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# Nanoscale Architectural Engineering for High-Performance Solid Oxide Fuel Cells

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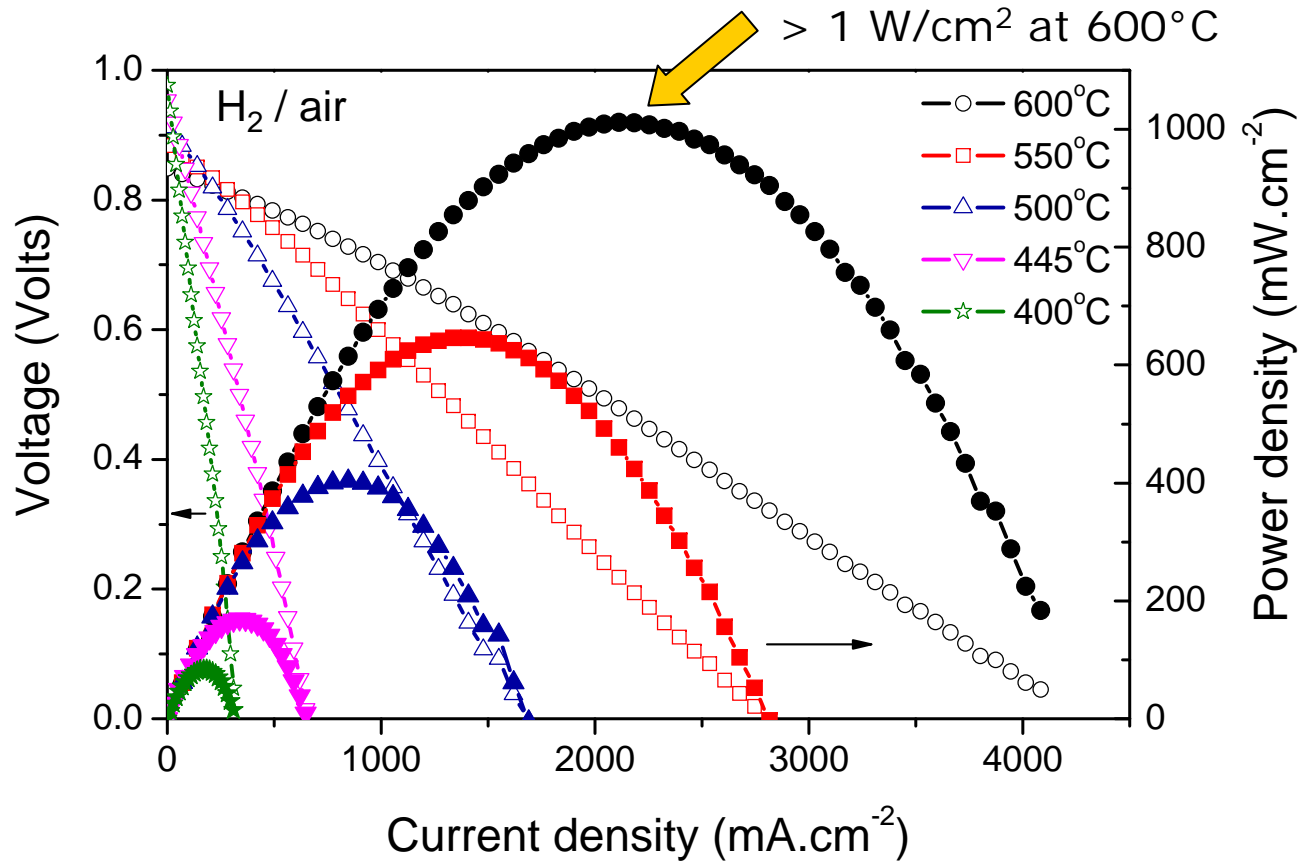
# Vision and Objectives

- Fuels cells are the most efficient, clean way to convert from chemical to electrical energy
- Solid oxide fuel cells offer fuel flexibility
- Potential near-term CO<sub>2</sub> emissions reduction (due to high efficiency)
  - No need to wait for hydrogen
- Barrier is cost
  - What matters is not *absolute* cost
  - It is cost/power (at 'reduced' temperatures)
- Dramatic improvements in performance
  - Imply lower cost/power and acceptance

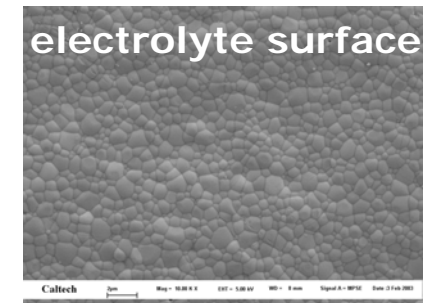
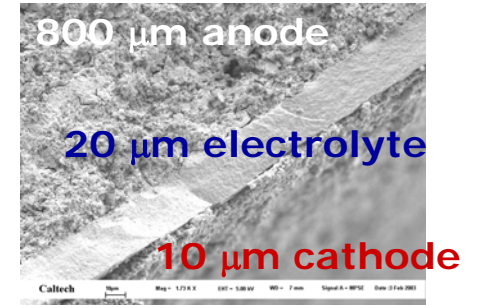


# State-of-the-art SOFCs

Conventional powder processing



Ni-SDC | SDC | BSCF



High power density reproduced in other labs

SDC = samaria doped ceria

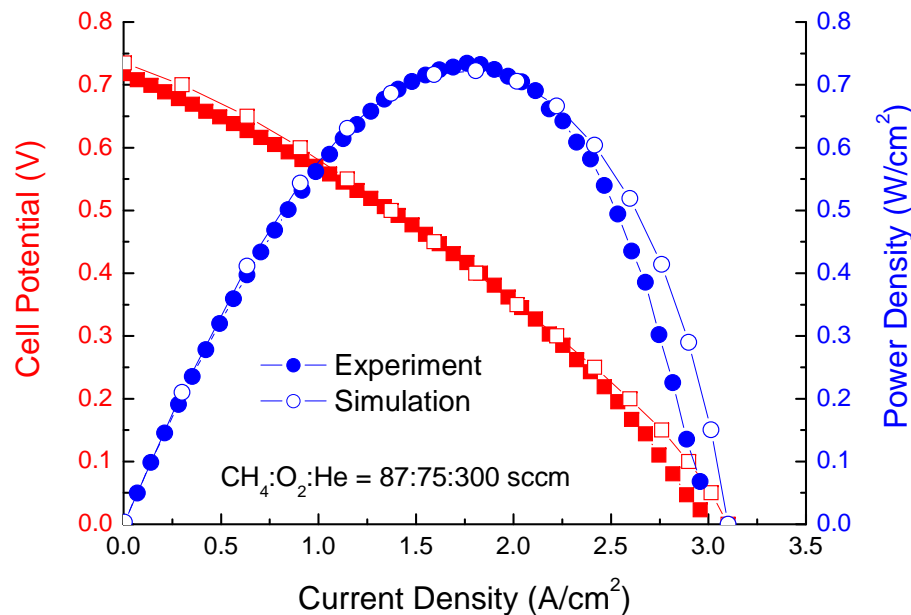
BSCF = Ba<sub>0.5</sub>Sr<sub>0.5</sub>Co<sub>0.8</sub>Fe<sub>0.2</sub>O<sub>3-δ</sub>

Z. Shao and S. M. Haile, *Nature* **431**, 170-173 (2004).



# Computational Modeling

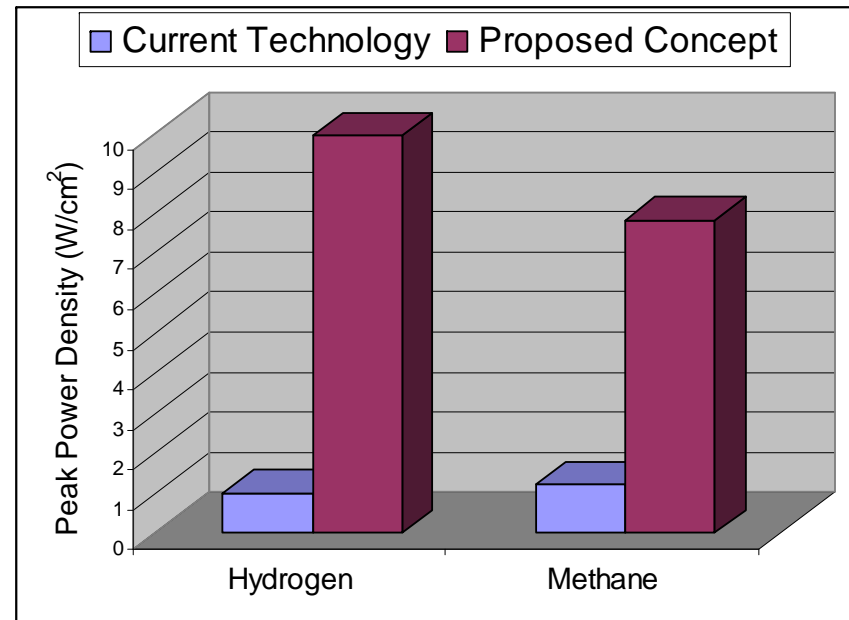
## Model validation



- Parameters obtained independently
- Model predicts experimental results

## Model predictions

- architectural design
- 10x increase in power



Based on fundamentals



Y. Hao, Z. Shao, J. Mederos, W. Lai, D. G. Goodwin and S. M. Haile, *Solid State Ionics* **177**, 2013-2021 (2006).

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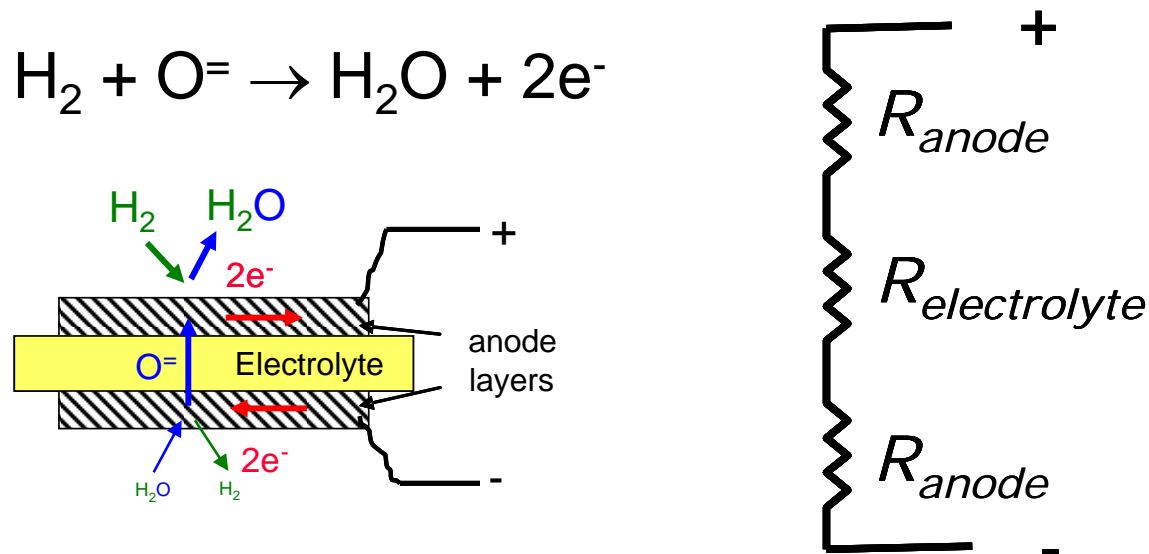
# Hypotheses

- Fuel electro-oxidation occurs on ceria surface, not limited to triple points
- Of the electrodes, anode is rate limiting
  - Cathode is fastest component
- Cathode is surface area limited
  - Bulk diffusion is rapid
- Electrolyte is grain boundary limited
- Prove hypotheses:
  - Lasting science & technological advances



# Hydrogen electro-oxidation

- Impedance measurement

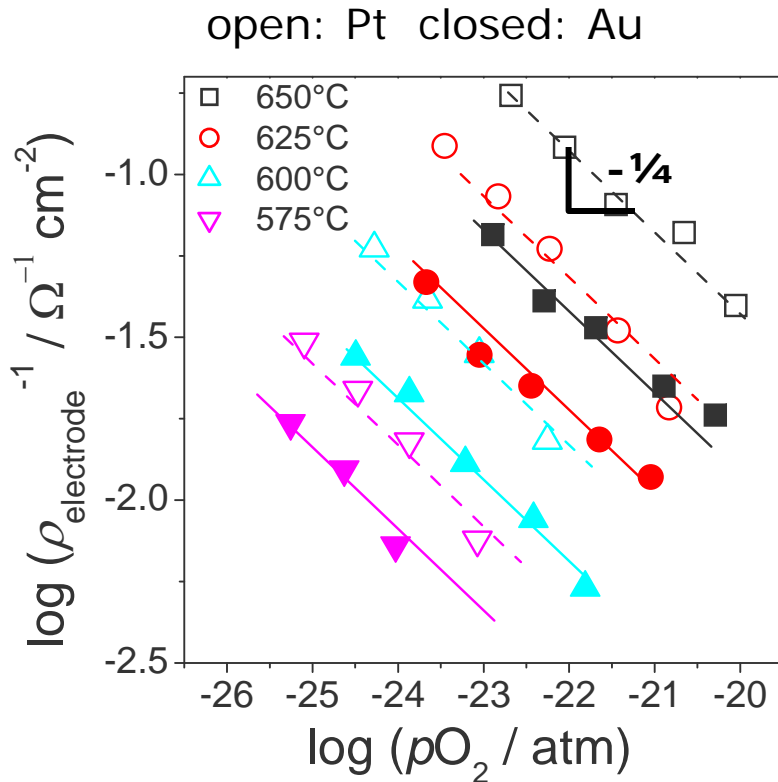


- Measurement also yields

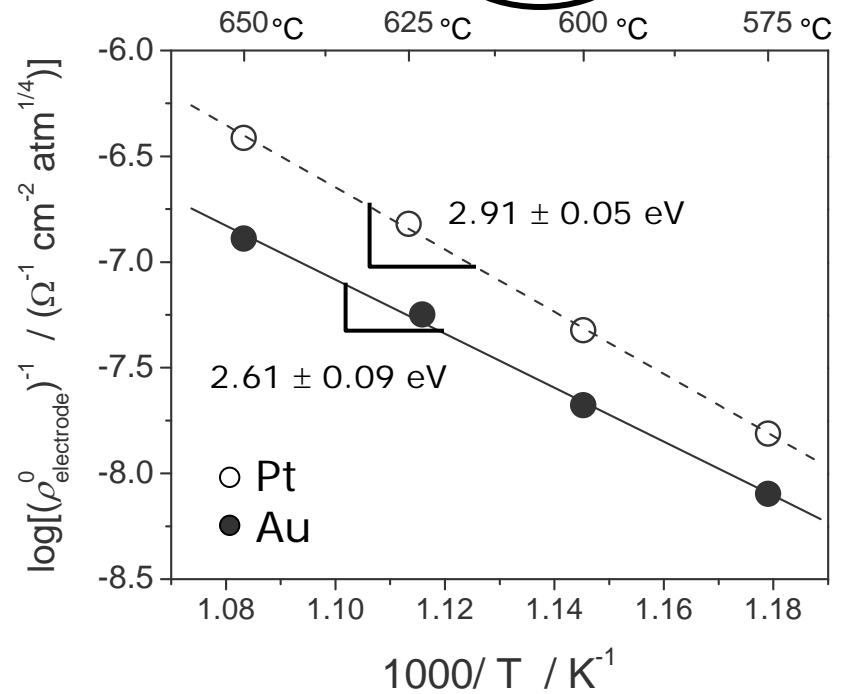
- ionic conductivity, electronic conductivity, electronic charge carrier concentration



# Hydrogen electro-oxidation



fit to  $1/\rho_{\text{electrode}} = 1/\rho_{\text{electrode}}^0 \cdot P_{\text{O}_2}^{-1/4}$



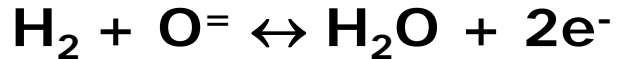
very different metals, similar behavior

matches electronic conductivity

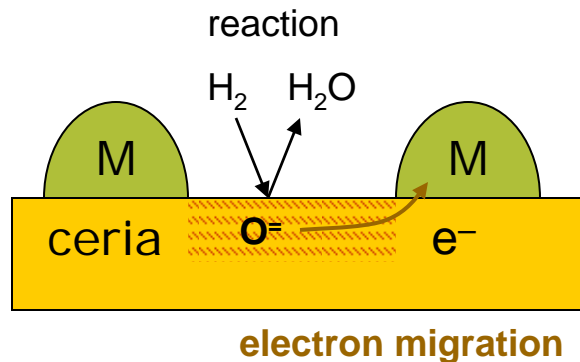
	$\sigma_{\text{electronic}}^0$
Pt SDC15 Pt	2.41 ± 0.01 eV
Au SDC15 Au	2.76 ± 0.05 eV



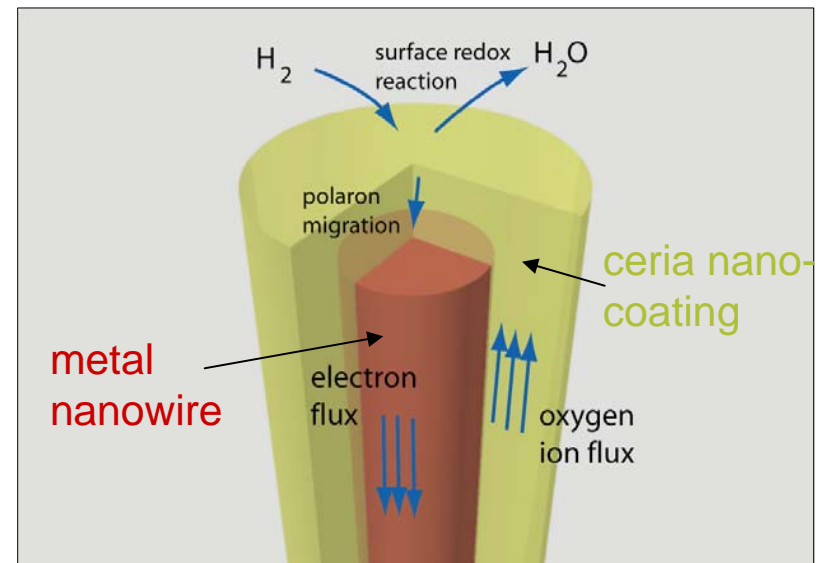
# Hydrogen electro-oxidation



- Independent of metal
- Activation energy matches  $\sigma_{\text{electronic}}$
- Reaction on ceria
- Rate-limiting step:



## Target architecture

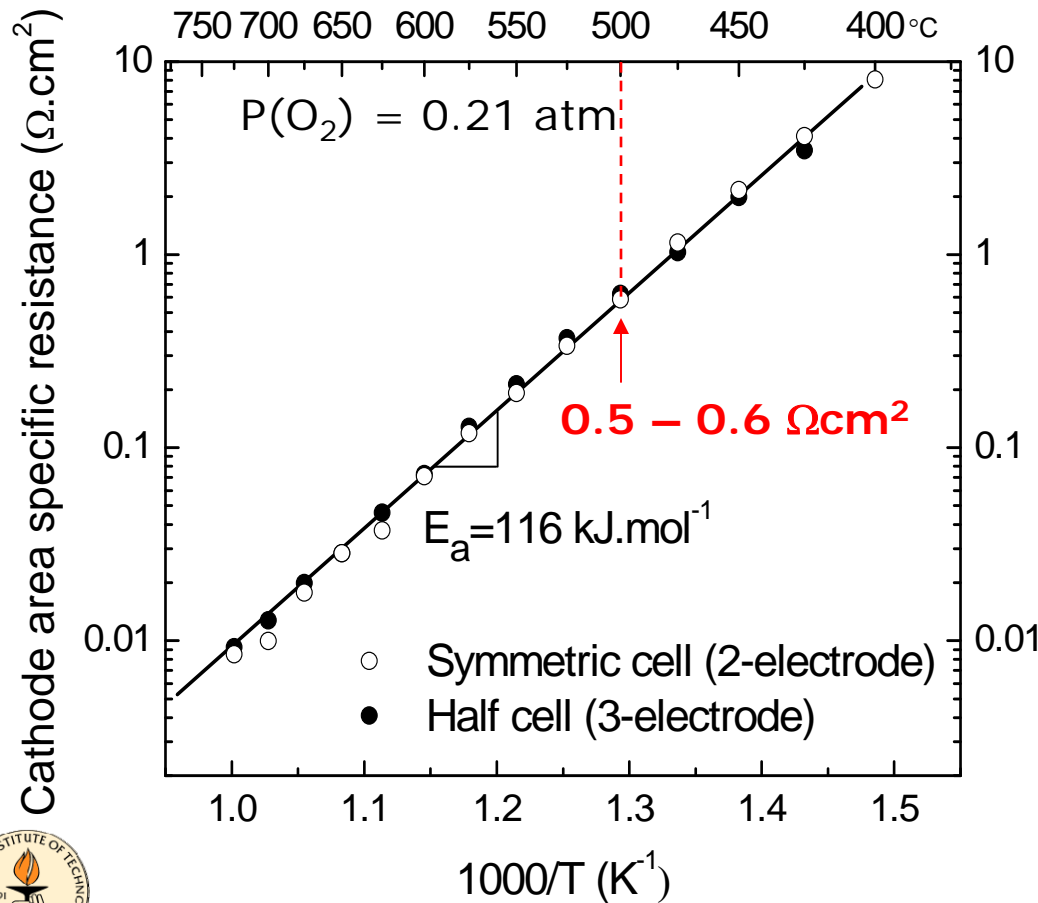
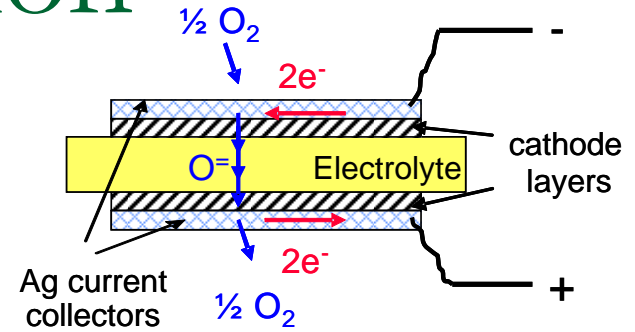
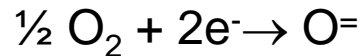


- "Triple points" not required
- Flexibility in choice of metal
- Oxide coating stabilizes structure
- Ceria is non-coking



# Oxygen electro-reduction

## ■ Impedance measurement



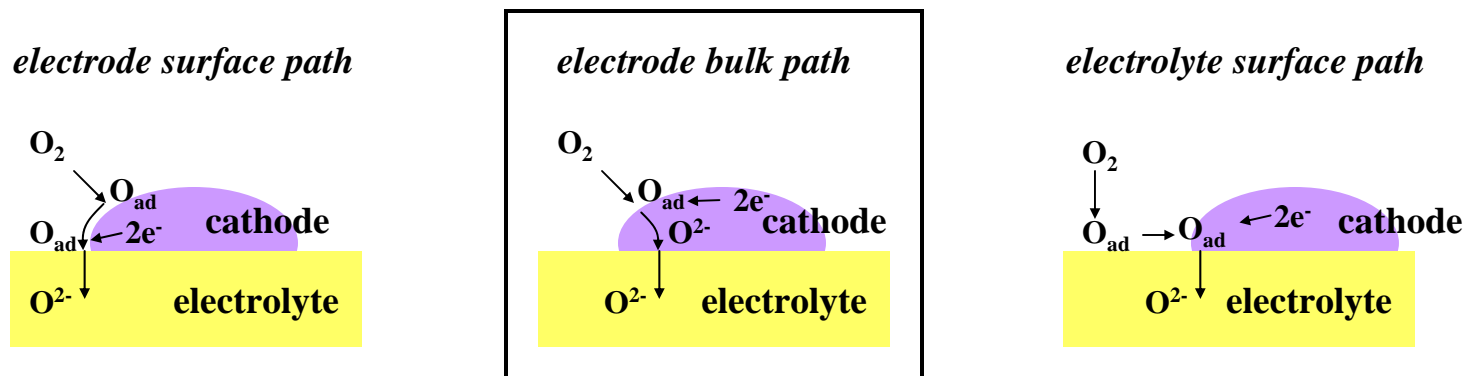
- Activation energy matches that for oxygen surface exchange ( $113 \text{ kJ} \cdot \text{mol}^{-1}$ )
- Exchange rate measured indep'ly by  $\text{O}_2$  permeation
- Bulk diffusion is fast ( $46 \text{ kJ} \cdot \text{mol}^{-1}$ )
- Other 'advanced' cathodes
  - $(\text{PrSm})\text{CoO}_3$ :  $5.5 \Omega \cdot \text{cm}^2$
  - $(\text{LaSr})(\text{CoFe})\text{O}_3$ :  $48 \Omega \cdot \text{cm}^2$

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# Oxygen electro-reduction

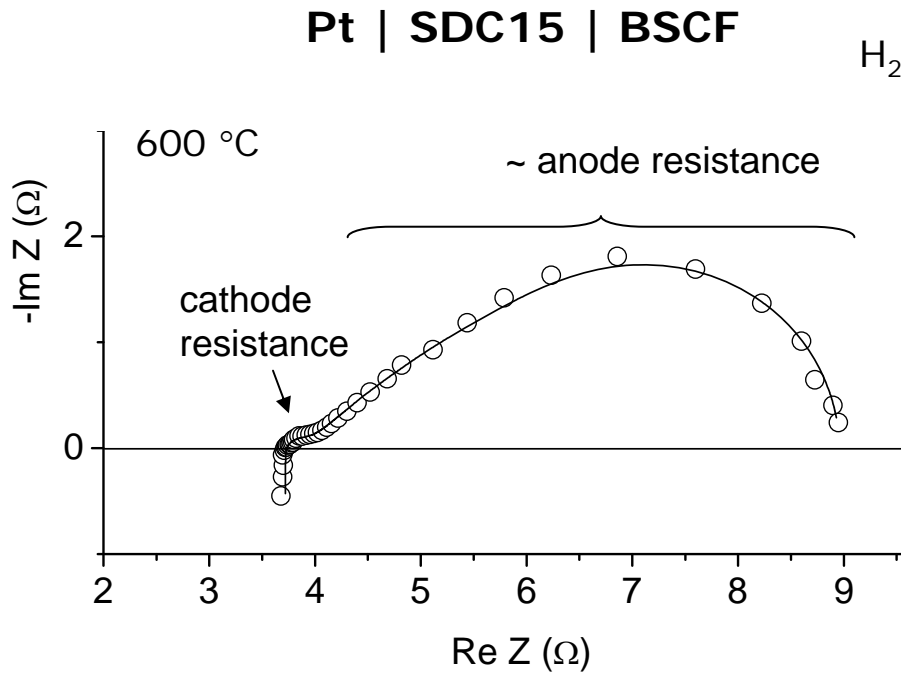
- Reaction pathways



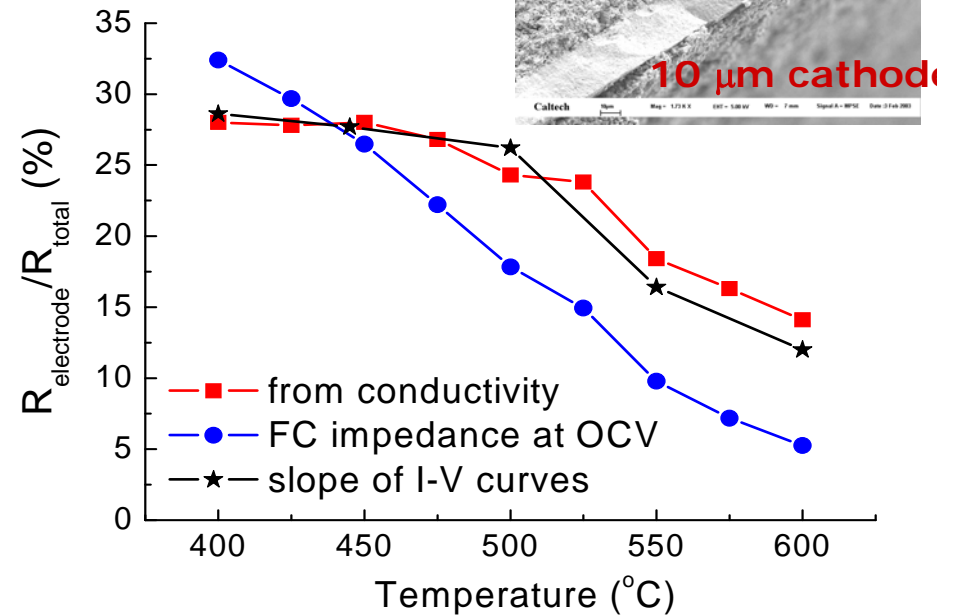
- $(Ba_{0.5}Sr_{0.5})(Co_{0.8}Fe_{0.2})O_{3-\delta}$ 
  - Exceptionally high oxygen vacancy diffusivity
  - Exceptionally high vacancy concentration ( $\delta \sim 0.4$ )
  - No indication of vacancy ordering/clustering
  - Surface related step is rate-limiting ← maximize surface area



# Performance limiters



Ni-SDC | SDC | BSCF



- Depending on the cell (electrode fabrication)
  - Anode can dominate: slow electro-oxidation reactions
  - Electrolyte can dominate: resistive grain boundaries
  - Cathode is always negligible



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# Target fuel cell architecture

- Anode

- High surface-area, porous metal *coated with doped ceria*
- Overall thickness?

- Electrolyte

- 10  $\mu\text{m}$ ; clean or parallel grain boundaries

- Cathode

- High surface-area, porous BSCF
- Overall thickness?

