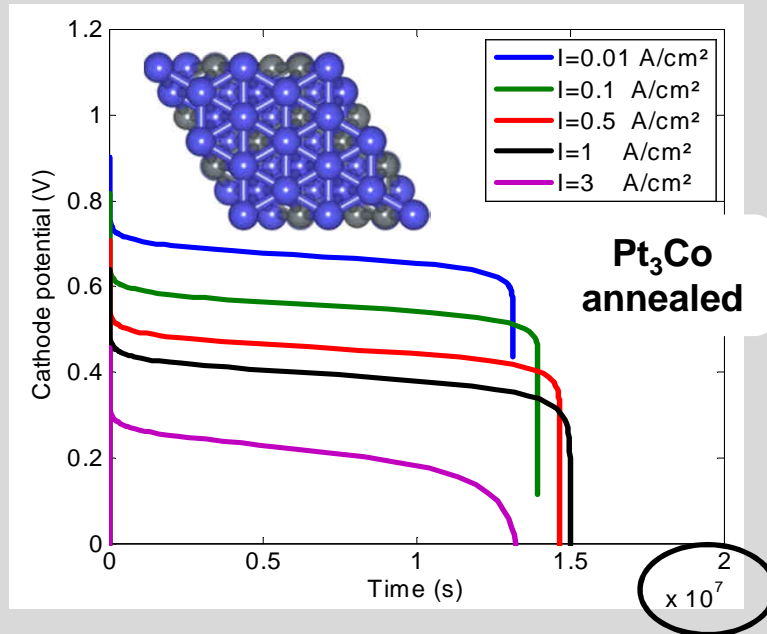


Materials performance rank

$$PtCo > Pt_3Co > Pt > PtCo_3$$

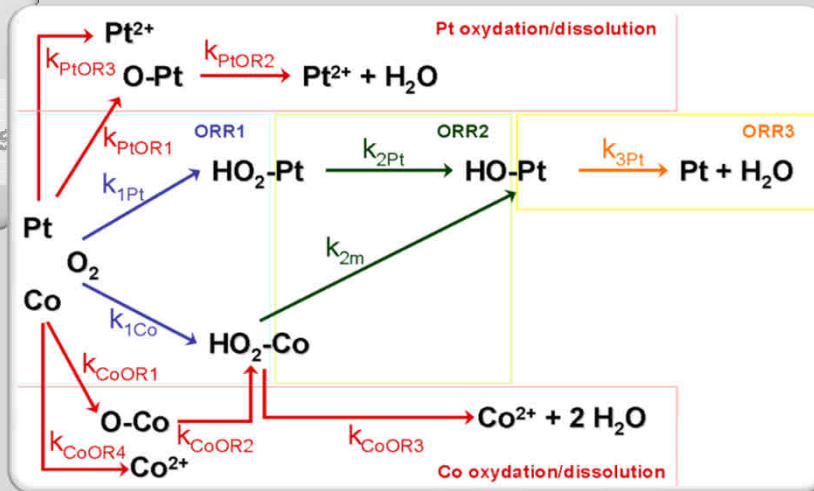
# Example #3: catalyst stability “benchmarking” (1/2)

□ The model suggest operating currents providing maximal catalyst durability.



~5500 h

~1100 h



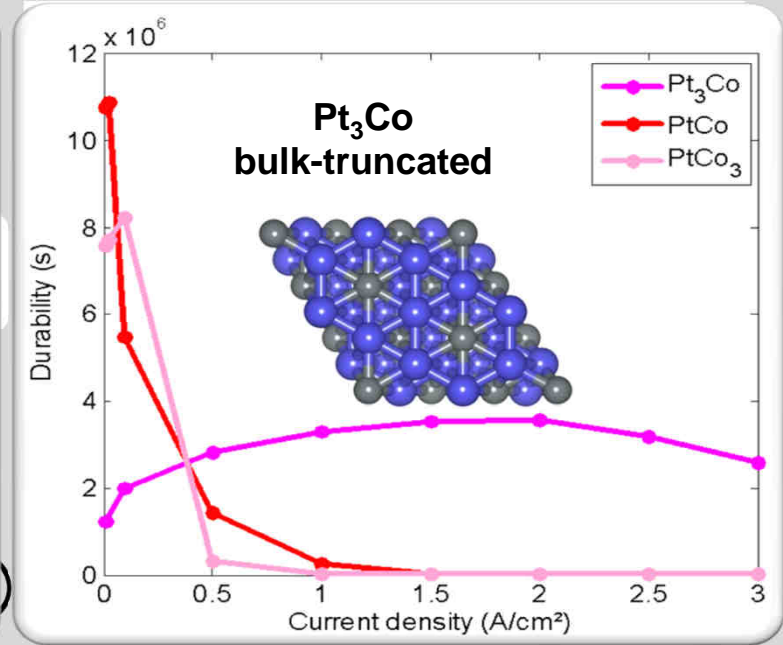
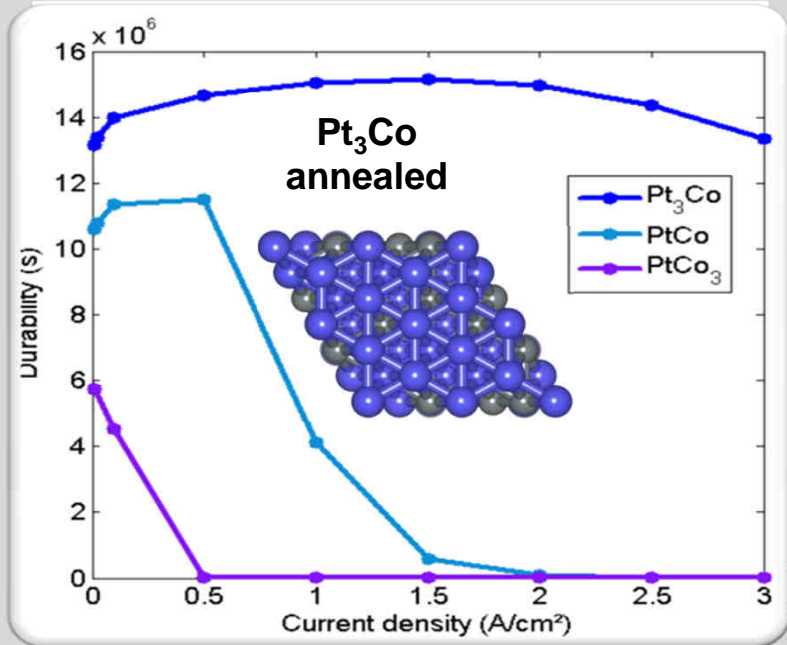
➤ ORR mechanism appears strongly coupled to material (both Pt and Co) degradation → **elementary kinetic steps with time-dependent rates.**

➤ HO intermediate adsorbs preferentially on Pt.

➤ Co dissolves better than Pt when the two materials coexist at the surface (“sacrificial” mechanism).

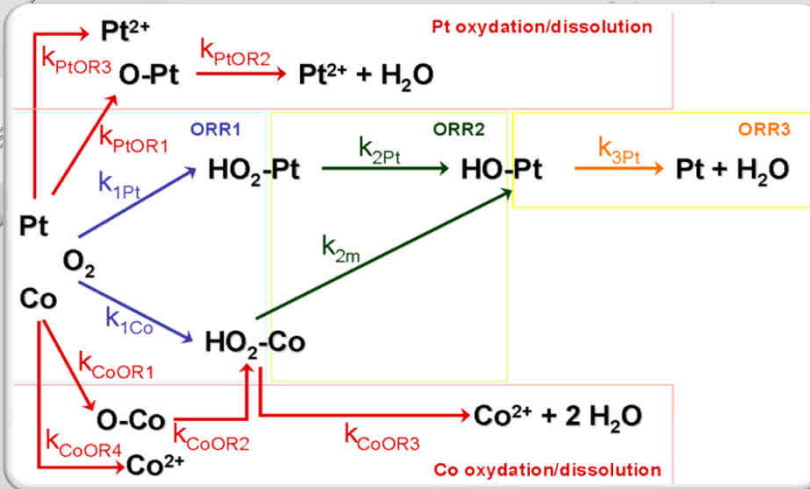
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Becoming a scientist

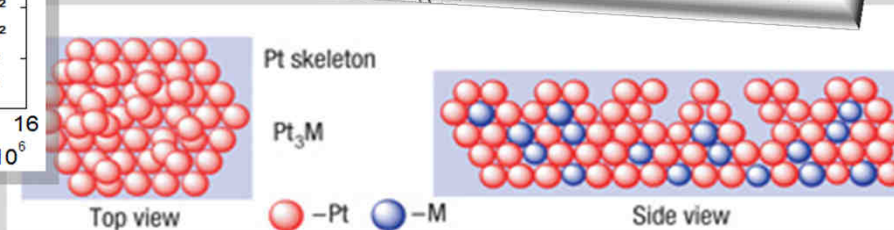
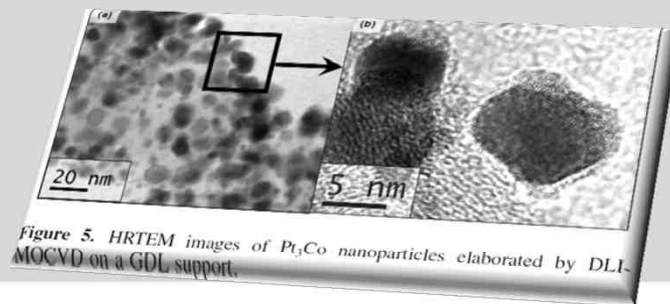
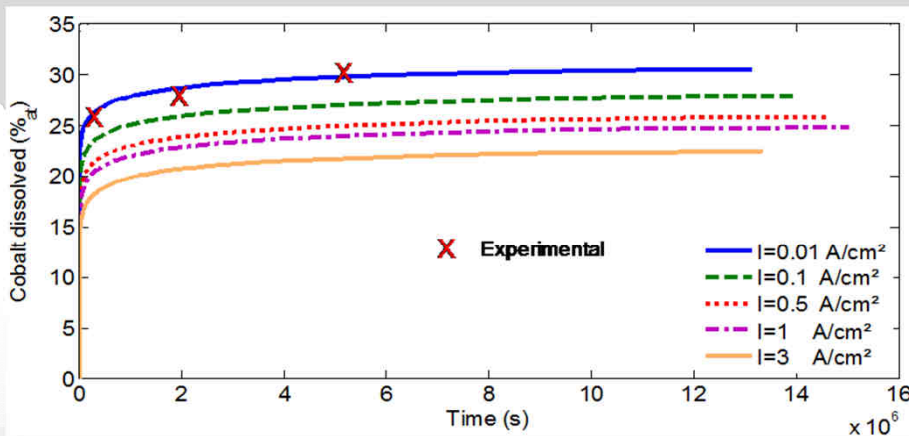
Research motivations

Research contribution

Perspectives

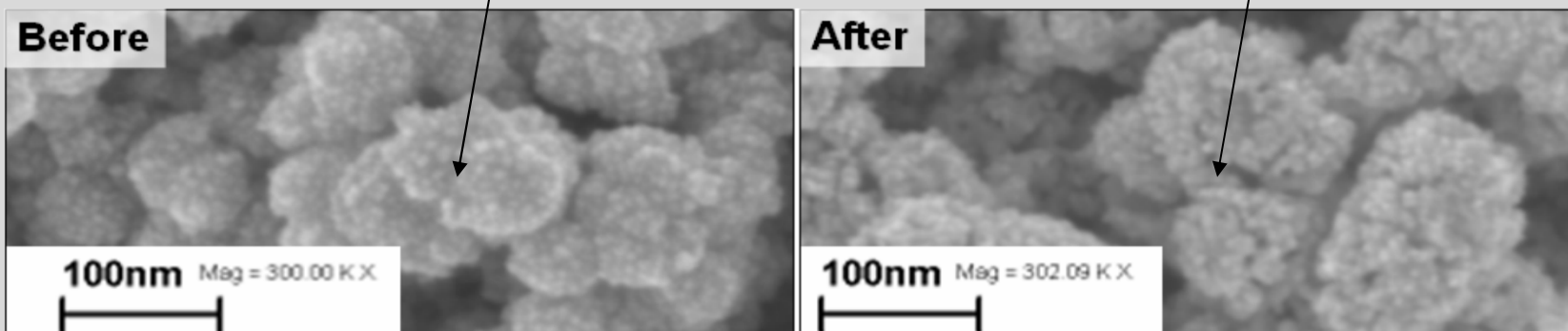
# Example #3: catalyst stability “benchmarking” (2/2)

- ❑ Predicted impact of current on dissolved Co amount from a bulk-truncated  $Pt_xCo_y$ .
- ❑ Predicted and experimental degradation impact on structure: becomes more and more as an “emmental cheese” or “skeleton”-structure.



Bulk-truncated structure

Skeleton-like structure



FEG-SEM images of our DLI-MOCVD  $Pt_3Co$  electrode before and after aging





# Example #4: impact of CO poisoning on anode $Pt_xCo_y$ stability

□ CO effects on structural stability of  $Pt_xCo_y$  catalysts.



Becoming a scientist

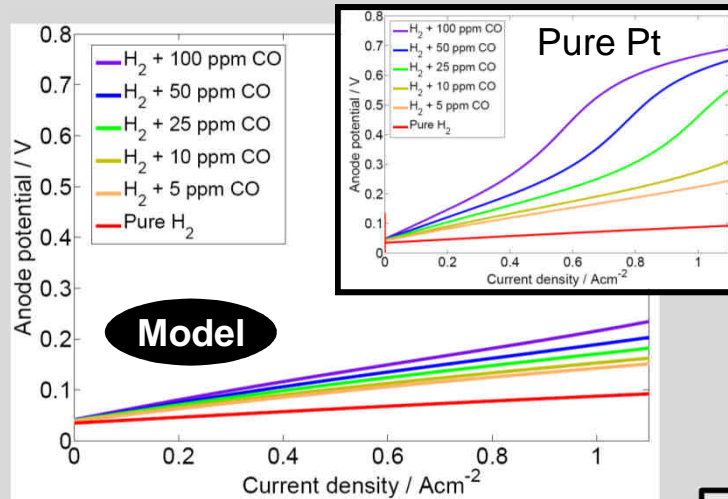
Research motivations

Research contribution

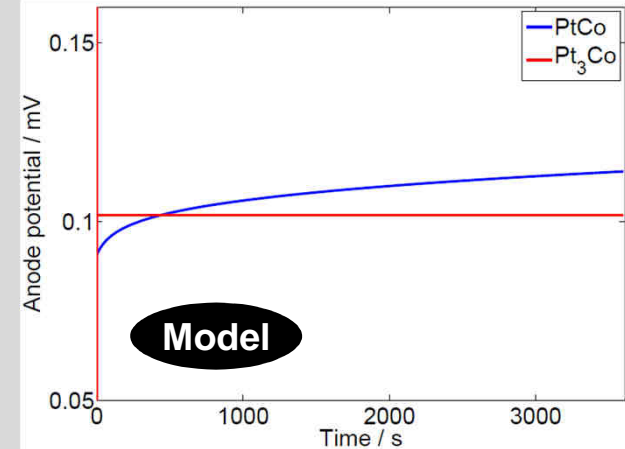
Perspectives

S.K.Cheah, P. Gelin, O. Lemaire, A.A. Franco, *ECS Trans.*, **25** (35), 275 (2010).

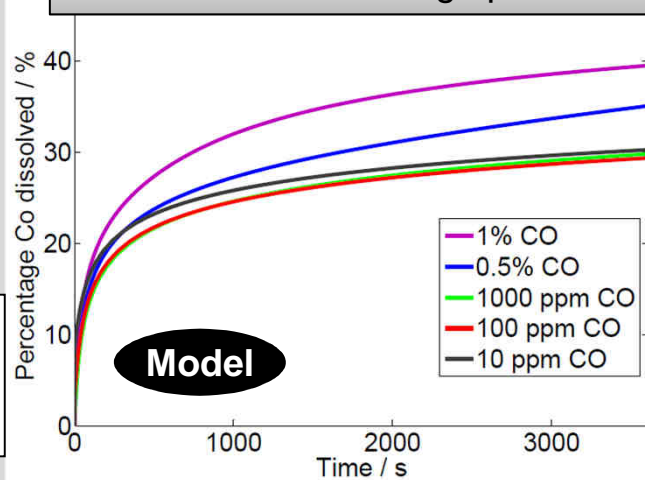
Pt<sub>3</sub>Co catalyst has high CO tolerance



PtCo shows degrading performance with time



Co dissolved due to high potential



**Experiments**

- Electrochemical half cell setup
- 3 samples go through same procedures except sample (a) was applied 20 mA of current under H<sub>2</sub>+50 ppm CO feed gas, sample (b) was applied 20 mA of current under pure H<sub>2</sub> feed gas, and sample (c) was left under OCV under H<sub>2</sub> feed gas

Results HPCL / ICP

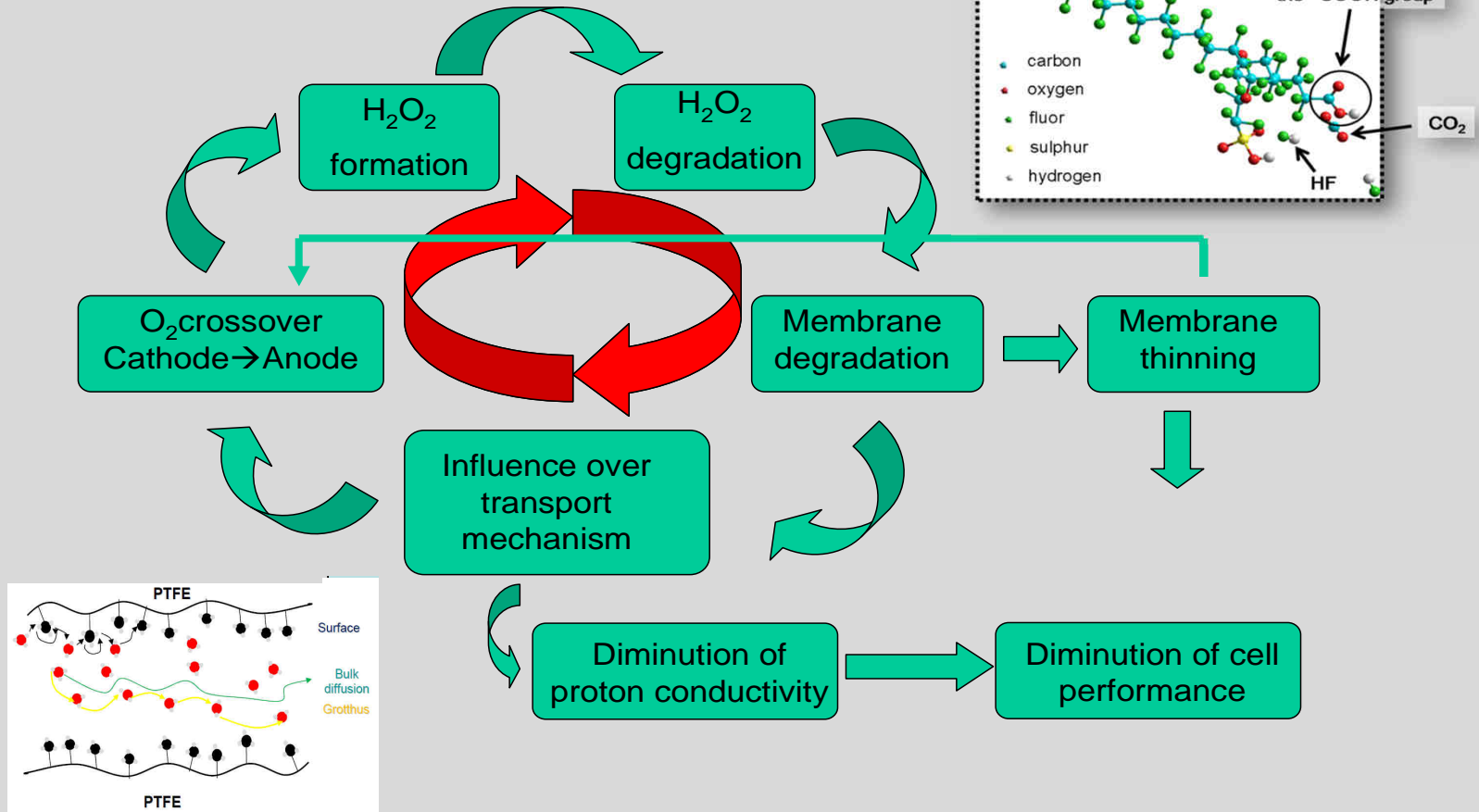
Samples	(a)	(b)	(c)
Co <sup>2+</sup> concentration in electrolyte (mg/L)	<b>0.67</b>	0.39	0.36

Co dissolved into the electrolyte due to high potential due to Co poisoning!!

# Example #5: PEM aging

□ PEM degradation: elementary kinetic model of the PEM side chain degradation (detailed description of anodic  $H_2O_2$  production, Fenton's reactions and side chain chemical degradation).

- Becoming a scientist
- Research motivations
- Research contribution
- Perspectives



A.A. Franco et al., *ECS Trans.*, **25** (1), 65 (2009).  
 R. Coulon, A.A. Franco, W. Bessler, *ECS Trans.*, **25** (35), 259 (2010).



Becoming a scientist

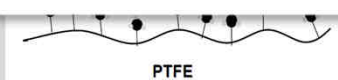
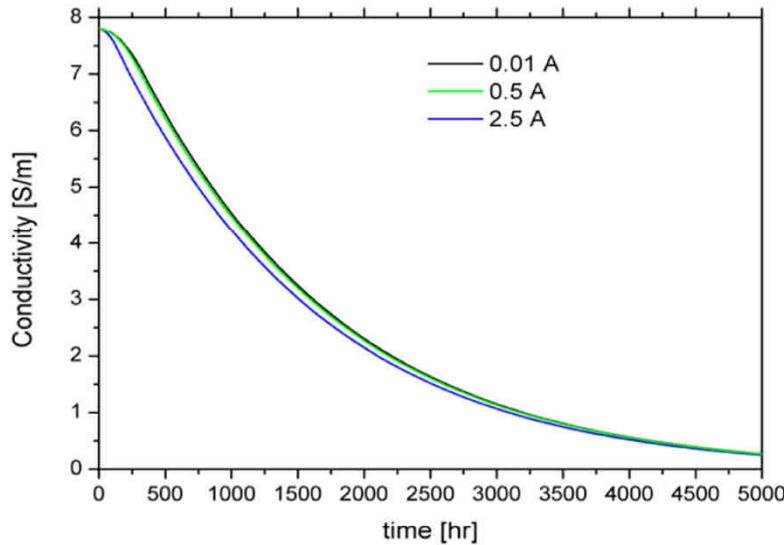
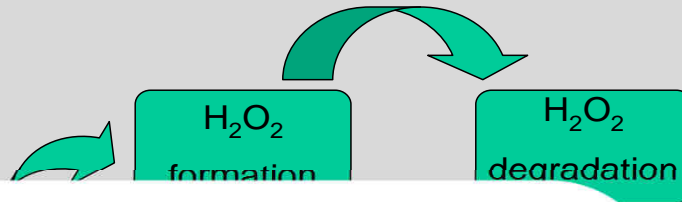
Research motivations

Research contribution

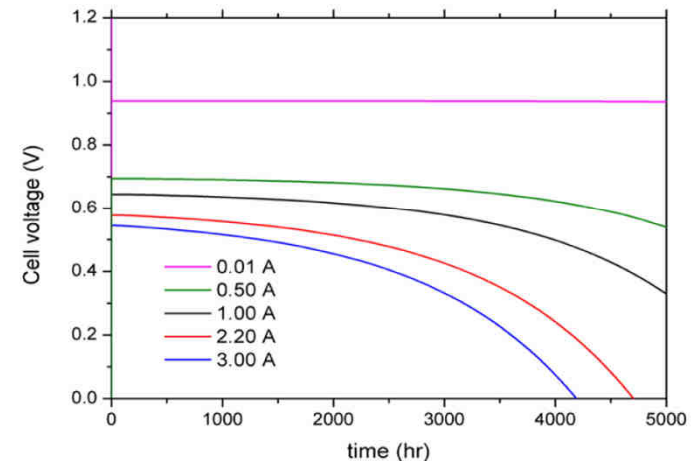
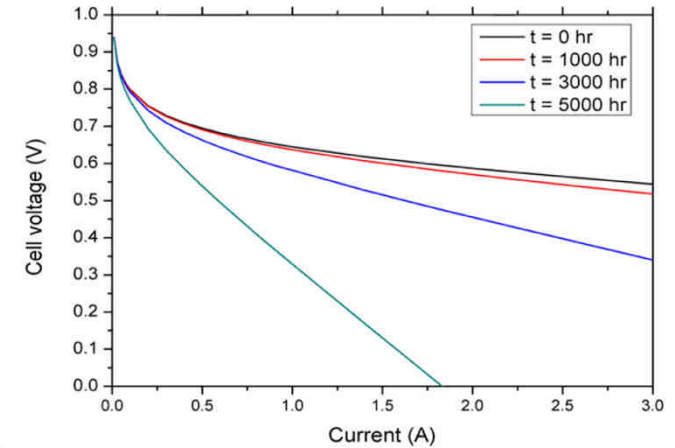
Perspectives

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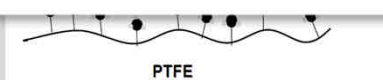
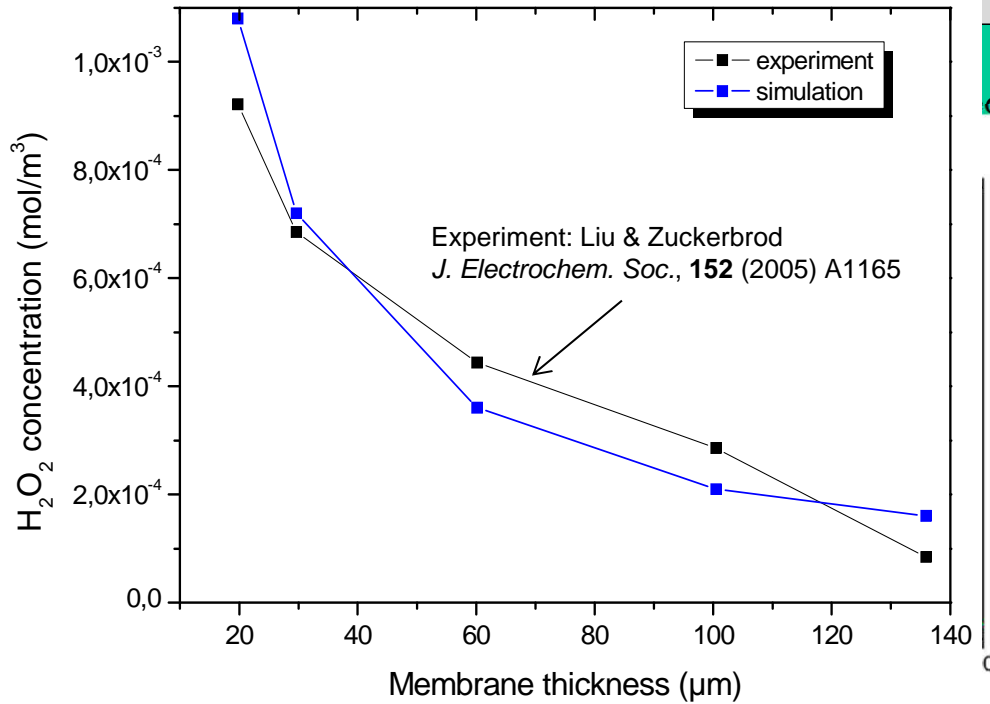
# Example #5: PEM aging



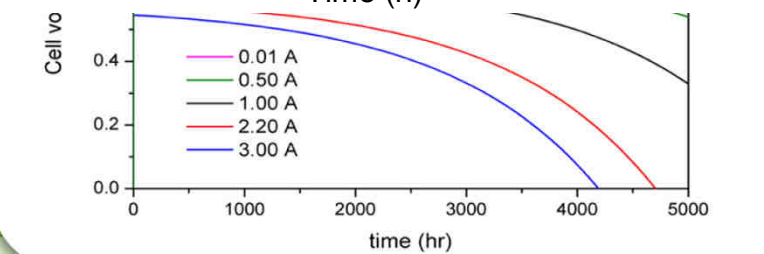
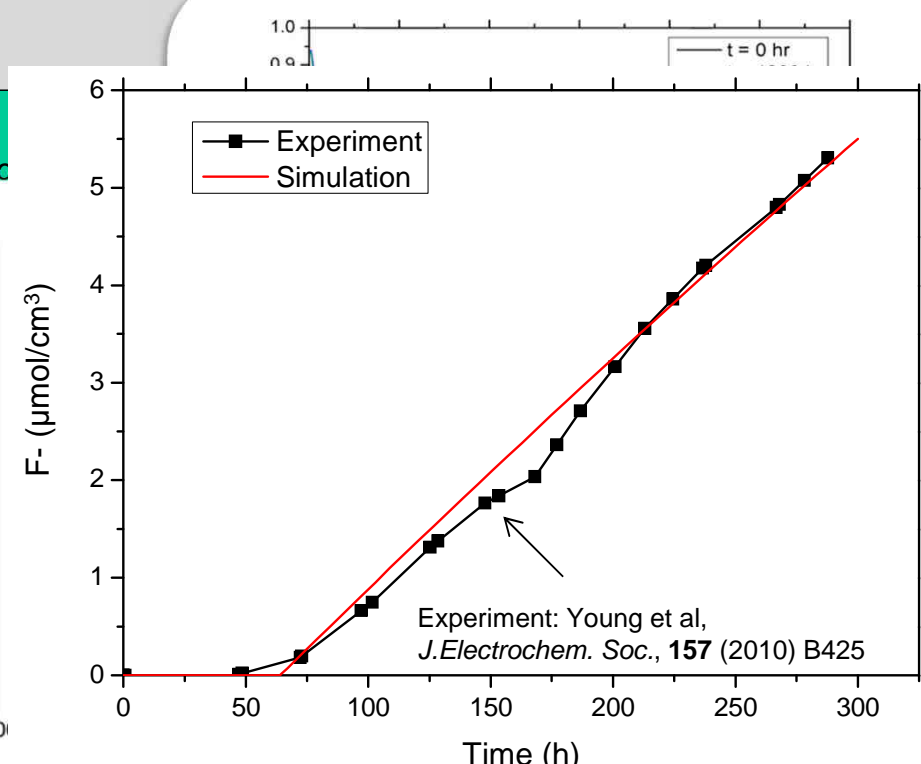
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A.A. Franco et al., *ECS Trans.*, **25** (1), 65 (2009).  
R. Coulon, A.A. Franco, W. Bessler, *ECS Trans.*, **25** (35), 259 (2010).





# Example #6: cathode C corrosion

□ C corrosion: elementary kinetic model of the oxides and CO<sub>2</sub> formation.

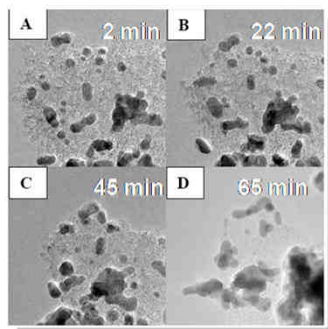
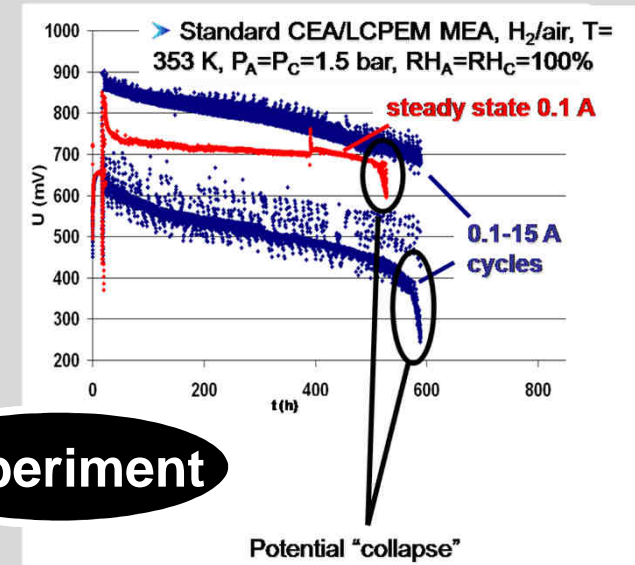
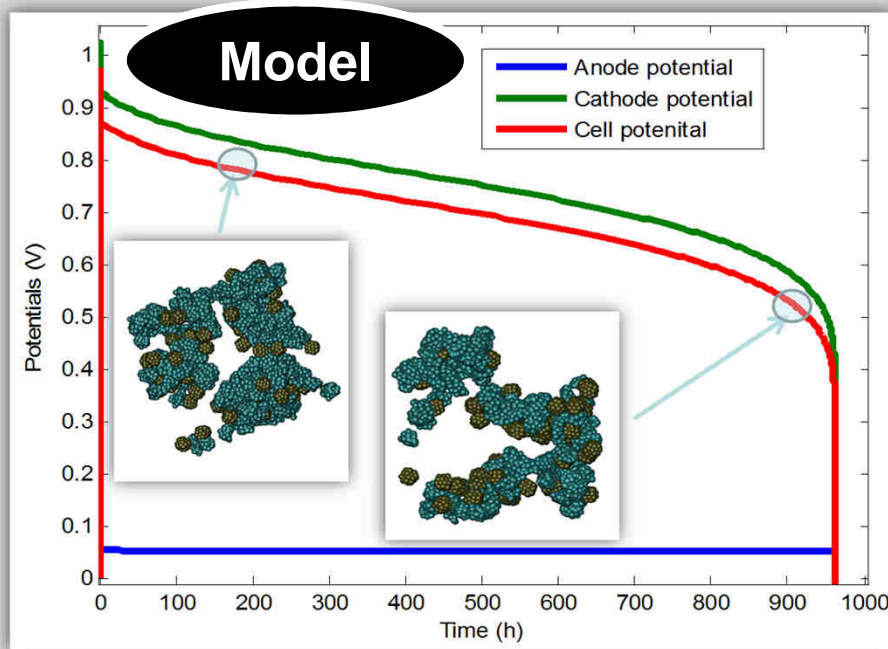


Becoming a scientist

Research motivations

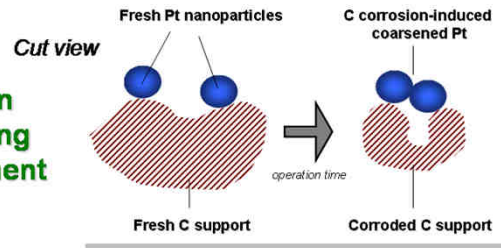
Research contribution

Perspectives



TEM images for 38 wt.% Pt/C (Tanaka) taken after (A) 2 min. (B) 22 min. (C) 45 min. (D) 65 min. under the electron beam (U=300keV).

**COR-driven Pt coarsening and detachment**



$$\frac{I}{S_{Pt}(t)} = F \sum_i v_i^{Far} \pm \frac{\partial \sigma}{\partial t}$$

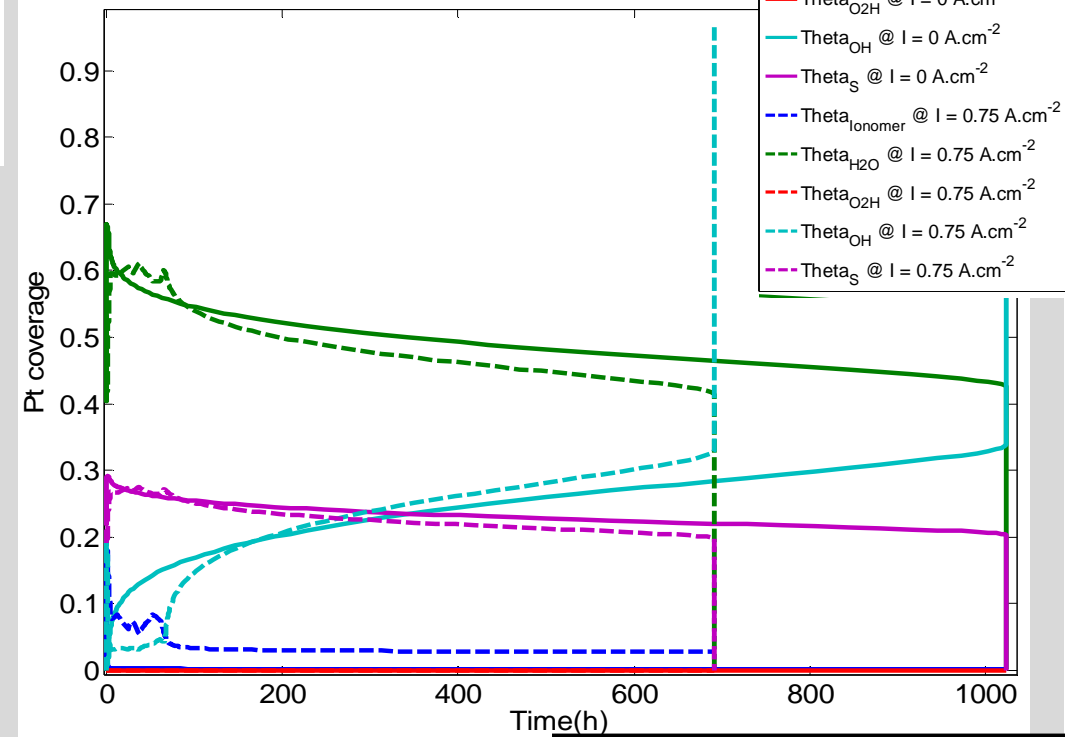
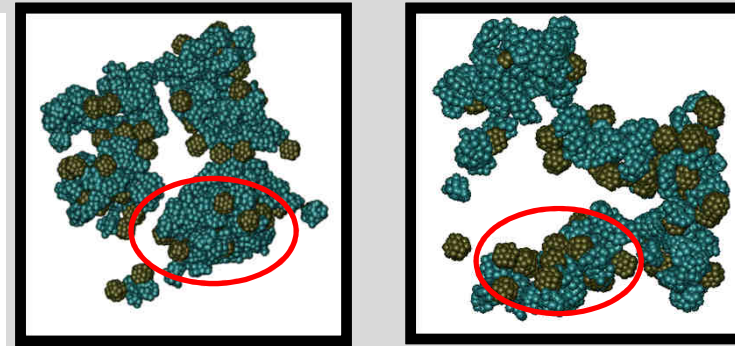
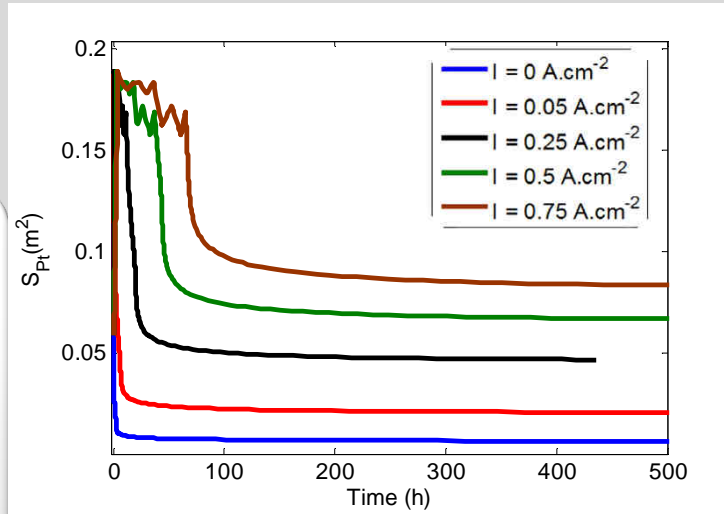
$$S_{Pt}(t) \downarrow \Rightarrow \psi_{Cathode}(t) \downarrow$$

I @ 0.1 A.cm<sup>-2</sup>  
 T = 300 K  
 P<sub>A</sub>=P<sub>C</sub>=1.5 bar  
 RH<sub>A</sub>=RH<sub>C</sub>=100%  
 S<sub>electrode</sub>=2 cm<sup>2</sup>  
 I/C=0.9  
 WP<sub>A</sub>= 0.1 mg.cm<sup>-2</sup>  
 WP<sub>C</sub>= 0.25 mg.cm<sup>-2</sup>  
 CO<sub>2</sub> @ anode = 0.01%

A.A. Franco et al., *J. Electrochem. Soc.*, **155** (4) B367 (2008).  
 K. Malek, A.A. Franco *in preparation* (2010).

# Example #6: cathode C corrosion

□ Impact of nominal current on Pt surface area evolution and ORR ad-species

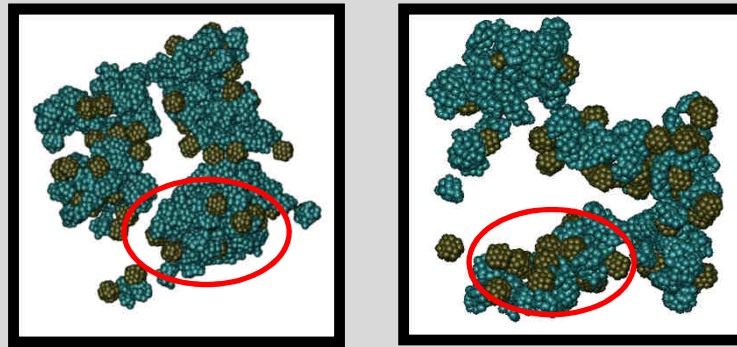
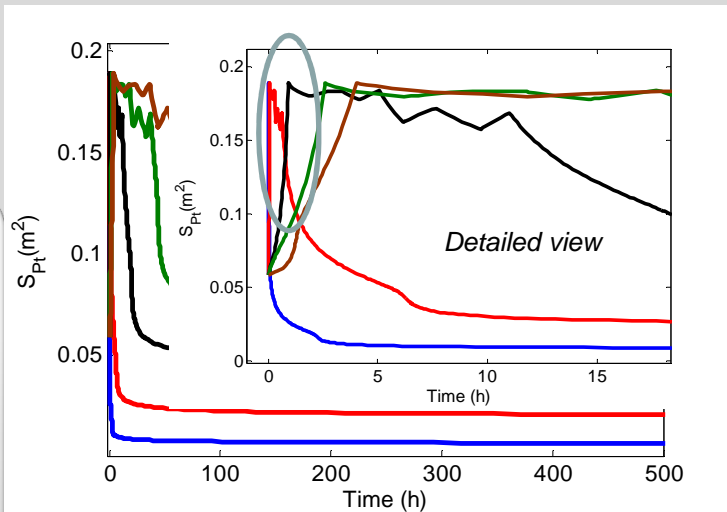


- ✓ C corrosion induces catalyst re-organization (and ad-species).
- ✓ At short-term, catalyst surface area increases with time: catalyst in smaller pores becomes exposed to water and ionomer. At long-term, catalyst surface area decreases (detachment).
- ✓ OH coverage increases with time → effective catalyst activity decay.
- ✓ Ionomer coverage higher at high current → stronger poisoning effect.

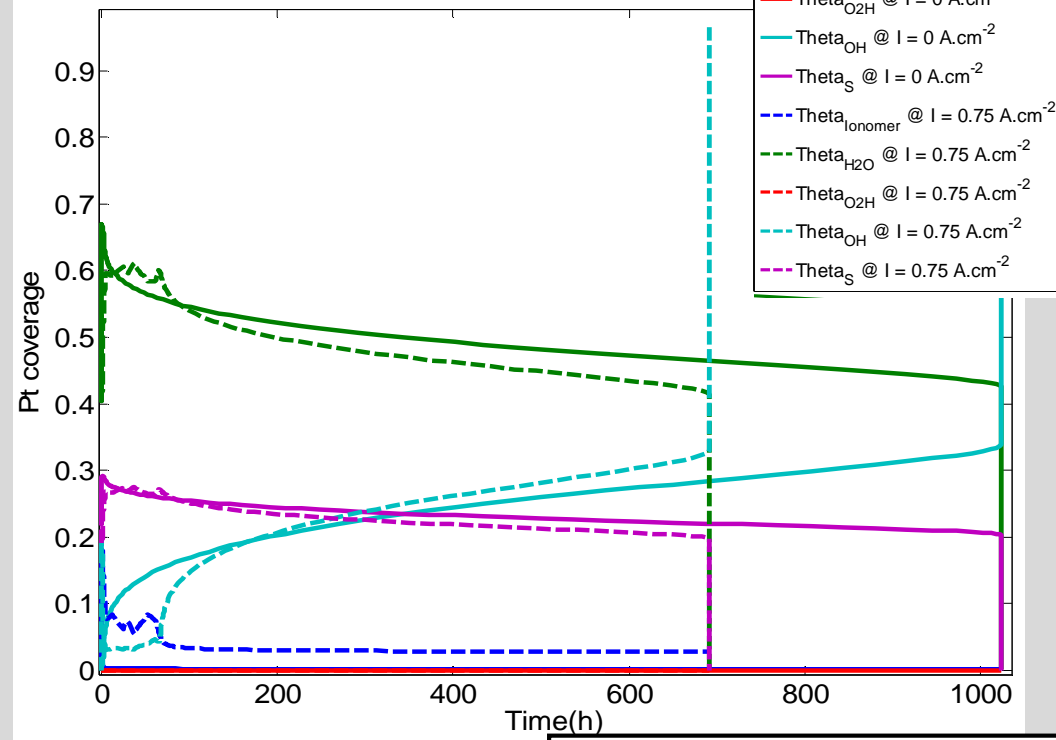
K. Malek, A.A. Franco *in preparation* (2010).

# Example #6: cathode C corrosion

□ Impact of nominal current on Pt surface area evolution and ORR ad-species



- Theta<sub>Ionomer</sub> @ I = 0 A.cm<sup>-2</sup>
- Theta<sub>H<sub>2</sub>O</sub> @ I = 0 A.cm<sup>-2</sup>
- Theta<sub>O<sub>2</sub>H</sub> @ I = 0 A.cm<sup>-2</sup>
- Theta<sub>OH</sub> @ I = 0 A.cm<sup>-2</sup>
- Theta<sub>S</sub> @ I = 0 A.cm<sup>-2</sup>
- - - Theta<sub>Ionomer</sub> @ I = 0.75 A.cm<sup>-2</sup>
- - - Theta<sub>H<sub>2</sub>O</sub> @ I = 0.75 A.cm<sup>-2</sup>
- - - Theta<sub>O<sub>2</sub>H</sub> @ I = 0.75 A.cm<sup>-2</sup>
- - - Theta<sub>OH</sub> @ I = 0.75 A.cm<sup>-2</sup>
- - - Theta<sub>S</sub> @ I = 0.75 A.cm<sup>-2</sup>

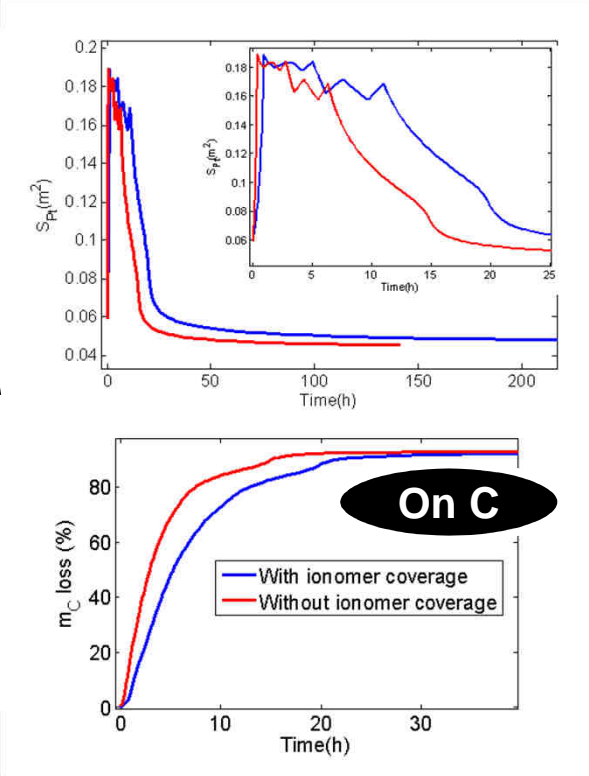
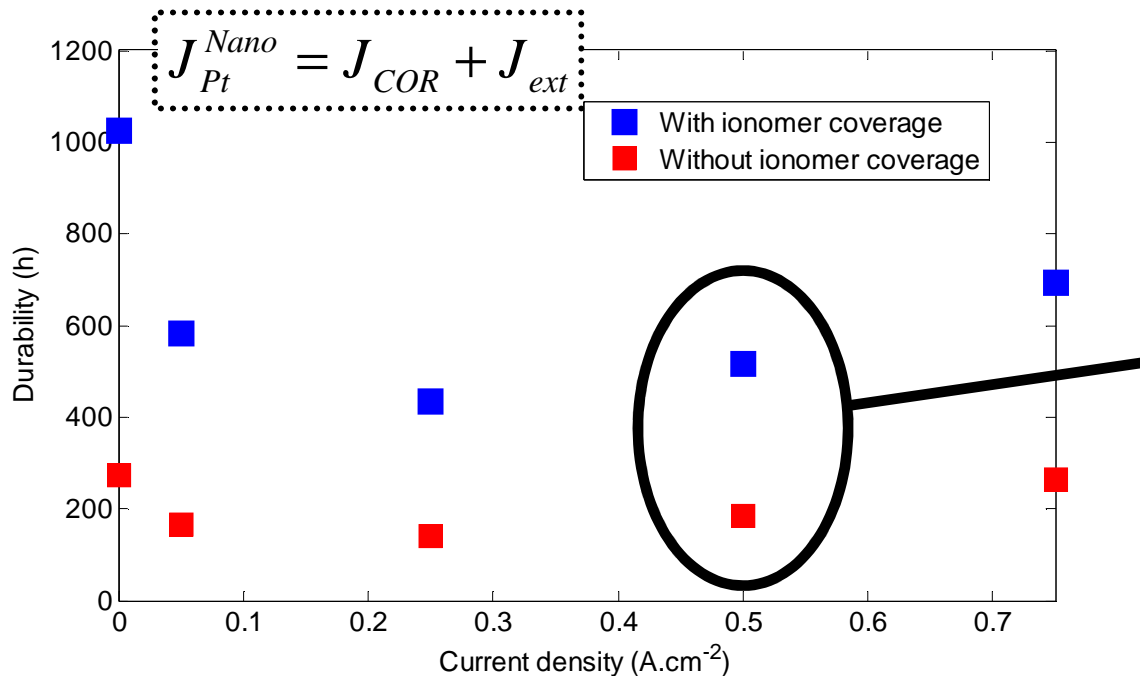


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K. Malek, A.A. Franco *in preparation* (2010).

# Example #6: cathode C corrosion

□ Impact of ionomer adsorption on C and Pt on corrosion kinetics.



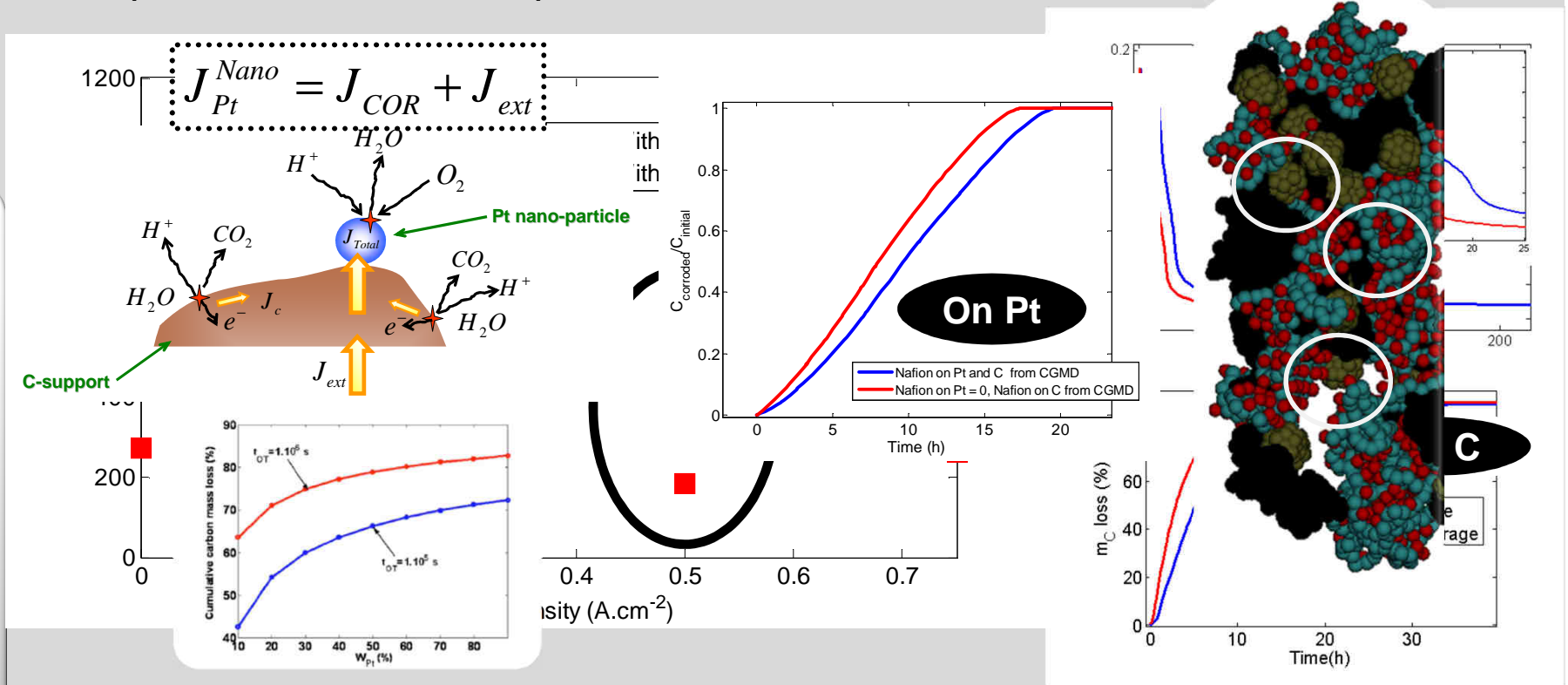
- ✓ Ionomer adsorption on both Pt and C slows down C corrosion and associated catalytic activity loss → extremely important role of the ionomer chemical nature in electrode degradation!
- ✓ Pt catalyzes C corrosion: C corrosion increases as the Pt ORR activity increases (electron pumping mechanism\*)
- ✓ Ionomer adsorption on Pt slows down ORR activity → C corrosion rate is slowed down.

A.A. Franco et al., *J. Electrochem. Soc.*, **155** (4) B367 (2008).  
 K. Malek, A.A. Franco in preparation (2010).



# Example #6: cathode C corrosion

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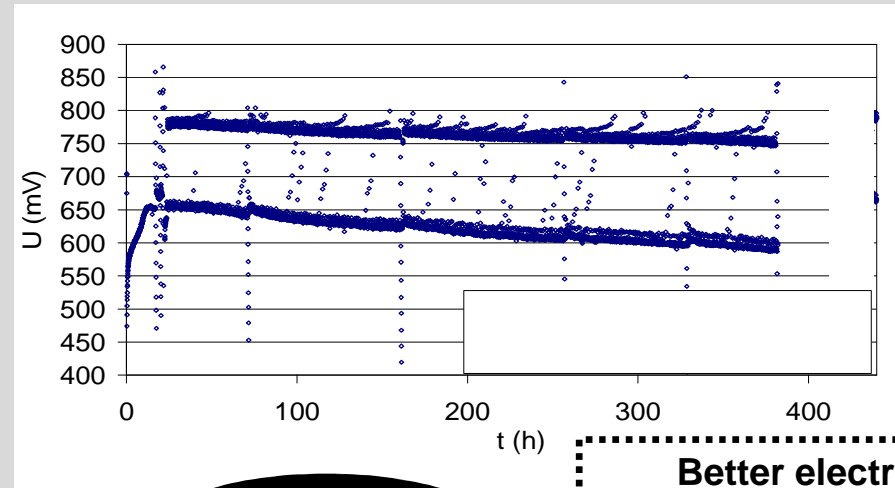
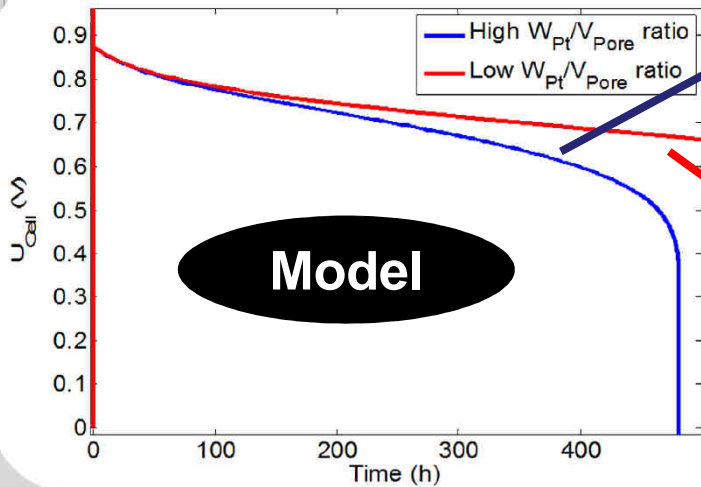
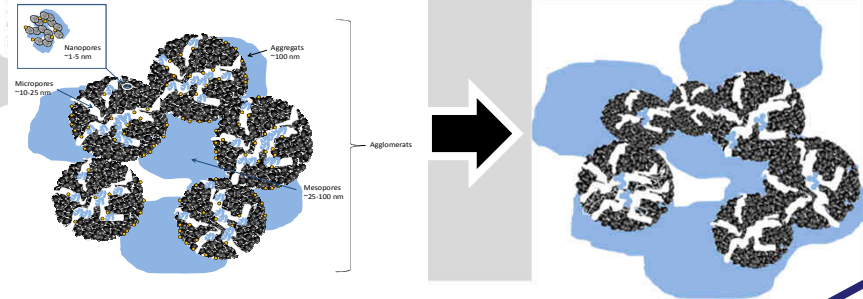
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A.A. Franco et al., *J. Electrochem. Soc.*, **155** (4) B367 (2008).  
K. Malek, A.A. Franco in preparation (2010).

# Example #7: impact of $W_{Pt}/V_{pore}$ ratio on performance decay @ $I_{min}-I_{max}$ cycle

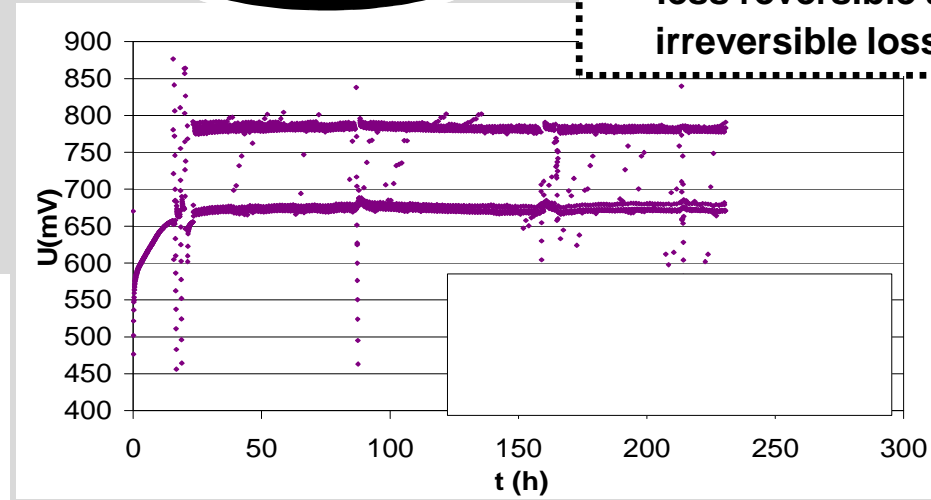
□ Impact of water flooding on performance decay well reproduced by the model: the increase of Pt loading per unit of pore volume enhances potential decay (flooding, Pt dissolution and C corrosion).  
 Courtesy S. Escribano & R. Vincent (CEA/LCPEM)

Components for Polymer electrolyte fuel cells and Electrolysers.



**Experiment**

Better electrode mesostructuration → less reversible and irreversible losses

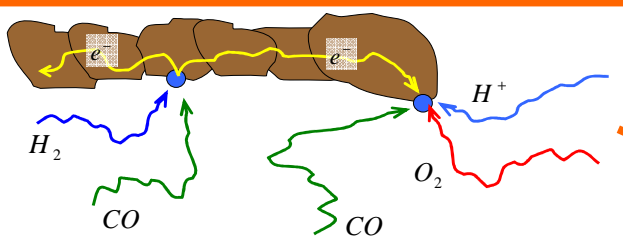
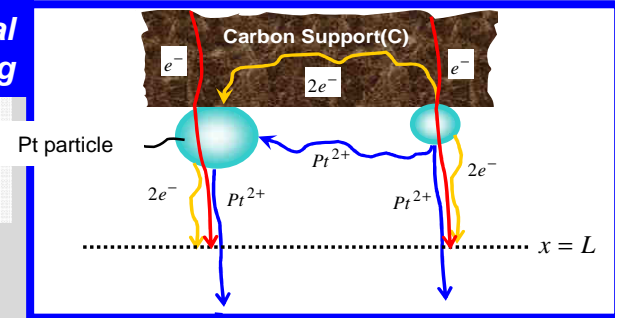
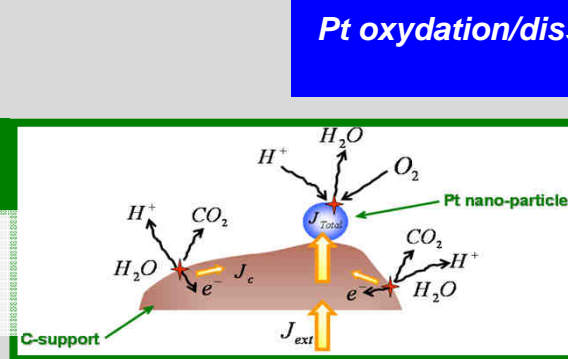


A.A. Franco et al., *J. Electrochem. Soc.*, **154** (7) B712 (2007).  
 A.A. Franco et al., *J. Electrochem. Soc.*, **155** (4) B367 (2008).

# Example #8: competition between materials aging mechanisms (1/2)

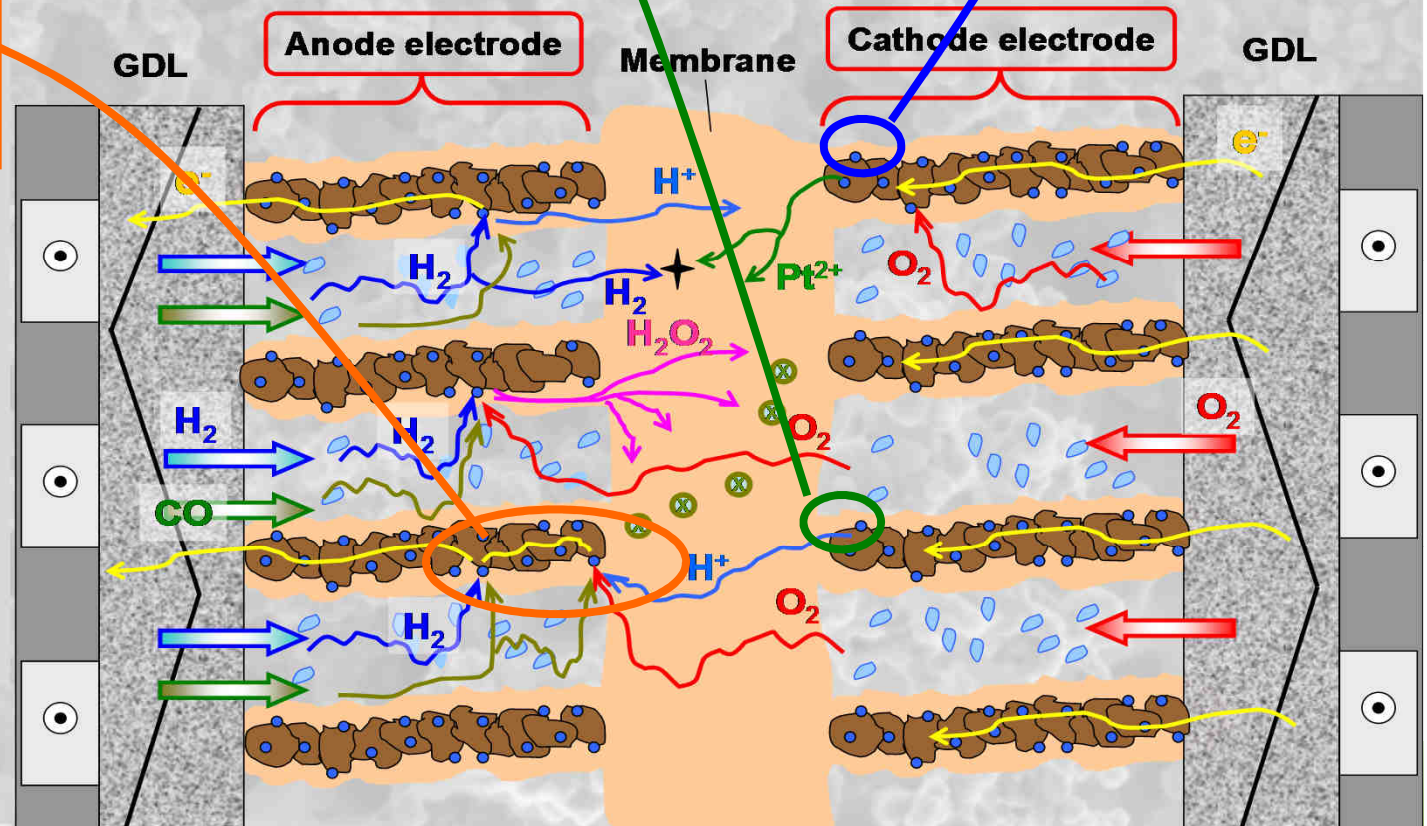
## Cathode catalyst C-support corrosion

A.A. Franco, M. Gerard, *J. Electrochem. Soc.*, **155** (4) B367 (2008)



## Competition between local ORR and CO-catalyst poisoning

A.A. Franco et al, *ECS Trans.*, **13** (15) 35 (2008)  
 A.A. Franco et al, *Electrochimica Acta*, **54** (22) 5267 (2009).



- Water
- Pt<sup>0</sup> crystallites
- Fenton's cations



# Example #8: competition between materials aging mechanisms (2/2)

Square cycle 0.1-0.5 A.cm<sup>-2</sup>  
 (period=30 min).  
 T = 300 K  
 P<sub>A</sub>=P<sub>C</sub>=1.5 bar  
 RH<sub>A</sub>= RH<sub>C</sub>=100%  
 WPt<sub>A</sub>= 0.1 mg.cm<sup>-2</sup>  
 WP<sub>C</sub>= 0.25 mg.cm<sup>-2</sup>

- ❑ Non uniformities of aging mechanisms can now be resolved.
- ❑ Deconvolution between the different contributions to the global potential decay.
- ❑ Validated by TEM characterizations.



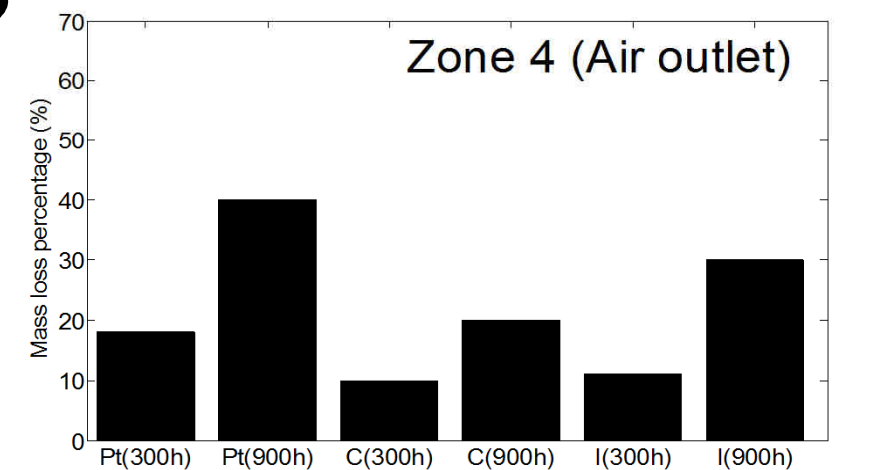
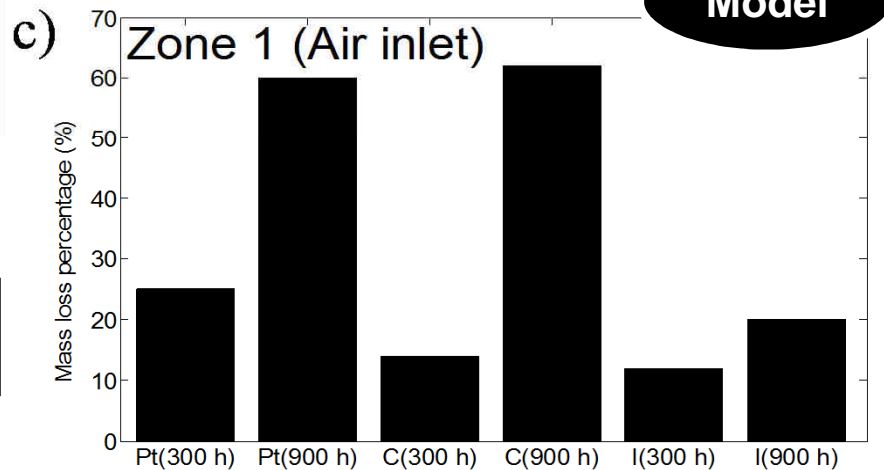
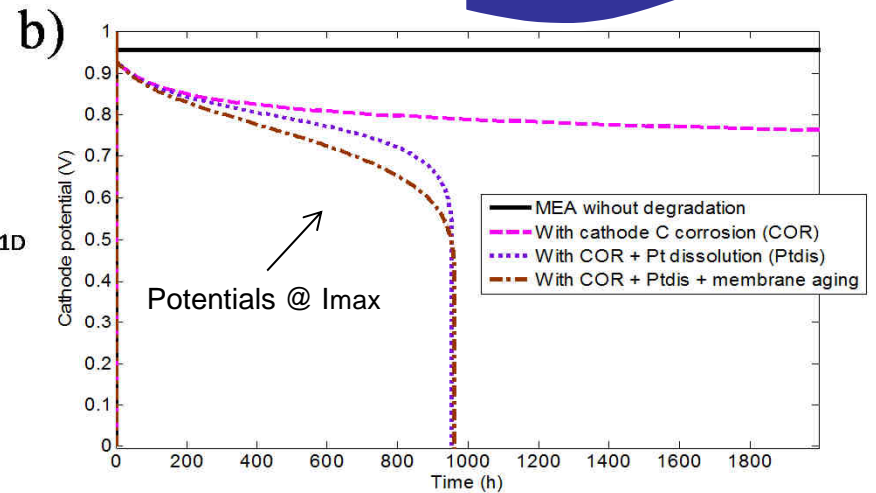
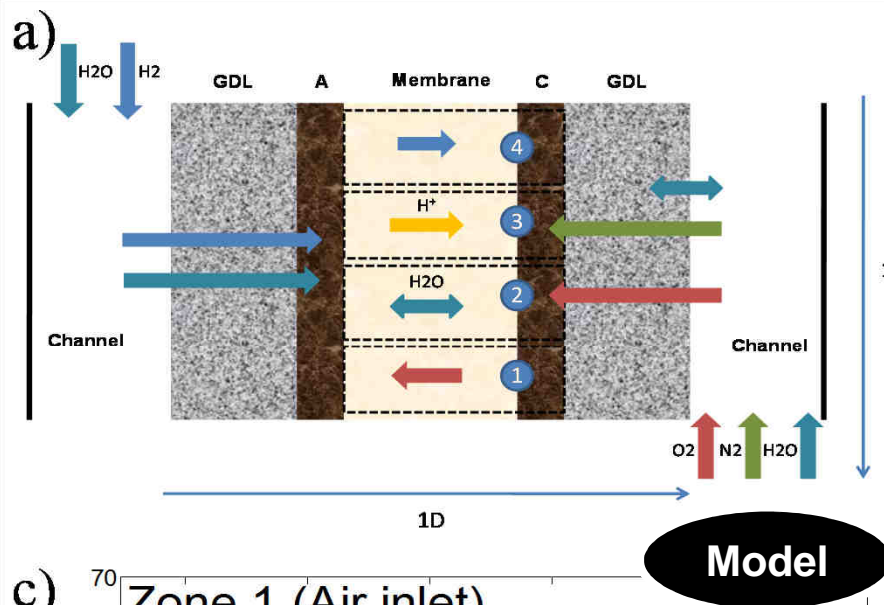
Becoming a scientist

Research motivations

Research contribution

Perspectives

A.A.Franco et al., *J. Electrochem. Soc.*, in preparation (2010).





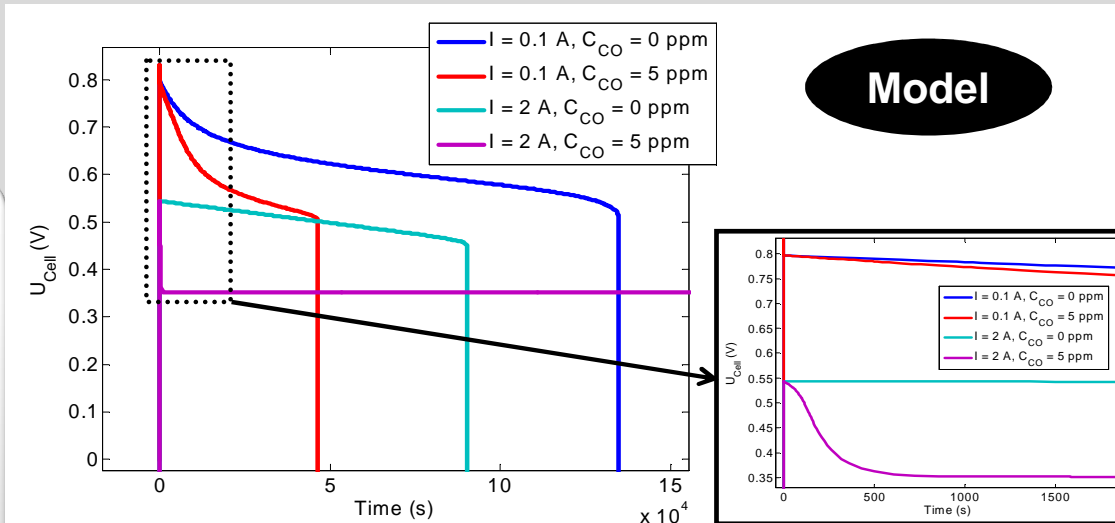
# Example #9: impact of external contaminants on MEA durability



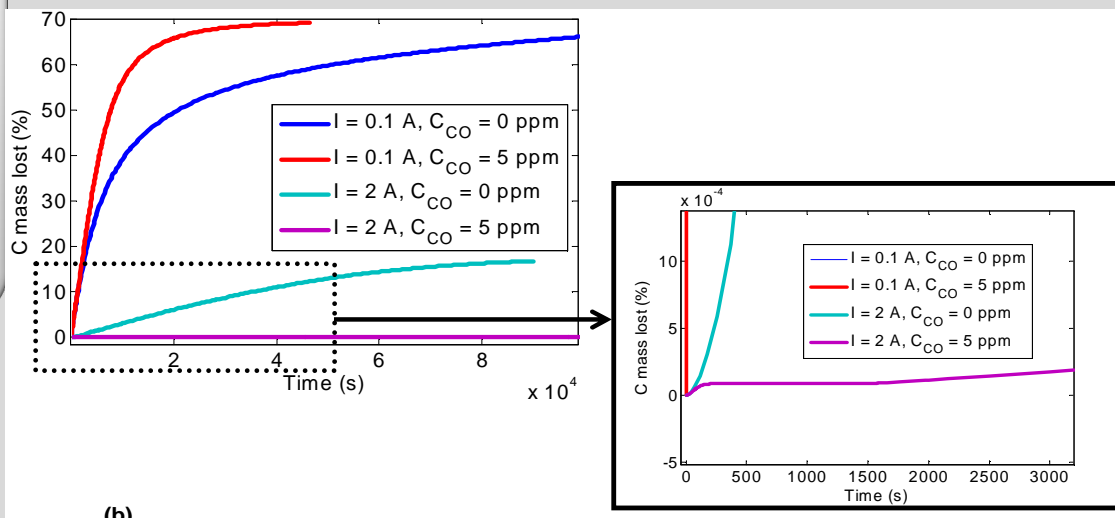
Becoming a scientist  
Research motivations

Research contribution  
Perspectives

□ Impact of current and CO concentration on cell potential evolution.



✓ For low currents, the potential decay rate increases as the CO concentration increases (strong CO poisoning effect).  
✓ For higher currents and high CO concentrations, cell potential stabilizes after a strong short-term decay.

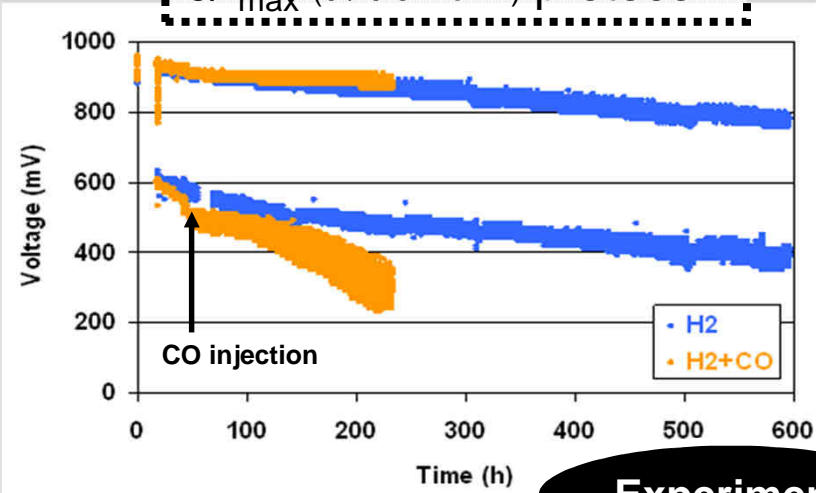


✓ For low currents, C mass loss increases as the CO concentration increases (more H<sub>2</sub>O<sub>2</sub> production in the anode → more PEM degradation → more crossover).  
✓ For higher currents and high CO concentrations, C mass loss and PEM degradation is mitigated.

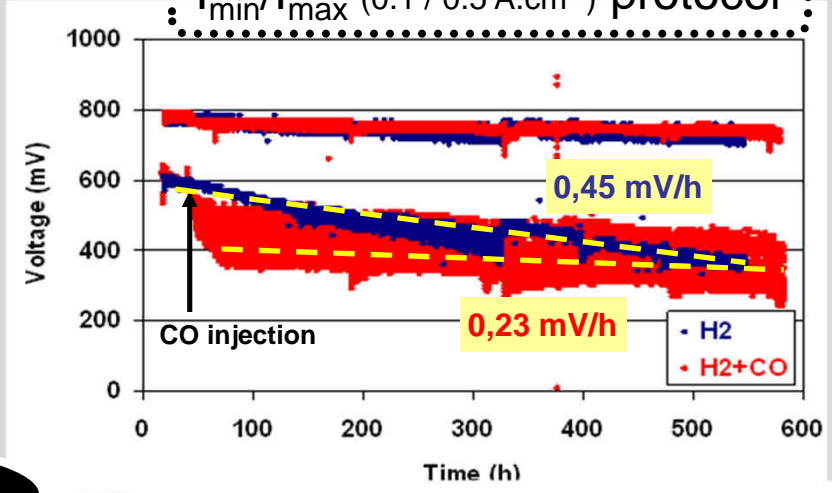
# Example #9: impact of external contaminants on MEA durability

❑ Degradation under pure H<sub>2</sub> and H<sub>2</sub> + CO (5ppm): experiments (complimented with XPS and TEM).

0/I<sub>max</sub> (0 / 0.5 A.cm<sup>-2</sup>) protocol

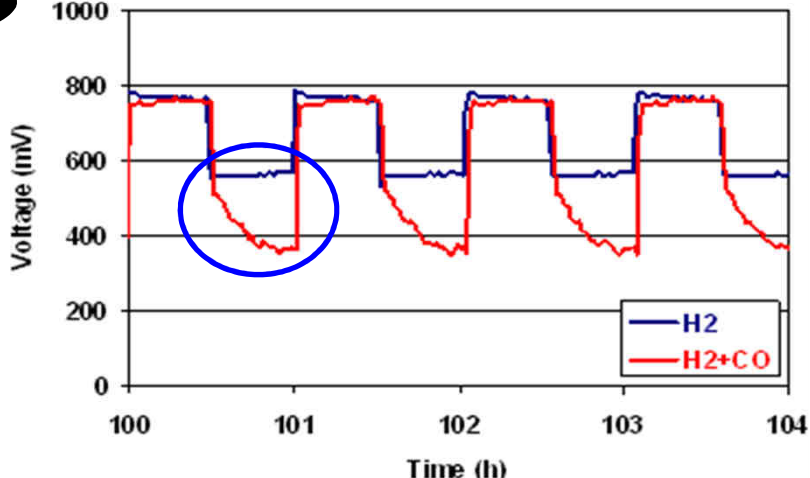


I<sub>min</sub>/I<sub>max</sub> (0.1 / 0.5 A.cm<sup>-2</sup>) protocol



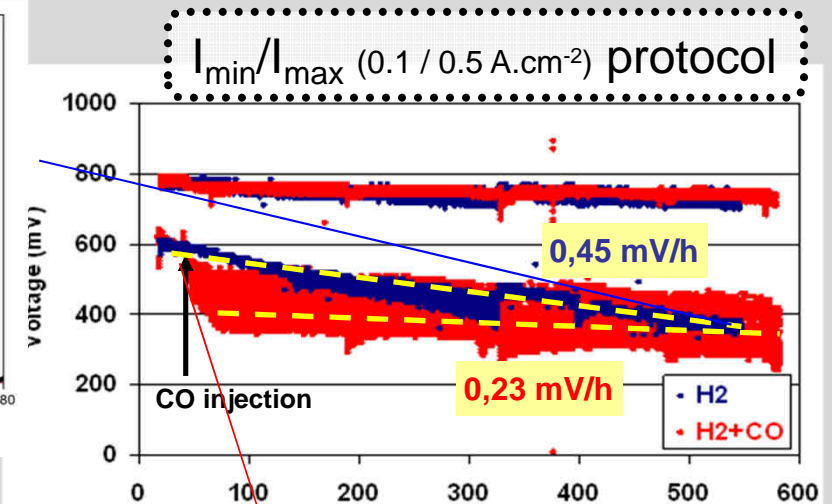
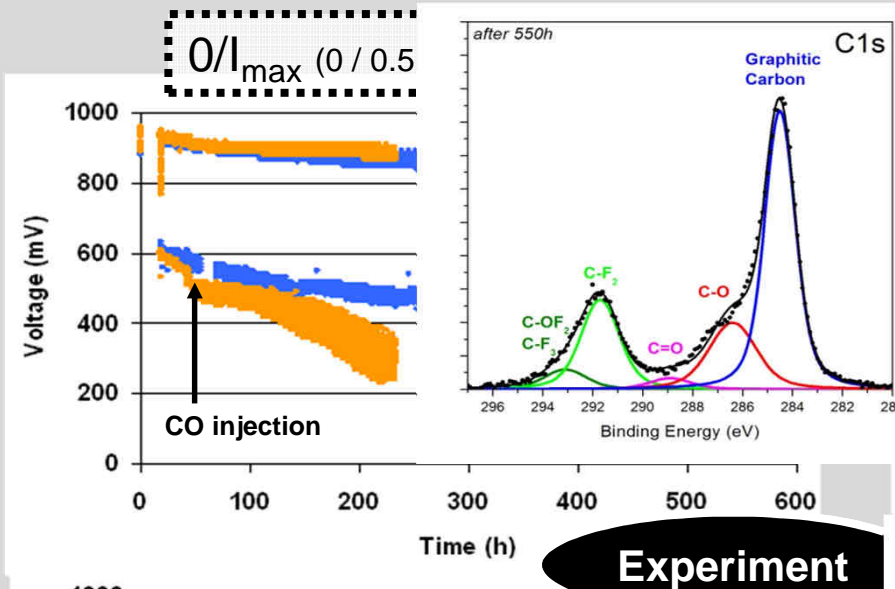
**Experiment**

- ❑ CO reacts with O<sub>2</sub> (to give CO<sub>2</sub>) decreasing
  - the anodic ORR rates and thus decreasing the proton pumping effect → mitigation of cathode carbon corrosion
  - the anodic H<sub>2</sub>O<sub>2</sub> production → mitigation of PEM degradation



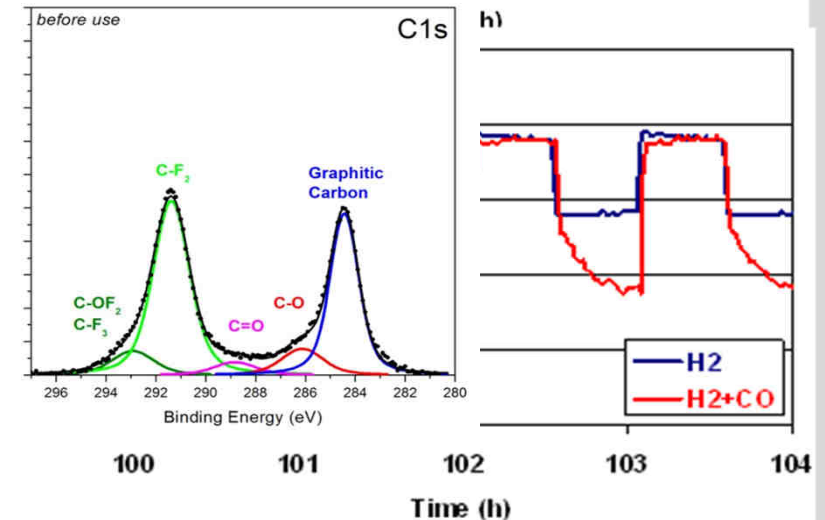
## Example #9: impact of external contaminants on MEA durability

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# Example #9: impact of external contaminants on MEA durability



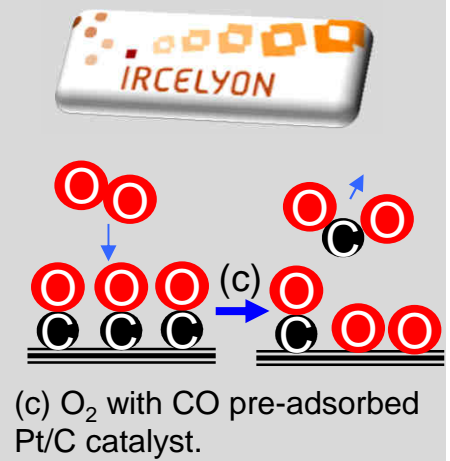
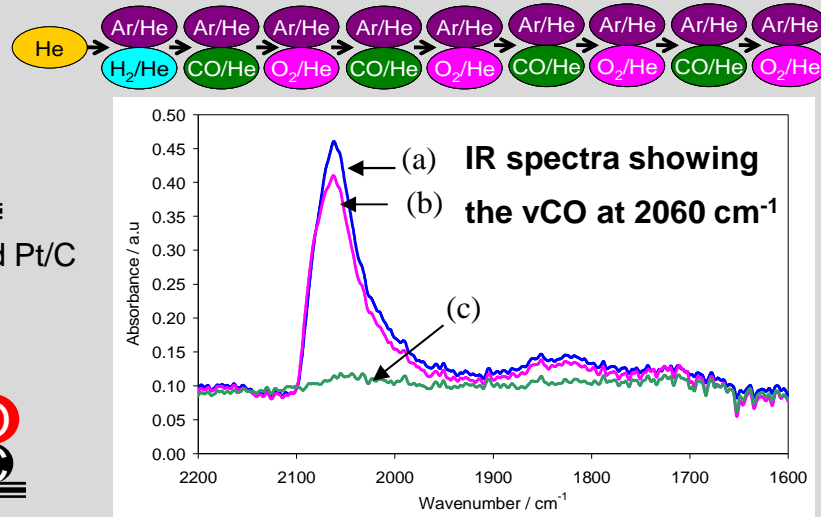
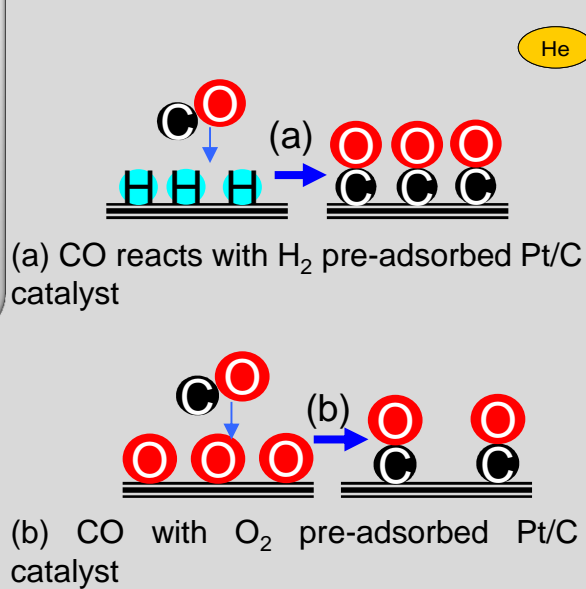
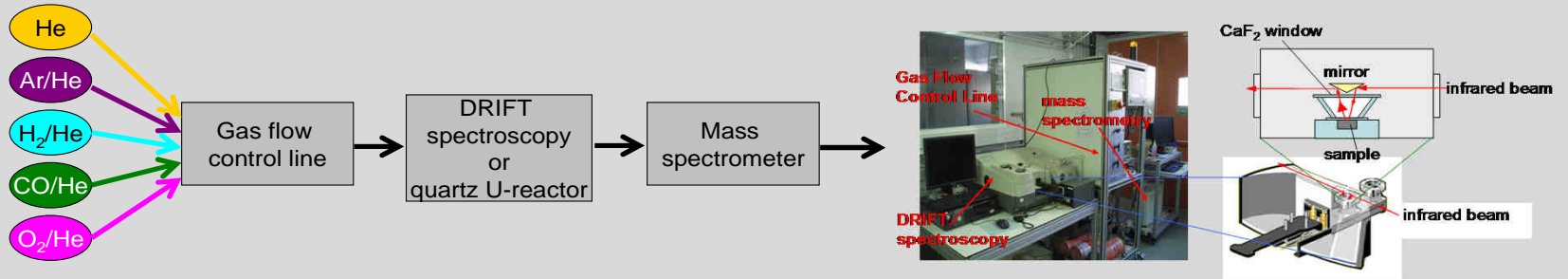
- ❑ CO+O<sub>2</sub> ≠ O<sub>2</sub>+CO mechanism experimentally demonstrated using coupled DRIFT-spectroscopy/mass spectrometry and electrochemical half cell.
- ❑ Air bleeding of CO: very low performance reaction vs. using CO to remove O<sub>2</sub> from the surface
- ❑ Air bleeding can strongly contribute on cathode C corrosion (cf. A.A. Franco et M. Gerard, *J. Electrochem. Soc.* 2008), and CO can be used to remove crossover O<sub>2</sub> to mitigate C corrosion:

Becoming a scientist

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Research contribution

Perspectives



A.A.Franco et al., *Electrochim. Acta*, **54** (22), 5267 (2009).  
 S. K. Cheah, P. Gelin, O. Lemaire, A.A.Franco, *in preparation* (2010).





Becoming  
a scientist

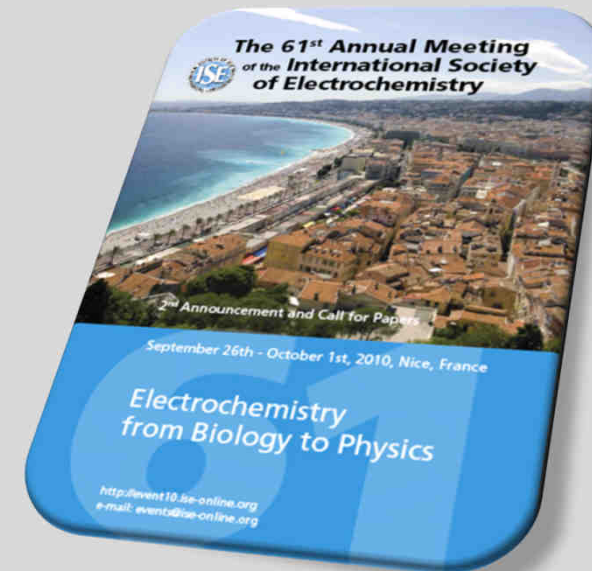
Research  
motivations

Research  
contribution

Perspectives

# My scientific production 2003-2005 (PhD) + 2006-2010

- ❑ 23 papers published in international journals (+ 5 submitted).
- ❑ 3 book chapters (Pan Stanford-Imperial College, Woodhead-Cambridge, Springer)
- ❑ 1 book edition, internationally recognized contributors (Pan Stanford)
- ❑ 14 patents filed (+ 6 under application)
- ❑ 18 invited presentations in international conferences
- ❑ 30 oral presentations in international conferences
- ❑ Organization of 3 international conferences
- ❑ Several invited seminars in universities/institutes (Stanford University, NRC...).
- ❑ July 2008: invited presentation to Prof. Bernard Bigot (CEA High Commissioner)
- ❑ Young Scientist Award Finalist 2005 (International Society of Solid State Ionics)





Becoming  
a scientist

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contribution

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# Conclusions

- ❑ CEA multiscale/multiphysics model MEMEPhys<sup>®</sup> allows describing the nanomaterials (e.g. Pt, Pt<sub>x</sub>M<sub>y</sub> catalysts, C support, PEM...) degradation in in situ PEMFC conditions, on the basis of an *ab initio*-based elementary kinetics/non-equilibrium thermodynamics framework (bottom-up approach):
  - analysis of competitive aging mechanisms and cell durability prediction (**without using empirical Butler-Volmer approach**).
- ❑ In practice:
  - experimental observables (polarisation curves, EIS...) from first principles: useful for experiments interpretation.
  - microstructure-performance-durability relationships for the MEA materials: useful for materials design
- ❑ Re-usable/evolutive approach:
  - possibility of refining physics in a given module without changing the rest of the model.



# Conclusions



Becoming  
a scientist

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- Today, we illustrated the capabilities of our approach through some application examples, including:
  - **Benchmarking** of PEMFC electrocatalysts (activity and durability)
  - **Anode CO contamination enhances the degradation of  $Pt_xCo_y$  catalysts.**
  - Possibility of **using CO anode contamination as a mitigation method** of cathode C corrosion and PEM degradation.
  - Revealing the crucial role of **ionomer mesostructure on C corrosion** kinetics
  - Revealing the crucial role of **liquid water on the degradation mechanisms.**



- Becoming a scientist
- Research motivations
- Research contribution
- Perspectives**

# Perspectives of my research

## □ Technical perspectives:

### ✓ Refining MEMEPhys<sup>®</sup> modules:

- further detailed descriptions of transport phenomena and electrochemistry -e.g. solvent and ionomer impact on reactions- (ongoing)
- implementation of new phenomena (mechanical stresses, thermal issues)
- continuation of experimental validation (e.g. EU project PREMIUM ACT)
- interpolated relationships for simplified models → stack perspective

### ✓ Improvement of global MEMEPhys<sup>®</sup> model:

- structural identifiability analysis
- symplectic discretization methods (e.g. EU project MMM@HPC or joint thesis with LAGEP?)
- user-friendly interface for non-specialists (including experimentalists).
- commercialization perspective within 3-4 years



# Perspectives of my research



□ Technical perspectives:

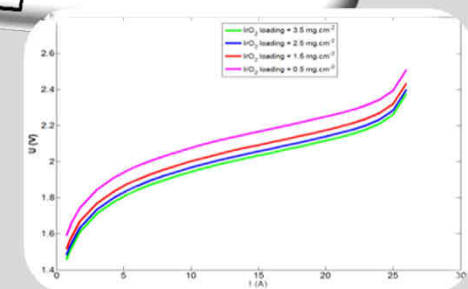
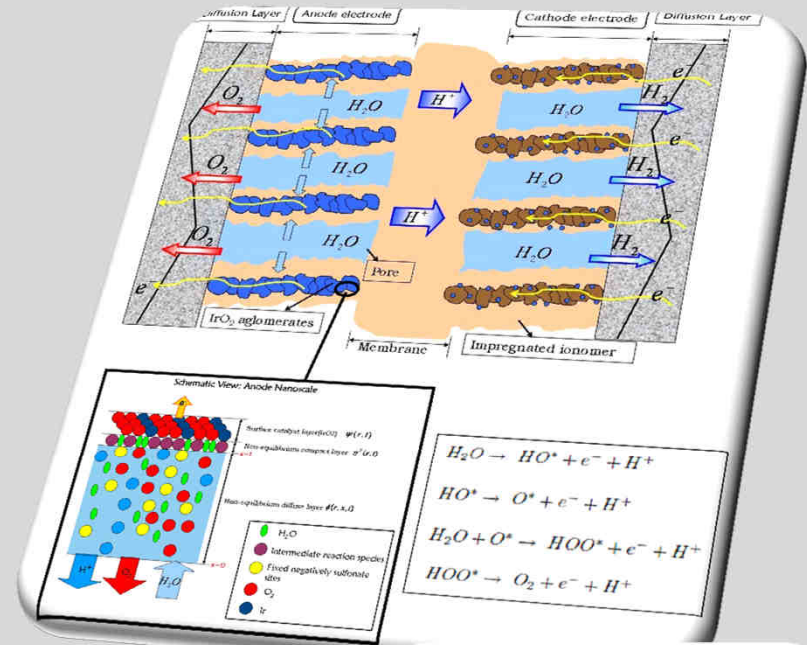
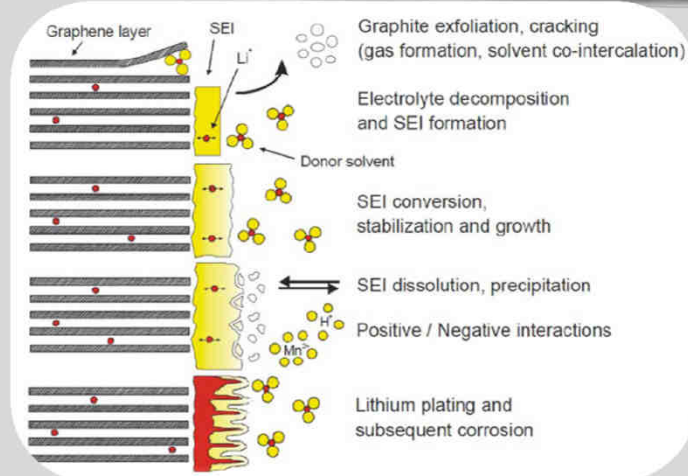
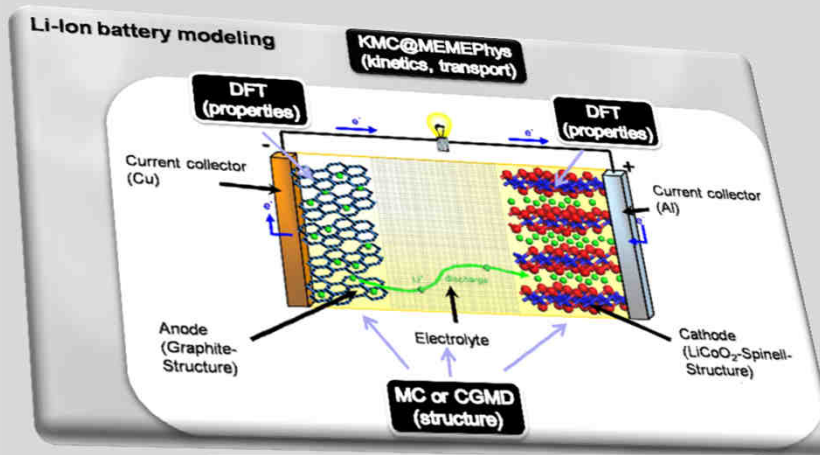
✓ extension of this model for PEM-Water Electrolysers (PEMWE) and Li-ion batteries → my ongoing activities.

Becoming a scientist

Research motivations

Research contribution

Perspectives





Becoming  
a scientist

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# Perspectives of my scientist life

## □ Scientist perspectives:

- ✓ continue propagating “multiscale” and “network” modeling approaches within the electrochemistry community
- ✓ continue helping into the international recognition of my laboratory
- ✓ continue managing the Modeling Group and contributing on deciding on the CEA research strategies
- ✓ teaching to young students

# Acknowledgements

- Prof. Alfredo Juan and Prof. Jean Bletry for providing this opportunity to realize my dream
- Prof. Christian Jallut and Prof. Bernhard Maschke for their great lessons during my PhD
- Dr. Florence Lefebvre-Joud for proposing me this position and Nicolas Bardi (head of the LCPEM during 2007-2009) for his support.
- Dr. Olivier Lemaire (head of the LCPEM) and Dr. Florence Mattera (head of the DEHT) for their support.



- All my colleagues in the Modeling Group and in LCPEM (special thanks to Christine Nayoze, Remi Vincent, Federico Nores, Valentina Vetere...)
- All my collaborators inside and outside CEA (special thanks to Tetsuya Mashio, Atsushi Ohma, David Loffreda, Philippe Sautet, Nicolas Fouquet, Kourosh Malek, Wolfgang Bessler, Valerie Parry, Patrick Gelin, Gerard Gebel...)
- All my students and postdocs
- All the members of the jury
- All my family and friends all around the world
- *And mi princesa...*





# My becoming a scientist...



My first hydrogen machine (first patent)...

4 Y/O



8 Years Old

T0

My dream: to become a physicist...



Becoming a scientist

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12 Y/O



16 Years Old

My Physics studies and other machines...

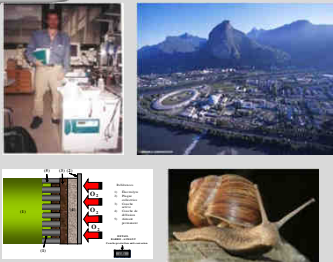


19 Y/O



24 Years Old

My arrival to France and 2002 stay at CEA...

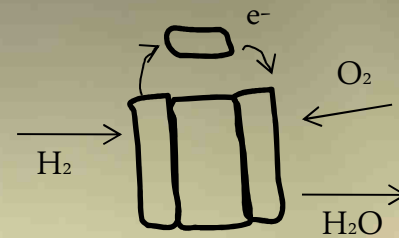


My young scientist life

TODAY: my H.D.R. defense day

32 Years Old





MEMEphys

Gracias Maudsita,  
Mama y Papa, Tia,  
amigazos... por todo  
el aguante de  
siempre... Los quiero  
mucho!

**Thank you very much!**

[alejandro.franco@cea.fr](mailto:alejandro.franco@cea.fr)