



# ADVANCING FUEL CELLS FOR OPERATION ON NATURAL GAS

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Research Centre  
for Gas Innovation

cleaner energy for a sustainable future

V Workshop of the RCGI  
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# Thanks to our Sponsors & Research Team

- Shell



- FAPESP



**Fabio Coral Fonseca (PI) - SOFC**

- Francisco Tabuti
- *Ivan Kourskischko - post-doc Fapesp*
- *Marina F Machado*
- *Leticia P Reis Moraes*

**Estevam V. Spinacé – PEM electrocatalysts**

**Almir O. Neto – PEM electrocatalysts**

- Vanderlei S. Bergamaschi
- Júlio Nandenha
- *Julio Cesar Martins da Silva – post-doc*

**Thiago Lopes (FAPESP Young Investigator) – low and mid temperature electrochemical systems**

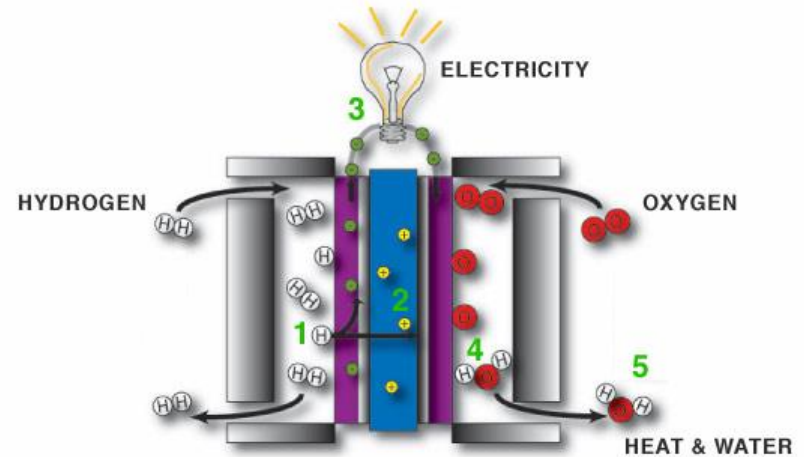
- *Otávio Beruski – post-doc FUSP*

**Elisabete I. Santiago – PEM membranes / MEA's**

- Edgar Ferrari Cunha
- *Bruno R. Matos – post-doc*
- *Roberta Isidoro – post-doc (CNPq)*

# Fuel Cell - Background

Fuel cells are the most efficient devices for the direct conversion of chemical energy of fuels into electricity.

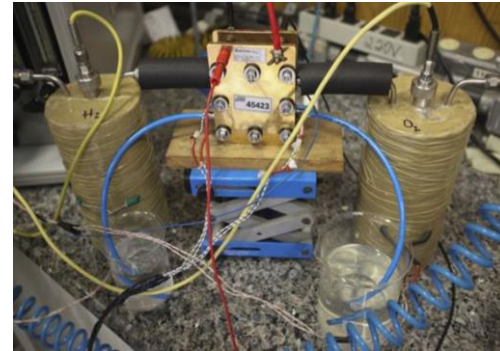


PEMFC	$\text{H}_2 \rightarrow 2\text{H}^+ + 2\text{e}^-$	$\text{H}^+ \rightarrow$	$2\text{H}^+ + \frac{1}{2} \text{O}_2 + 2\text{e}^- \rightarrow \text{H}_2\text{O}$
SOFC	$2\text{O}^{2-} + 2 \text{H}_2 \rightarrow 2\text{H}_2\text{O} + 4\text{e}^-$	$\leftarrow 2\text{O}^{2-}$	$\text{O}_2 + 4\text{e}^- \rightarrow 2\text{O}^{2-}$

# Project 12 – Goals

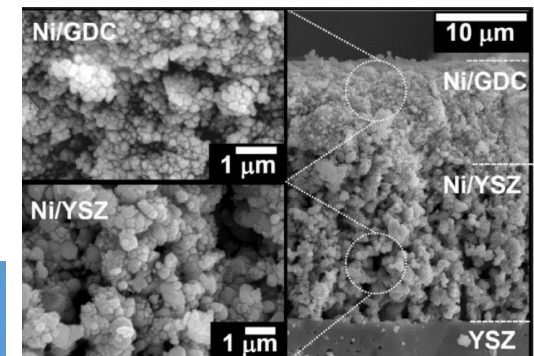
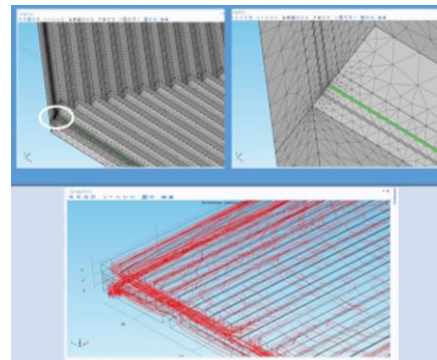
## i) PEMFCs

- more efficient anodes for direct methane and for H<sub>2</sub>-rich gas mixtures;
- membranes for high operating temperatures.



## ii) SOFCs

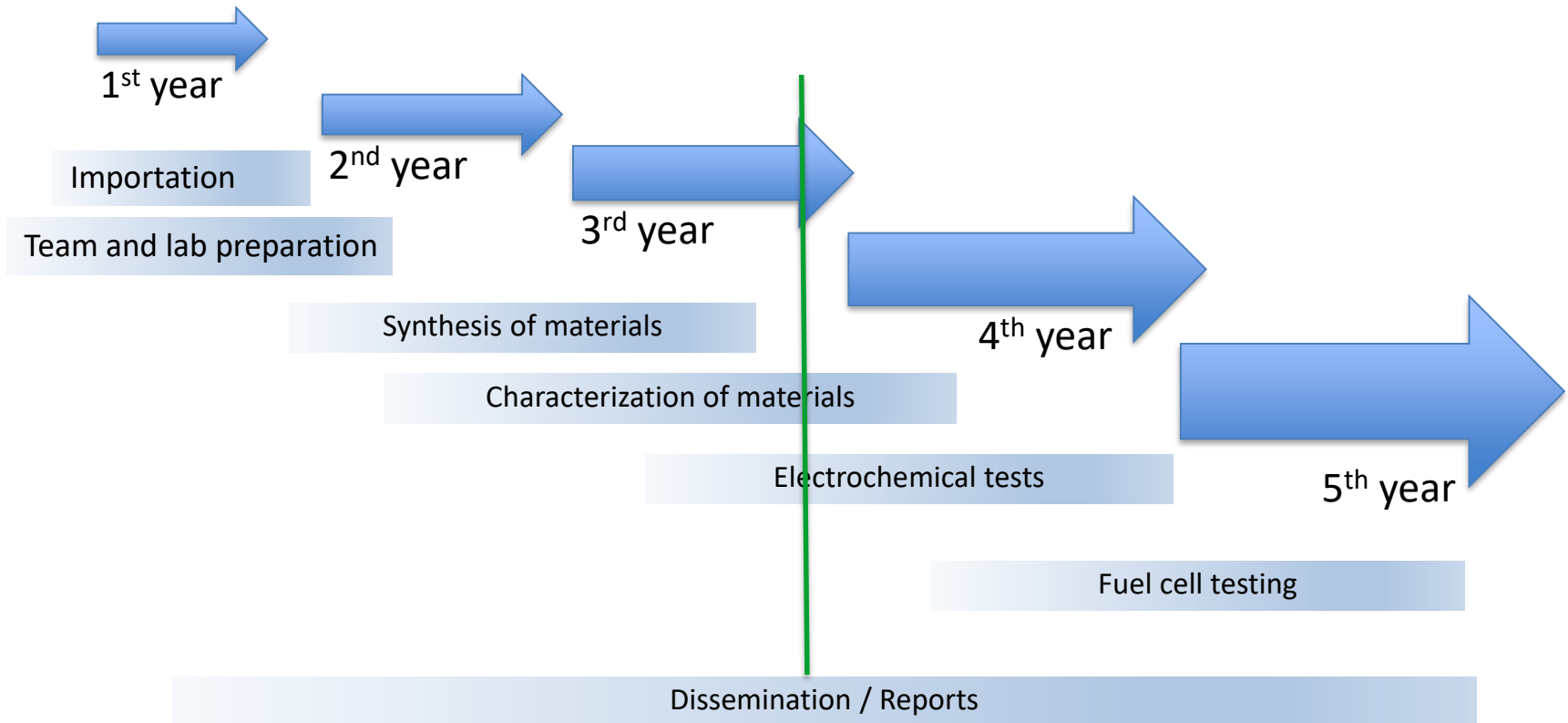
- anodes resistant to carbon deposition (coking) for direct natural gas SOFCs.



## iii) Numerical simulations

- flow field optimization.

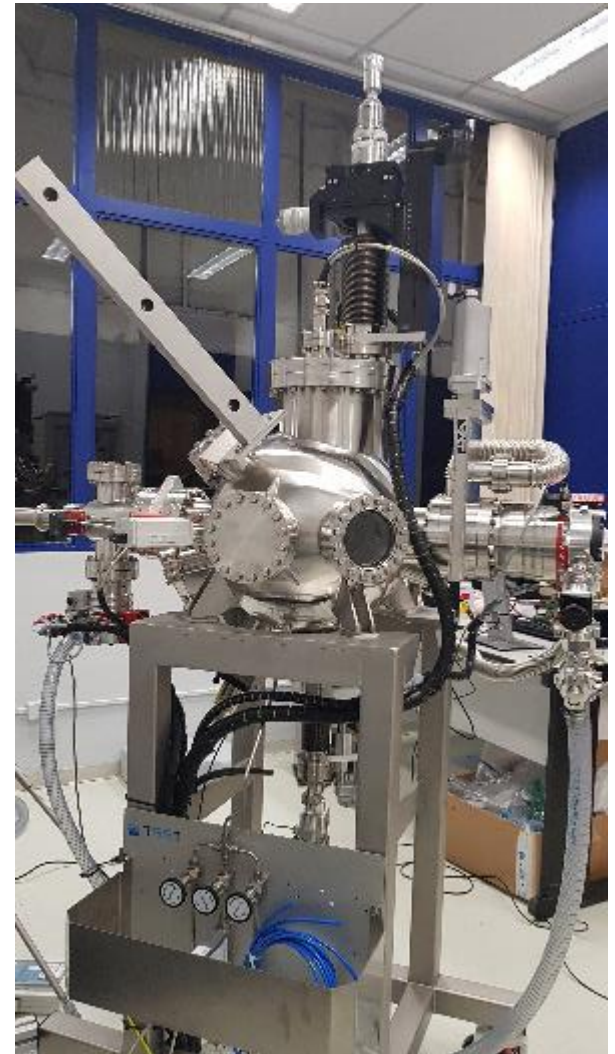
# Project 12 – Timeline and Deliverables



# Fuel Cells @ IPEN/RCGI

- **Recent Achievements**

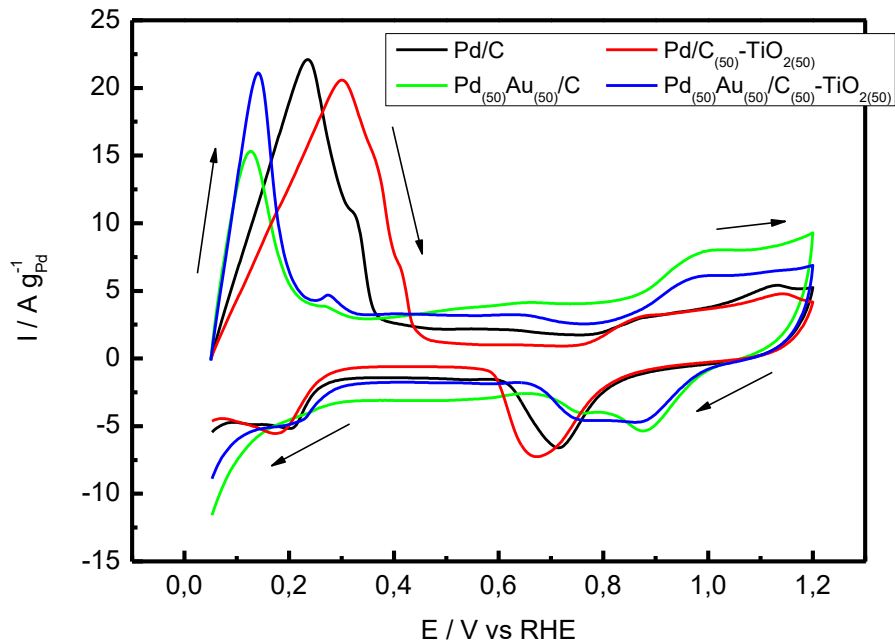
- Post-doc hiring
  - Candidate selected
  - Still awaiting for Fapesp approval
- Pulsed Laser Deposition
  - 1<sup>st</sup> year equipment – finally installed
  - Great help from RCGI and Shell
    - Lab preparation (gas line and electrical installation)
  - Thank you very much Camila and Luis
- Still missing the importation of one (very important) equipment WDS (wavelength-dispersive X-ray spectrometer)



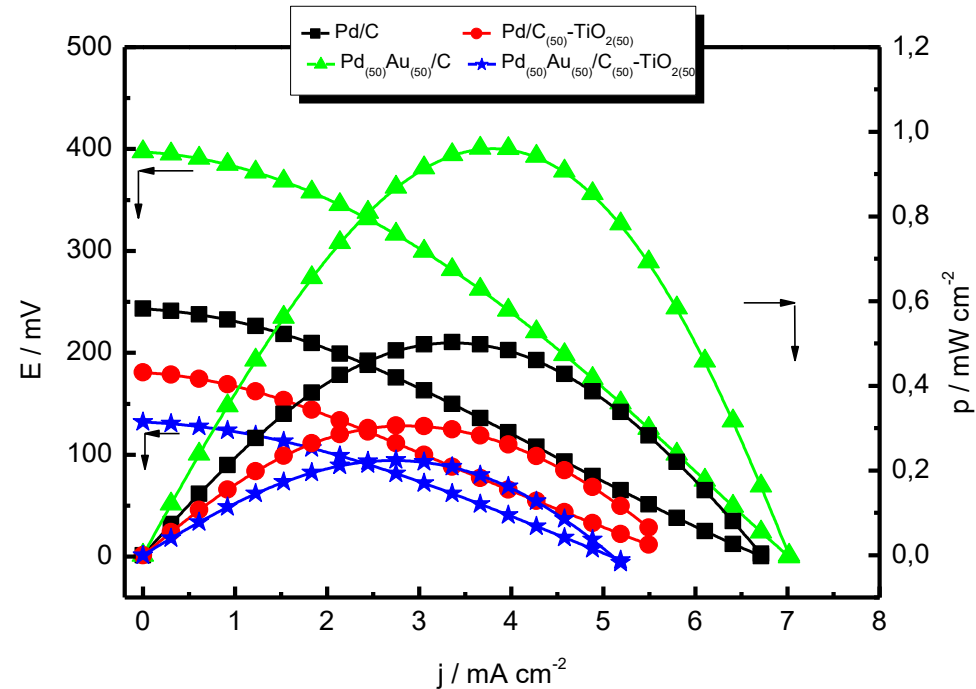
# Project 12 – Challenges in Oxidizing CH<sub>4</sub> @ Low Temperature Fuel Cells

## Fundamental Electrochemistry

Adsorption properties of CH<sub>4</sub> on ≠ electrocatalysts

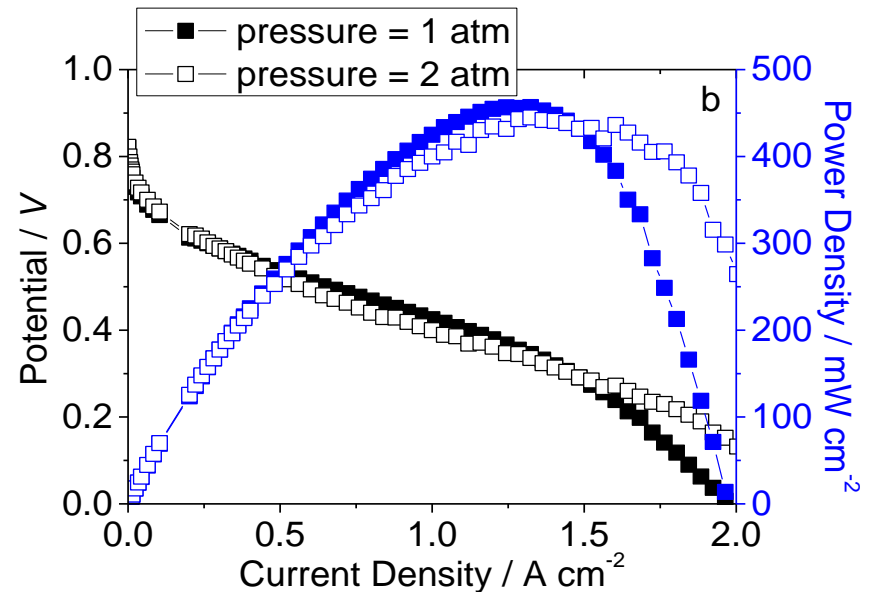
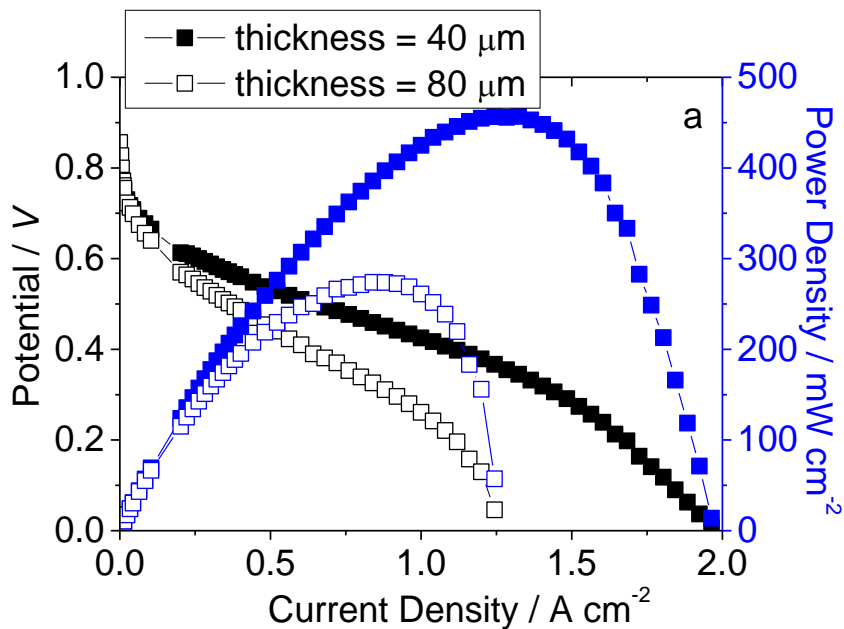


## @ a single PEM Fuel Cell



# Project 12 – PEM for High Operating T (> 180 °C)

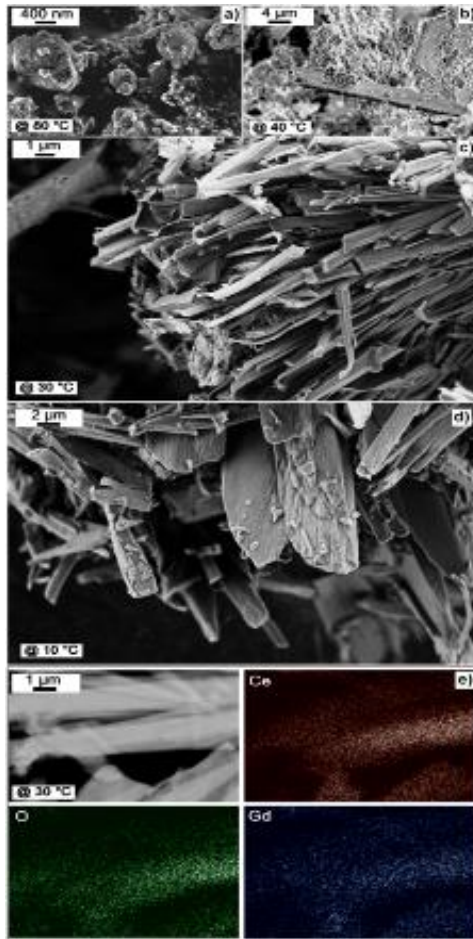
Polibenzimidazole (PBI) Membranes @ a single PEM fuel cell @ 180 °C



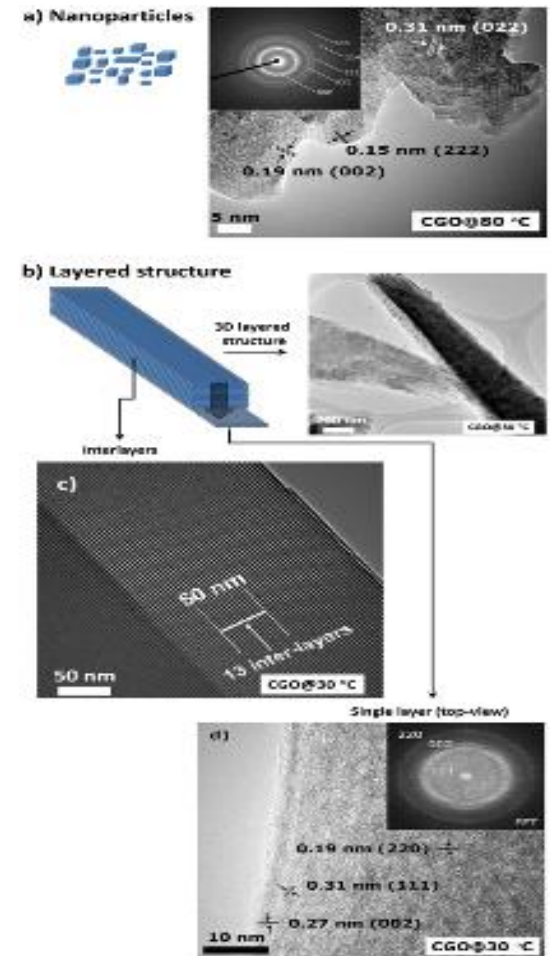


# Project 12 – Novel Materials for Direct Natural Gas SOFCs

Morphology optimization towards novel anode materials resistant to carbon deposition.

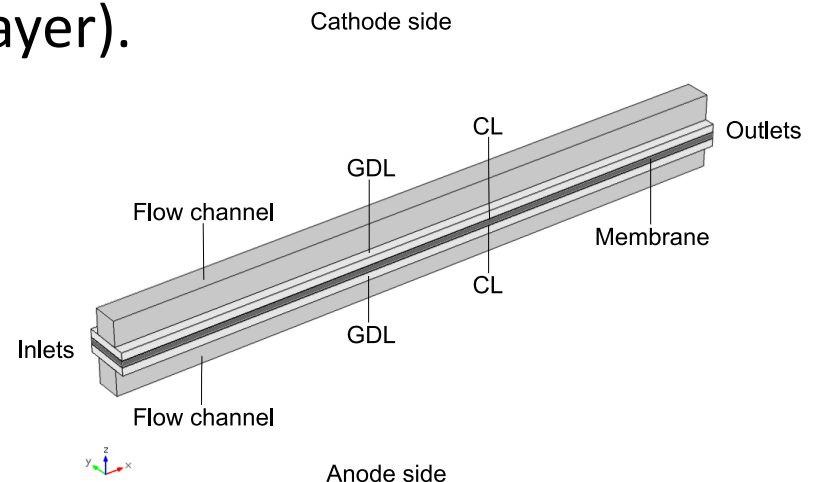
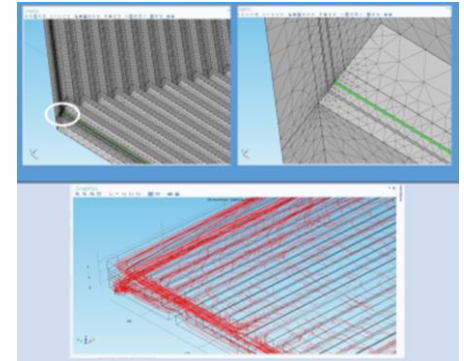


High resolution TEM images and elemental mapping of novel 2D gadolinium-doped ceria materials

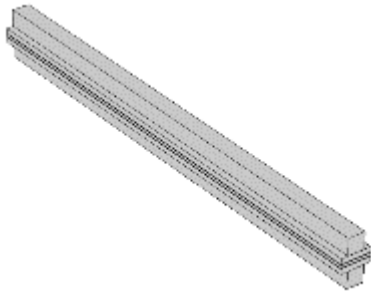


# Project 12 – Numerical Simulation and Optimization

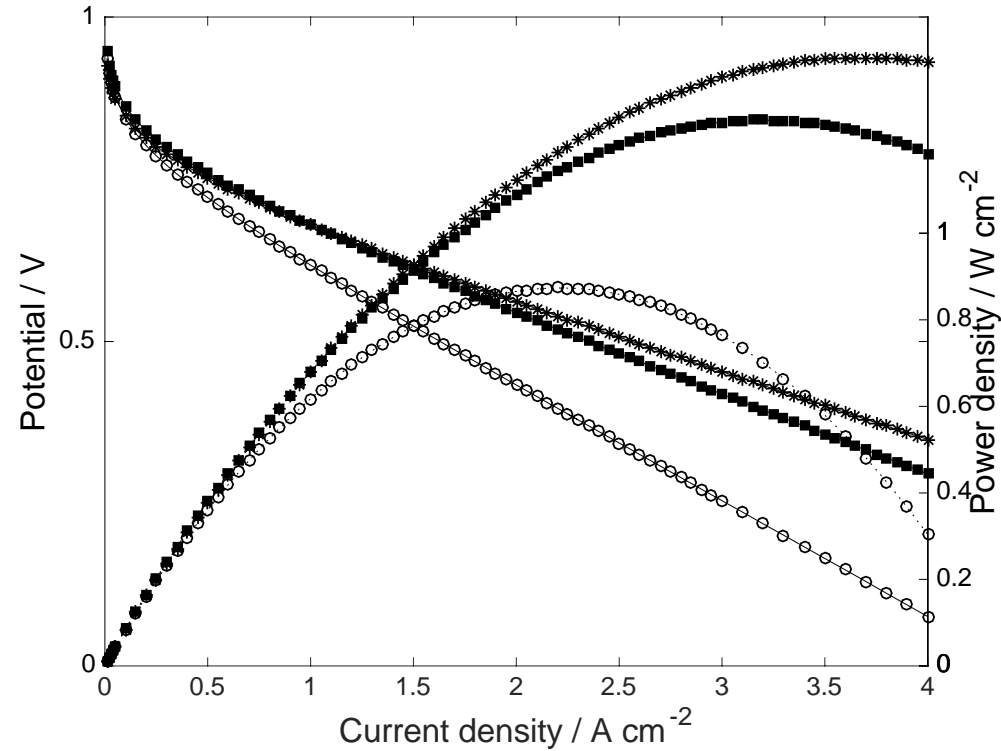
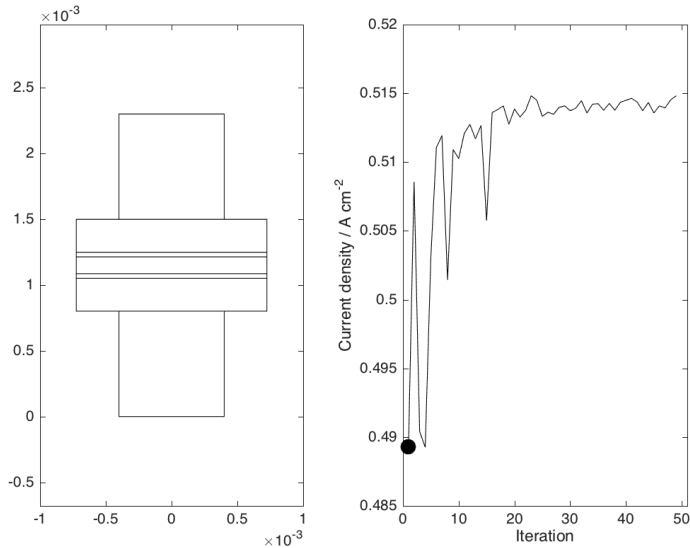
- Partnership between projects 8 and 12;
- Finite element method;
- Computational fluid dynamics;
- COMSOL Multiphysics;
- Shape optimization of the cathode cross section (flow channel and catalyst layer).



# Results: Single channel

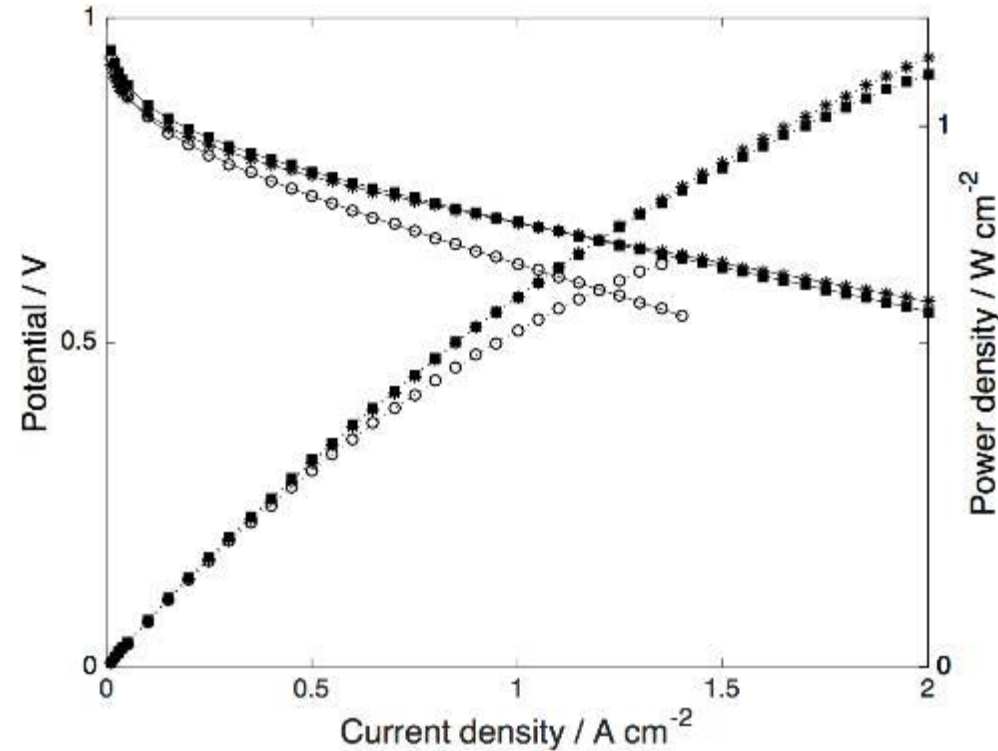
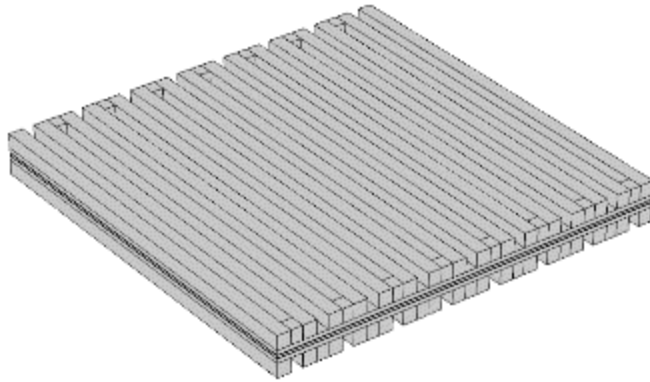


Shape optimization of PEMFC flow channel cross section



- Rectangular channel
- Optimized channel
- \* Optimized channel and CL

# Results: Single-channel serpentine



- Rectangular channel
- Optimized channel
- \* Optimized channel and CL

# Project 12 – Upcoming activities here

*Advancing fuel cells for operation on natural gas*

- ✓ Equipment importation not concluded: WDXRF (still awaiting at FAPESP);
- ✓ Integration of high-temperature membranes with optimized electrocatalysts for PEMFC running with methane
- ✓ Advancing the integration fuel cell and simulation groups (papers : *FUEL CELLS*, v. 17, p. 27, 2017; *PHYSICAL REVIEW FLUIDS*, v. 2, n. 103501, 2017 + another *under final revision for submission*);

# Project 12 – Publications (2018 up to August)

*Advancing fuel cells for operation on natural gas*

1. SILVA, P. S. M.; ESPOSITO, V.; MARANI, D.; DE FLORIO, D. Z.; MACHADO, I. F.; **FONSECA, F. C.** Thermochemical stability of zirconia-titanium nitride as mixed ionic-electronic composites. **CERAMICS INTERNATIONAL**, v. 44, n. 7, p. 8440-8446, MAY 2018.;
2. DA SILVA, ANDERSON G. M.; BATALHA, DANIEL C.; RODRIGUES, THENNER S.; CANDIDO, EDUARDO G.; LUZ, SULUSMON C.; DE FREITAS, ISABEL C.; **FONSECA, FABIO C.**; DE OLIVEIRA, DANIELA C.; TAYLOR, JASON G.; CORDOBA DE TORRESI, SUSANA I.; CAMARGO, PEDRO H. C.; FAJARDO, HUMBERTO V. Sub-15 nm CeO<sub>2</sub> nanowires as an efficient non-noble metal catalyst in the room-temperature oxidation of aniline. **CATALYSIS SCIENCE & TECHNOLOGY**, v. 8, n. 7, p. 1828-1839, APR 7 2018.
3. MARANI, DEBORA; REIS MORAES, LETICIA PORAS; GUALANDRIS, FABRIZIO; SANNA, SIMONE; DE FLORIO, DANIEL ZANETTI; ESPOSITO, VINCENZO; **FONSECA, FABIO CORAL.** Nucleation front instability in two-dimensional (2D) nanosheet gadolinium-doped cerium oxide (CGO) formation. **CrystEngComm**, v. 20, n. 10, p. 1405-1410, MAR 14 2018.
4. SANTOS, THAMYSCIRA H.; GRILO, JOAO P. F.; LOUREIRO, FRANCISCO J. A.; FAGG, DUNCAN P.; **FONSECA, FABIO C.**; MACEDO, DANIEL A. Structure, densification and electrical properties of Gd<sup>3+</sup> and Cu<sup>2+</sup> co-doped ceria solid electrolytes for SOFC applications: Effects of Gd<sub>2</sub>O<sub>3</sub> content. **CERAMICS INTERNATIONAL**, v. 44, n. 3, p. 2745-2751, FEB 15 2018.
5. DO REGO, ULISSES ALVES; **LOPES, THIAGO**; BOTT-NETO, JOSE LUIZ; TANAKA, AURO ATSUSHI; TICIANELLI, EDSON ANTONIO. Oxygen reduction electrocatalysis on transition metal-nitrogen modified tungsten carbide nanomaterials. **JOURNAL OF ELECTROANALYTICAL CHEMISTRY**, v. 810, p. 222-231, FEB 1 2018.

# Conclusions

*Advancing fuel cells for operation on natural gas*

- Equipment purchasing and team hiring are “permanent” activities;
- Project 12 follows the planned S-curve;
- Results are converted into publications supported by RCGI;
- RCGI staff support is essential and only gets better (Luis Moreira, Lyu, Victor, Gabriel, Claudenor, Romi, Julio, Karen...);
- We have an increasing need of additional PhD and MSc students to tackle RCGI challenges.



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