SMARTCat

Systematic, Material-oriented Approach using Rational design to develop break-Through Catalysts for commercial automotive PEMFC stacks

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PROJECT OVERVIEW

Project Information	
Call topic	SP1-JTI-FCH.2012.1.5 : New catalyst structures and concepts for automotive PEMFCs
Grant agreement number	325327
Application area (FP7) or Pillar (Horizon 2020)	Transport and refuelling infrastructure
Start date	01/06/2013
End date	31/05/2017
Total budget (€)	4,768,172.60
FCH JU contribution (€)	2,501,998.00
Other contribution (€, source)	
Stage of implementation	85%
Partners	CNRS; SINTEF, DTU, CEA, mxpolymers

PROJECT SUMMARY

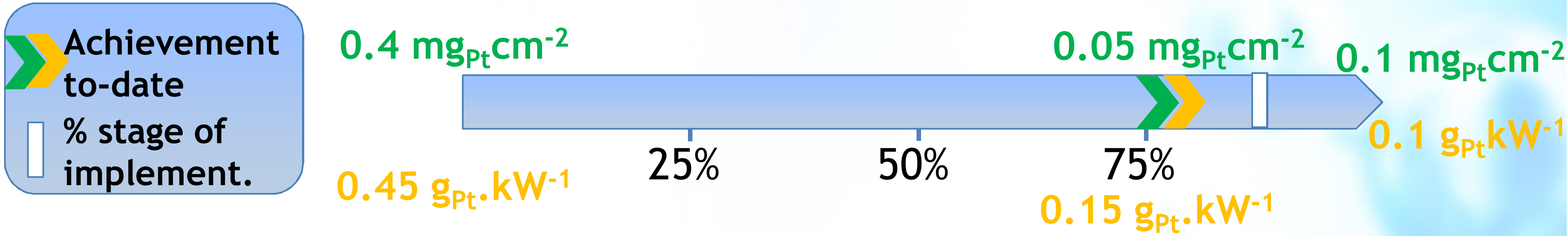
SMARTCat Project aims at:

- Reducing Pt content by combining it with cheaper elements, mainly common metal (Co, Cu, Ni) and Au as ternary alloy and/or core-shell nanocatalysts.
- Introducing new corrosion support able to operate at higher temperature (120 C)
- Predicting the “good” nanocatalyst composition, structure and activity, stability using DFT approach.
- Optimizing pilot MEA production (60 MEAs/day)
- Short stack (10 cells 220 cm^2 active area) evaluation in automotive application conditions.

Global positioning is targeted to provide multielement nanocatalysts, high temperature anticorrosion new supports and DFT methodology as a predictive tools, which will be an impact in FCH community and worldwide by conference invitations and new contracts with interested companies.

Application and market area are targeted to automotive application but stationary (APUs) and nomadic applications are expected to benefit from SMARTcat outputs.

PROJECT PROGRESS/ACTIONS
New Catalysts $Pt_xM_yAu_z$ (M=Ni, Cu, Co)



Aspect addressed	Parameter (KPI)	Unit	SMARTcat 2016	FCH JU Targets		
				Call topic	2017	2020
Pt reduction	Pt loading	$mg.cm^{-2}$	0.05(*)	0.1	0.1	0.1
	Pt loading	$g.kW^{-1}$	0.03(**)	0.1	0.1	-
	Pt loading	$g.kW^{-1}$	0.15 (***)	0.1		

(*) This value is demonstrated to be the ultimate lower Pt value suitable for automotive applications. It is not yet tested in stack conditions.

(**) @Pt loading of 0.05 $mg.cm^{-2}$ in single cell conditions

(***) @Pt loading of 0.18 $mg.cm^{-2}$ in stack conditions

Future steps:

Improved activity on oxide support

Durability of the catalyst

PROJECT PROGRESS/ACTIONS
New Catalysts $Pt_xM_yAu_z$ (M=Ni, Cu, Co)

SMARTCat

Achievement to-date

% stage of implement.

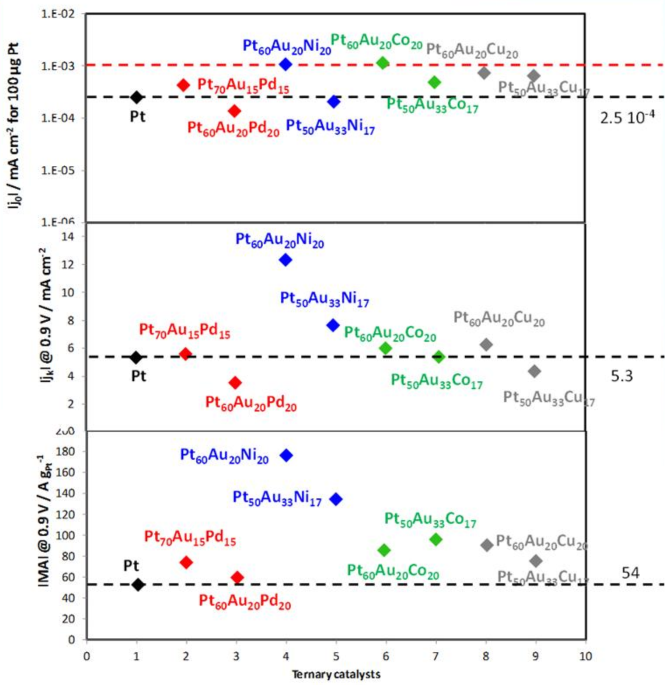
0.4 $mg_{Pt}cm^{-2}$ — 0.45 $g_{Pt}.kW^{-1}$

25% 50% 75%

0.05 $mg_{Pt}cm^{-2}$ — 0.15 $g_{Pt}.kW^{-1}$

0.1 $mg_{Pt}cm$ — 0.1 $g_{Pt}.kW$

Aspect addressed	Parameter (KPI)	Unit	SMART Cat 2016
Catalyst Electrochemical performance (@0.1 $mg_{Pt}cm^{-2}$)	Exchange current density j_0	$mA.cm^{-2}$	> 10^{-3}
	kin current j_k @0.9 V	$mA.cm^{-2}$	13
	mass activity @0.9 V	$A.g_{Pt}^{-1}$	180

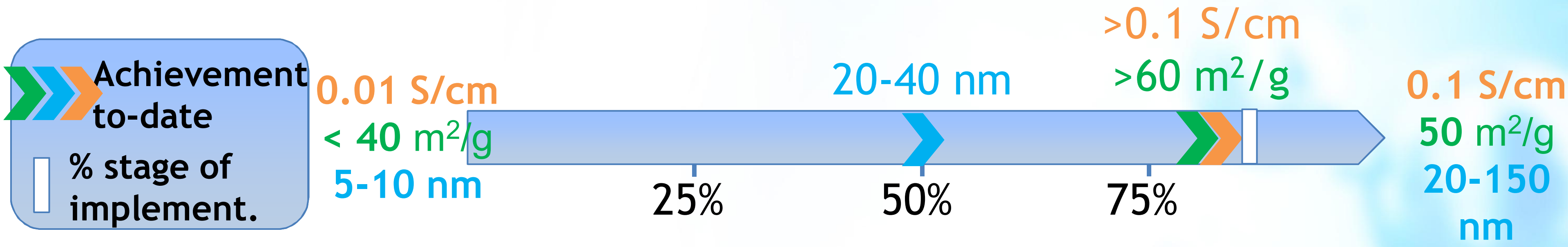


- Stability of $Pt_{60}Ni_{20}Au_{20}$/C ≈ $Pt_{50}Ni_{17}Au_{33}$/C ≈ Pt/C
- Stability of $Pt_{60}Cu_{20}Au_{20}$ > $Pt_{60}Co_{20}Au_{20}$ > $Pt_{60}Ni_{20}Au_{20}$/C

(S. Linkiang, «SMARTCat» PhD thesis 2016, CNRS)

- Perfect agreement with DFT calculations of DTU partner.

PROJECT PROGRESS/ACTIONS
Catalyst support



Aspect addressed	Parameter (KPI)	Unit	SMART Cat 2016	FCH JU Targets		
				Call topic	2017	2020
Conductivity	0.01-0.10	S/cm	>0.1	0.1		
Surface area	> 50	m^2/g	>60	50		
Pore size distribution	20-150	Nm	20-40	20-150		

Future steps:
Conductivity, surface area and pore size distribution may be further optimized by heat treatment and/or synthesis process conditions (flame spray pyrolysis)

PROJECT PROGRESS/ACTIONS
Catalyst support

Achievement to-date

% stage of implement.

0.01 S/cm
50 m^2/g
5-10 nm

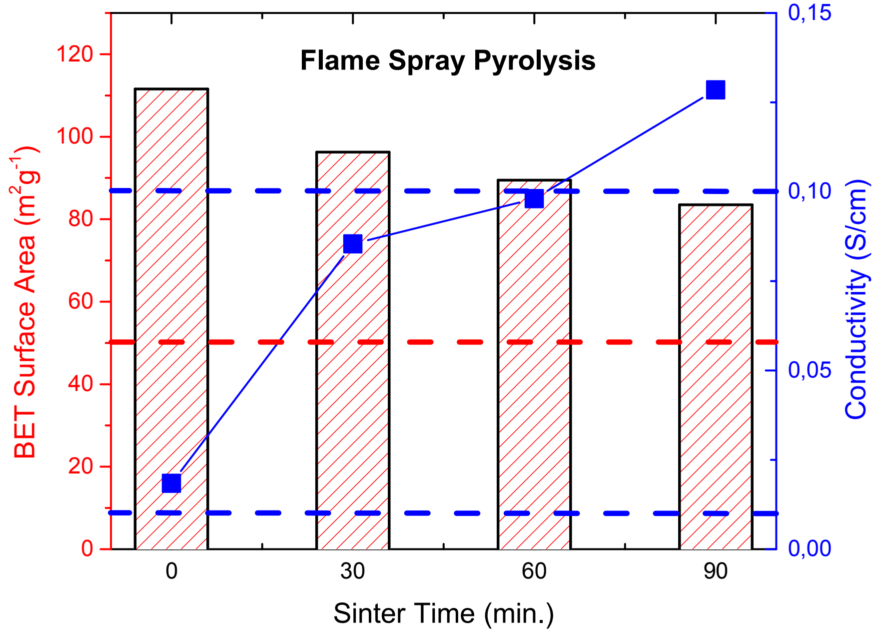
20-40 nm

>0.1 S/cm
>60 m^2/g

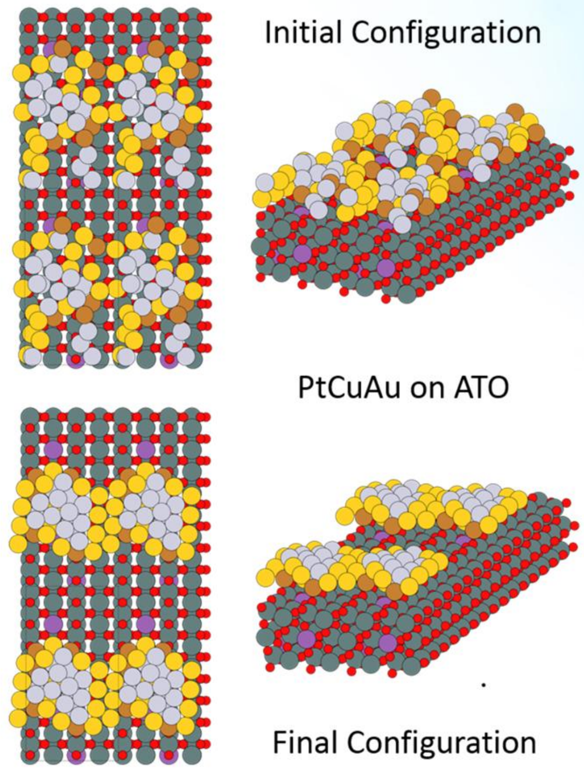
25% 50% 75%

0.1 S/cm
50 m^2/g
20-150 nm

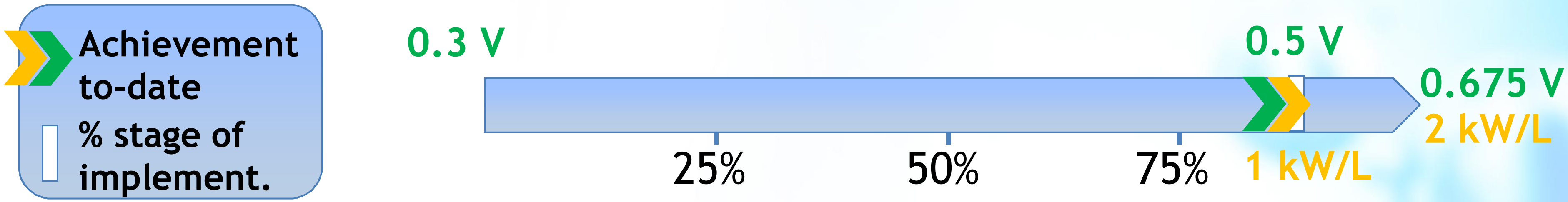
Effect of heat treatment at 550 °C for catalyst support material $Sn_{0.85}Sb_{0.15}O_2$



DFT predicts higher activity and stability of PtCuAu on ATO than Pt alone



PROJECT PROGRESS/ACTIONS
Short stack test (10 cells)



Aspect addressed	Parameter (KPI)	Unit	SMART Cat 2016	FCH JU Targets		
				Call topic	2017	2020
Single cell performance	Single cell power density	$W.cm^{-2}$	0.75	1	1	1
Stack performance	Average cell voltage (*) @1A	V	0.5	0.675 (**)	0.675	0.675
	Stack power density (*)	kW/L	1	2	2	-

(*) Operation using an unoptimised stack design working according to the European Harmonized Protocol conditions; 220 cm^{-2} active area; (**) at 1.5 A cm^{-2}

Future steps:
Lifetime of 5000h, Degradation rate of 20μV/h @0.5 A cm^{-2}

PROJECT PROGRESS/ACTIONS
Short stack test (10 cells)

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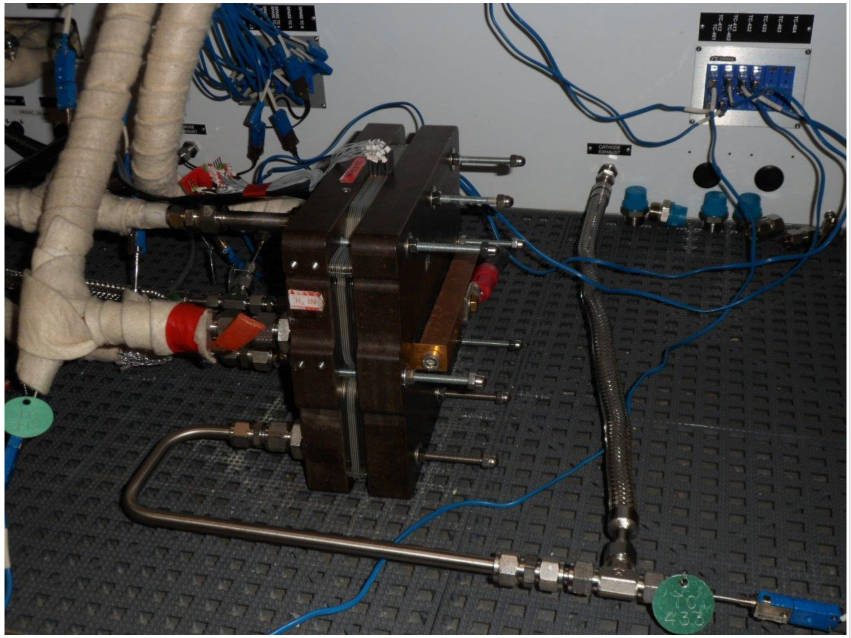
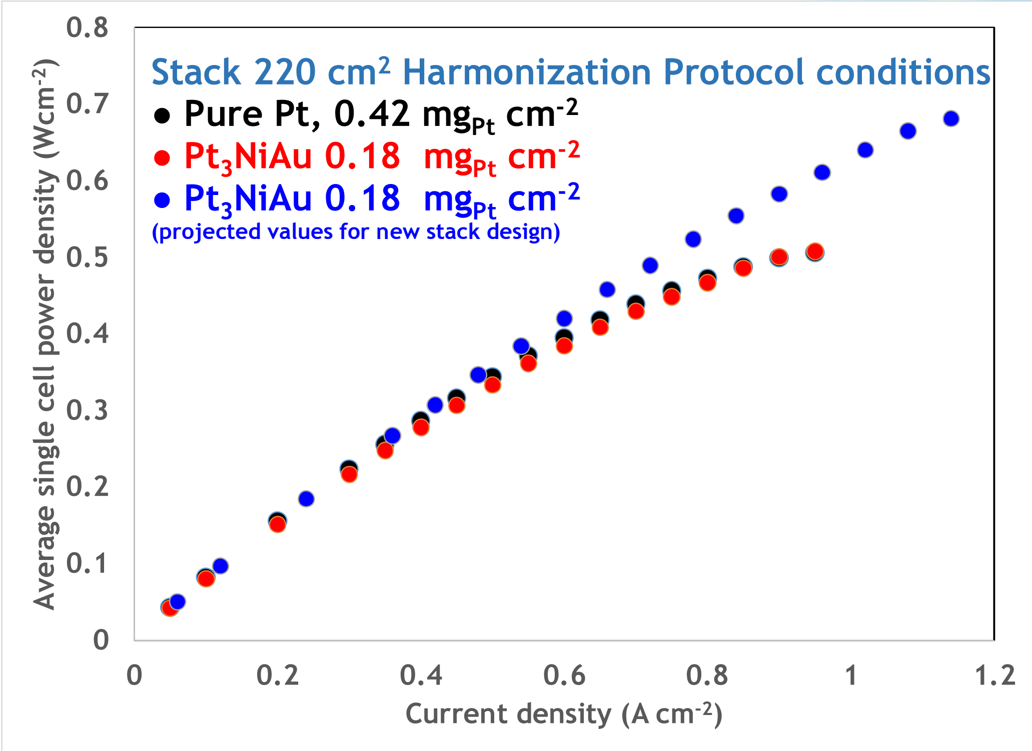
Achievement to-date

% stage of implement.

0.3 V | 25% | 50% | 75% | 0.5 V 1 kW/L | 0.675 V 2 kW/L



1.6 L 10 cell 220 cm^2 active area CEA stack operating using JRC European Harmonized Protocol



Stack degradation issue: ternary catalyst MEAs suffer less degradation. Nevertheless high RH/pressure of EHP conditions seem to induce higher degradation than dryer conditions (to be deepened and confirmed)

PROJECT PROGRESS/ACTIONS
MEA fabrication at pilot scale

Achievement to-date

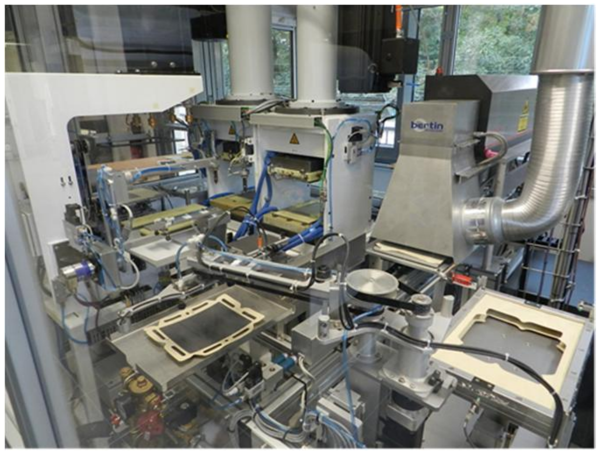
% stage of implement.

0 — 25% — 50% — 75% — 50 — -42 — 60 / -33

Aspect addressed	Parameter (KPI)	Unit	SMART Cat 2016	FCH JU Targets		
				Call topic	2017	2020
Automated MEA fabrication	Fabrication rate	#MEA/day	50	-	-	-
Membrane size reduction	Reduction rate	%	-42	-33%		

Future steps:

- Reaching 60MEA/day
- Reduction of membrane size: -76% vs 2013 to achieve membrane size = electrode size + 5%



Implementation of quality control procedure:

- 60 measurements per MEA
- Optical measurement
- Measurement precision: 20µm
- Process reproducibility: 100 µm
- (based on more than 100 MEA)

SYNERGIES WITH OTHER PROJECTS AND PROGRAMMES

Interactions with projects funded under EU programmes	
CATAPULT	Common meeting EFCD 2015 in Montpellier 2015
NANOCAT	Common meeting in Materials for Fuel Cells, Grenoble 2016
NANOCAT	Discussions with partner Tecnalia for collaboration on PVD
AUTOSTACK-CORE	Durability of stacks: Conditions of AUTOSTACK-CORE are more favorable than SMARTCat EHP. Ternary nanocatalysts improve durability (Pt_3NiAu and Pt_3CuAu)
Interactions with national and international-level projects and initiatives	
EERA JP H2FC	Presentation of new catalyst synthesis methods and DFT simulations at May 2015 Meeting in Copenhagen.

DISSEMINATION ACTIVITIES

Public deliverables

- 2.1 Report and/or scientific paper on the decoupling of strain, ligand and electronic effects in trimetallic core-shell nanoparticles
- D 2.2 Propose optimal trimetallic system, alloys and core shell with highest ORR activity (exchange current density $j_0 > 10^{-3}$ mA cm-2…
- D 3.2 Required amount (≤ 1 g) of catalysed support with improved conductivity > 1 Scm^{-1} …
- D 3.3 Required amount (≥ 1 g) of selected support with high stabilization of the metal particles through the metal-support interaction …
- D 4.4 60 MEAs per days capacity with an automatic and reproducible equipment

Conferences/Workshops

- 1 to be organised by the project

https://efcw2017.sciencesconf.org

- 2 in which the project has participated EFCD2015, Materials for Fuel Cell 2016

Publications: 8

- Styven Lankiang, Morio Chiwata, Stève Baranton, Hiroyuki Uchida, Christophe Coutanceau, Oxygen reduction reaction at binary and ternary nanocatalysts based on Pt, Pd and Au, *Electrochimica Acta* 182 (2015) 131-142

- Effect of Sb Segregation on Conductance and Catalytic Activity at Pt/Sb-Doped SnO 2 Interface: A Synergetic Computational and Experimental Study, Q. Fu , L. C. Colmenares Rausseo , U. Martinez , P. Inge Dahl , J. M. G. Lastra , P. E. Vullum , I.-H. Svenum , T. Vegge, *ACS Applied Materials and Interfaces* 7 (2015) 27782-27795

Thank You!

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