BERKELEY LAB
LAWRENCE BERKELEY NATIONAL LABORATORY

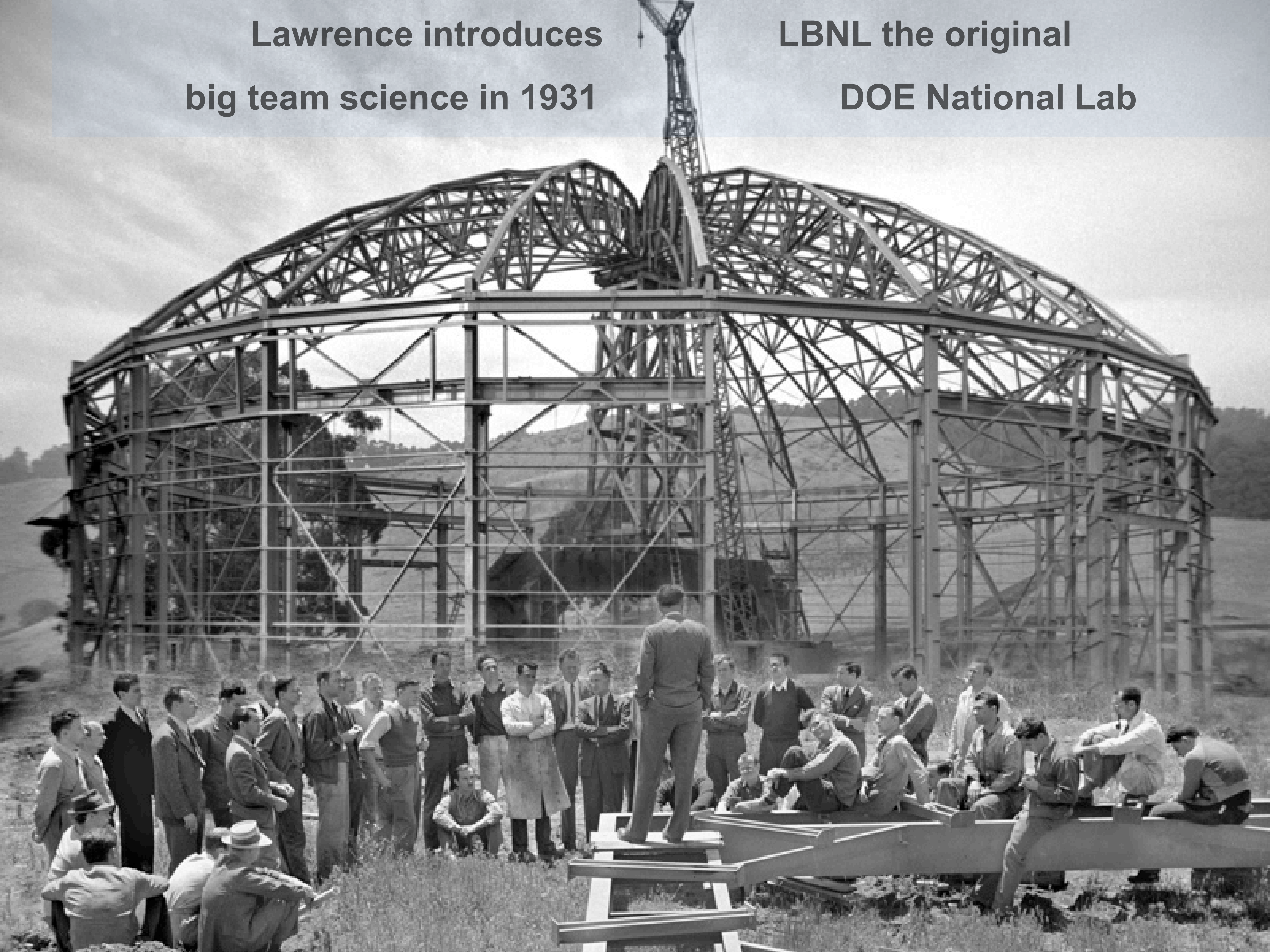
U.S. DEPARTMENT OF ENERGY

LBNL Fuel-Cell and Hydrogen Activities (FCTO) Overview

Ravi Prasher

Division Director
Energy Storage and Distributed Resources

HTAC meeting | April 7, 2016


Lawrence introduces
big team science in 1931
LBNL the original
DOE National Lab

Berkeley Lab Science Focus Areas

BIOSCIENCES

BASIC ENERGY SCIENCES

ENERGY TECHNOLOGIES

PHYSICAL SCIENCES

COMPUTING SCIENCES

- Mission: Perform analysis, research, and development leading to better energy technologies and reduction of adverse energy-related environmental impacts

- Budget: ~ $120 M

- No. of Staff: ~ 500

The long-term vision is "**lab-to-market-to-impact**"

Energy Technologies Area Organization

LIGTT (LBL Institute for Globally Transformative Technologies)
A. Gadgil

ETA
R. Ramesh
Associate Lab Director

Cyclotron Road
I. Gur

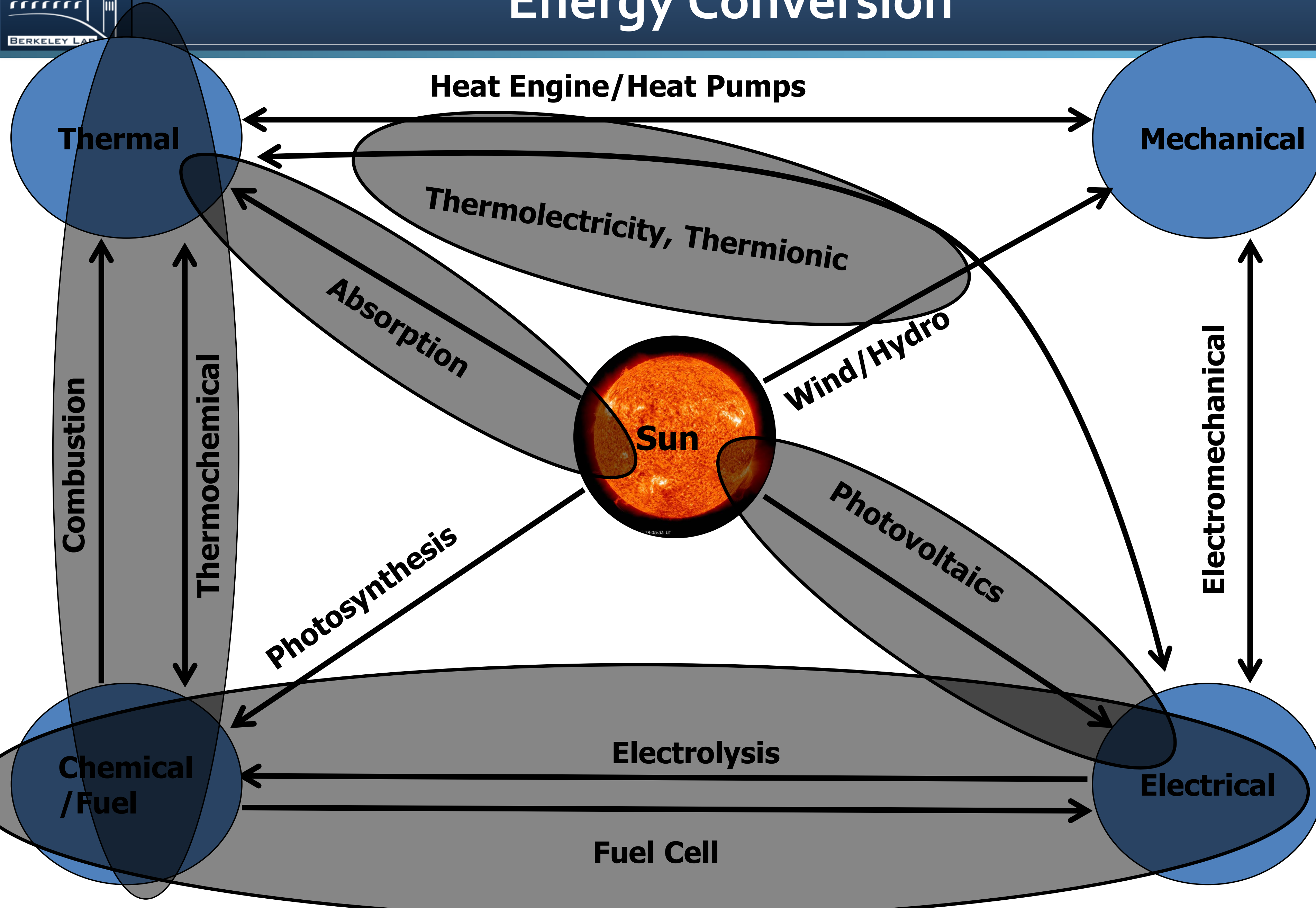
Buildings Technology & Urban Systems (BTUS)
M.A. Piette
Division Director

Energy Storage & Distributed Resources (ESDR)
R.S. Prasher
Division Director

Energy Analysis & Environmental Impacts (EAEI)
C. Goldman
Division Director

August 2015

Energy Conversion



Fuel-Cell-Technologies-Program Core Competences

- **Physics-based multiscale modeling with electrochemistry**
  - ↳ Advanced diagnostics and materials characterization
- **Manufacturing: analysis and detection of defects**
- **Energy analysis: total cost of ownership**
- **Hydrogen storage material development**
- **Photoelectrochemical generation of hydrogen: JCAP**

LBNL Hydrogen Activities

- **Fuel-Cell Subprogram**
  - 3 as prime organization
    - Fuel-cell performance and durability (FC-PAD) (diagnostics and modeling)
    - PECASE: Multiscale modeling of fuel-cell membranes (modeling)
    - Stationary fuel-cell cost and life-cycle analysis (analysis)
    - Integrated systems modeling of the interactions between stationary hydrogen, vehicle, and grid resources (analysis)
  - 3 as subcontractor
    - Alkaline-exchange membranes; SNL, NREL, CSM (diagnostics and modeling)
    - Manufacturing; NREL (modeling)
    - Tailored Low-PGM Catalysts; ANL (materials)
- **Hydrogen storage**
  - 2 as subcontractor
    - HyMARC (Hydrogen Materials - Advance Research Consortium); SNL, LLNL (materials and modeling)
    - Hydrogen Storage Characterization and Optimization Research Effort; NREL, PNNL (materials and diagnostics)
- **Hydrogen Production**
  - 1 as prime
    - PEC hydrogen generation; Stanford (analysis and materials)
  - 1 as subcontractor
    - Fermentation and Electrohydrogenic Approaches to Hydrogen Production; NREL, SNL, PSU (materials and diagnostics)
- **FCTO tech to market (T2M activities)**
- **Joint Center for Artificial Photosynthesis (JCAP)**
  - Carryover funds for H_2 production
- **H_2 based flow cells**
- **Metal supported SOFC**

Collaborators over past couple of years

Industry

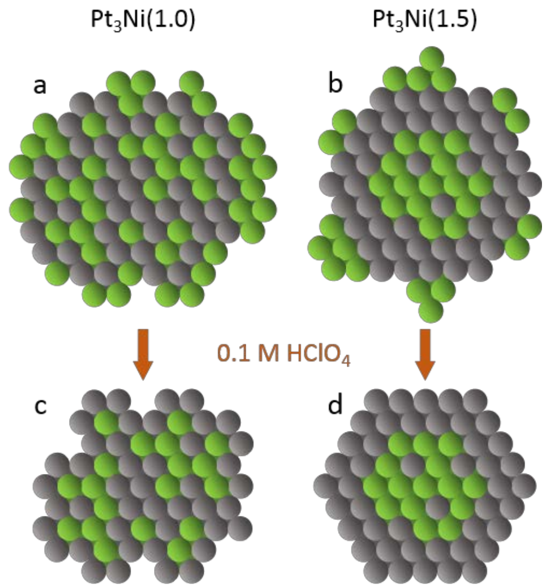
Academia

Labs

Fuel Cells R&D

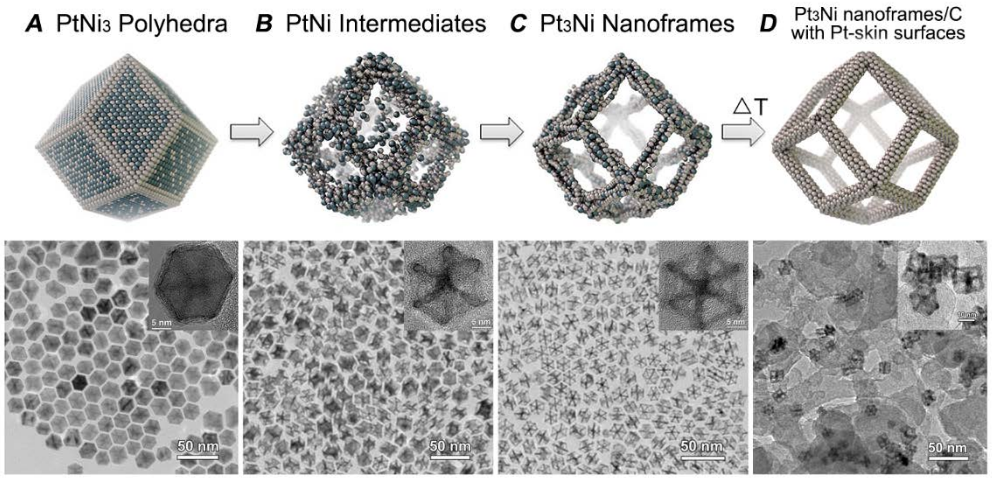
New Catalysts

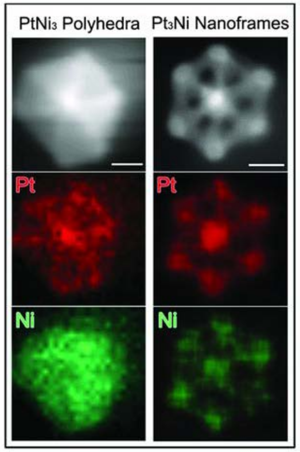
Models of nanoframe edges



Ni: Green
Pt: Gray

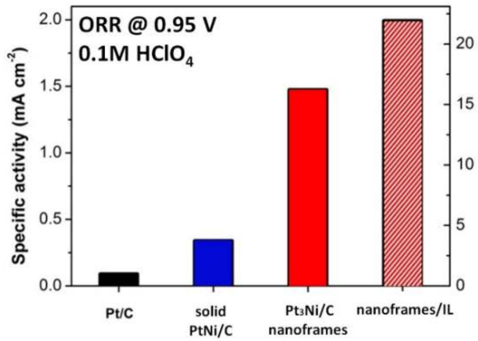
Evolution process from solid to hollow frame

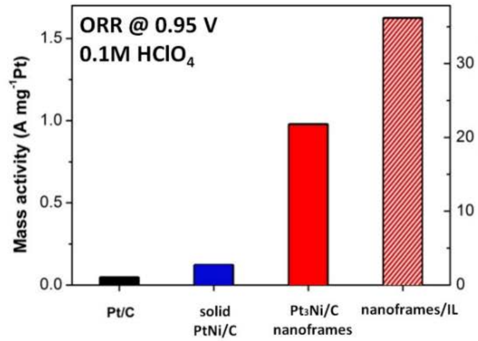




Pt segregated to edges

Excellent oxygen reduction activity



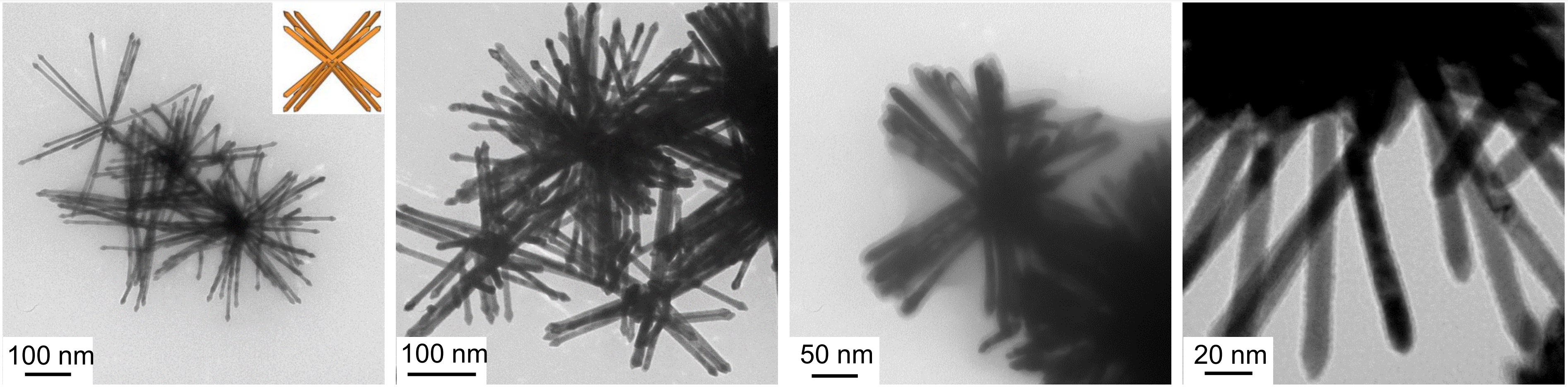


High intrinsic activity (mA/cm^2) ✖ **High surface area (cm^2/mg Pt)** = **High mass activity (mA/mg Pt)**

Becknell, et al. *J. Am. Chem. Soc.*, **137**, 2015

Chen, et al. *Science*, **343**, 2014

1-D Intermetallic Nanostructures

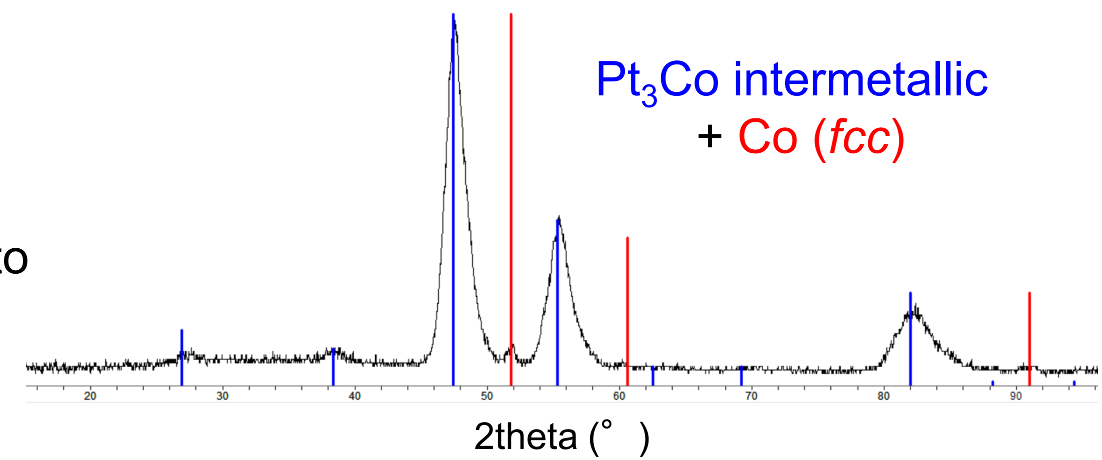


Synthesize Pt branches → Load branches with Co → Coat with ALD Al_2O_3 → Anneal 500°C in H_2/Ar

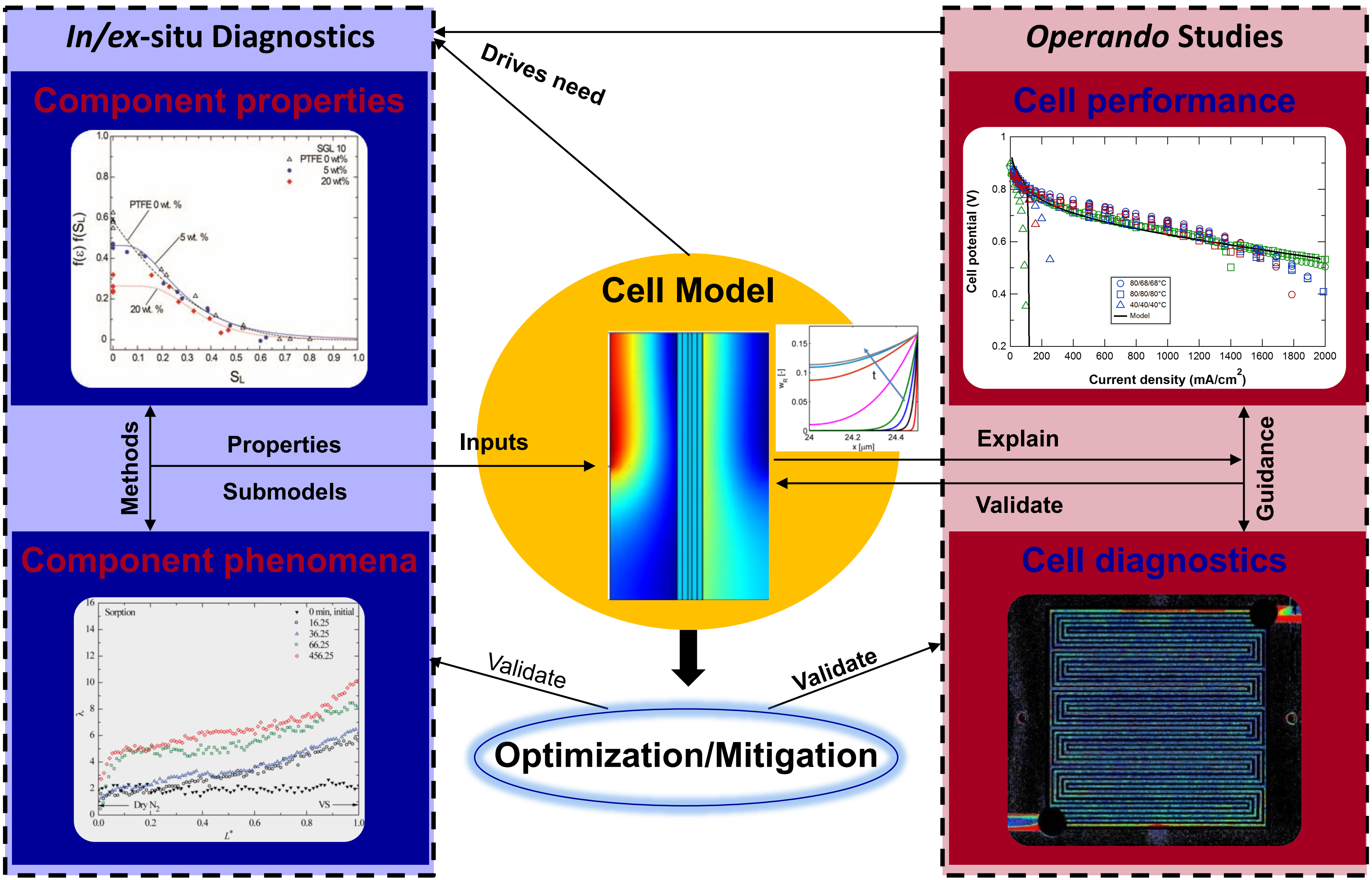
Goal: Attain high levels of mass activity and stability

- Intermetallics have demonstrated enhanced stability for ORR
- 1-D nanostructures are resistant to Ostwald ripening
- Pt-Co alloys are highly active for ORR

Annealing produces intermetallic Pt_3Co branches

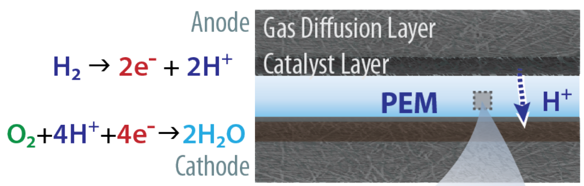


Analyzing Fuel-Cell Transport Phenomena



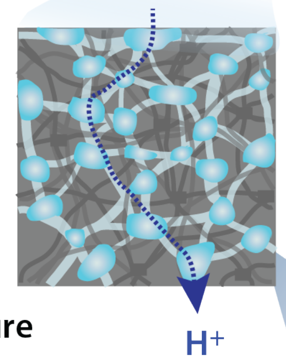
Multiscale Diagnostics of Fuel-Cell Membranes

Polymer-Electrolyte Fuel Cell (PEFC)



Proton-Exchange Membrane

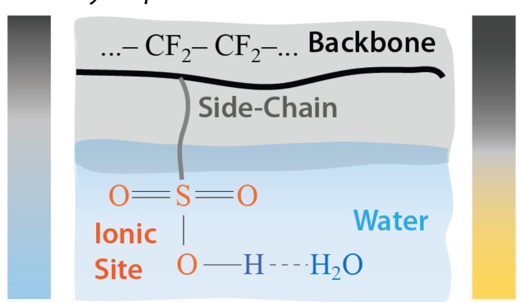
proton transport
in water network
key for performance



Chemical Structure

phase-separated with water

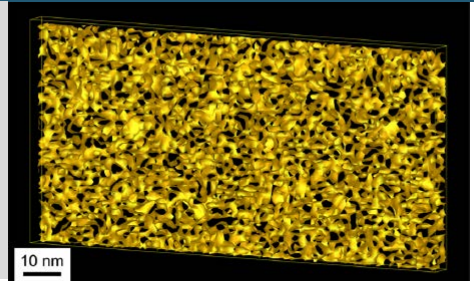
more Hydrophobic



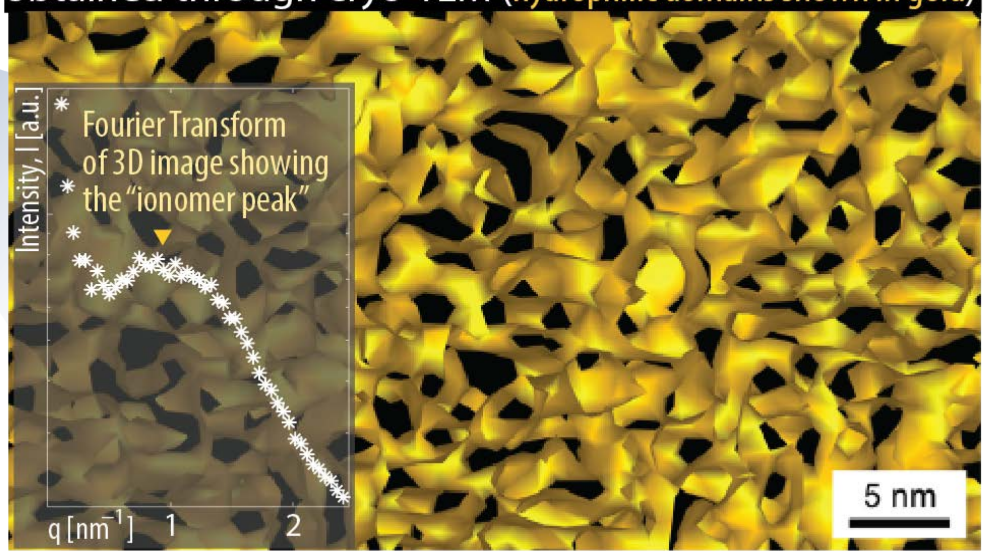
more Hydrophilic

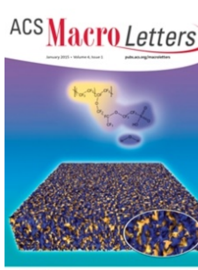
Modeling the transport of ionic/non-ionic species through membranes across multiple scales provides development design rules to materials manufacturers

First direct 3D imaging enables advanced computation of transport in the membrane and impact on cell performance



3D nanoscale morphology of as-cast hydrated Nafion obtained through cryo-TEM (hydrophilic domains shown in gold)

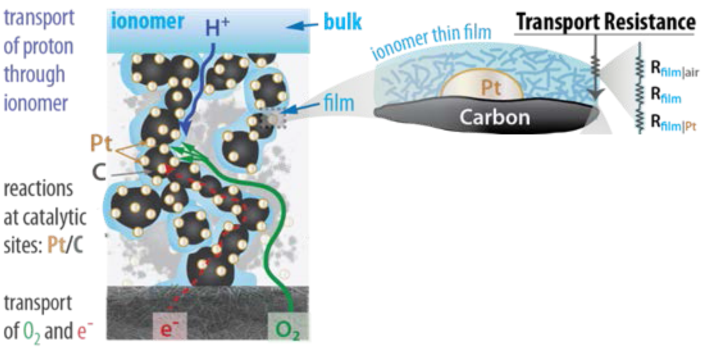


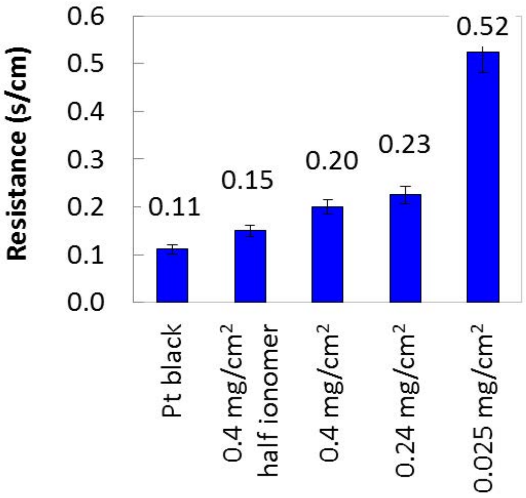


F.I. Allen, L.R. Comolli, A. Kusoglu, M.A. Modestino, A.M. Minor, A.Z. Weber, *ACS Macro Letters*, 4 (2015) 1-5 | DOI: 10.1021/mz500606

Transport Resistance at Low Pt Loadings

- **Increased local resistance with low Pt loadings is critical issue for cost reduction**
  - Measured by developed effective diffusivity experiment





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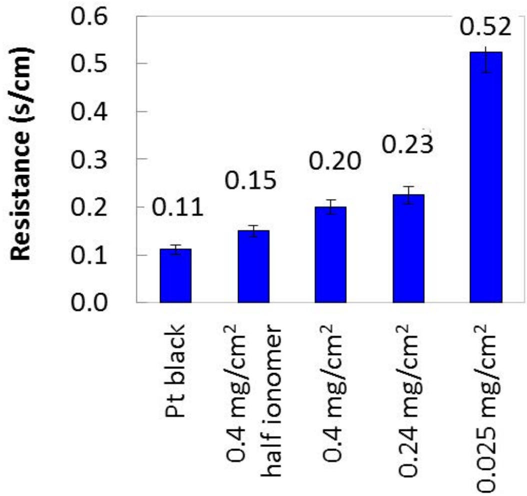
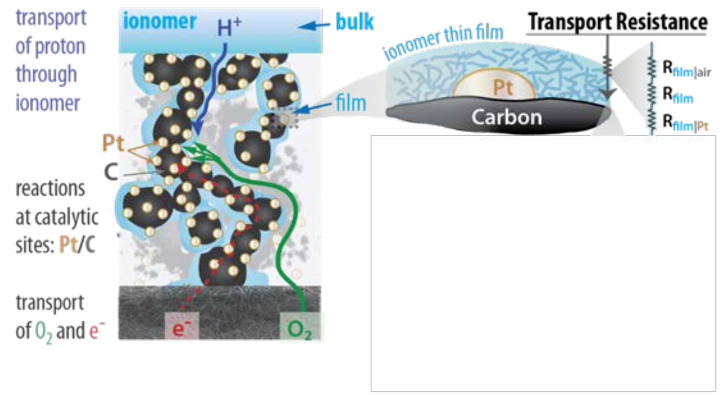
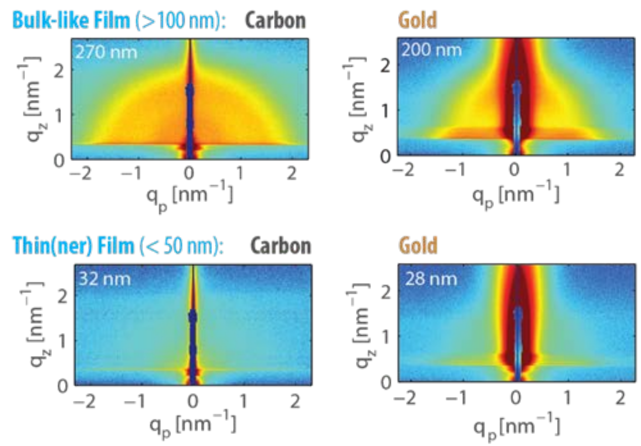


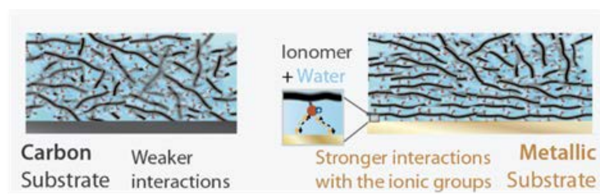
  - Correlating resistance to ionomer thin-film structure on model substrates
    - Elucidate limiting phenomena
    - Measure critical transport properties



Ionomer Film Moprhology Model Substrates

Hydrated morphology of ionomer film on substrates (Grazing-incidence SAXS)





Related Publications
A.Z. Weber and A. Kusoglu, *J. Mater. Chem. A* (2014) | DOI: 10.1039/c4ta02952f
A. Kusoglu *et al.*, *Adv. Functional Materials* (2014) | DOI: 10.1002/adfm.201304311

Transport Resistance at Low Pt Loadings

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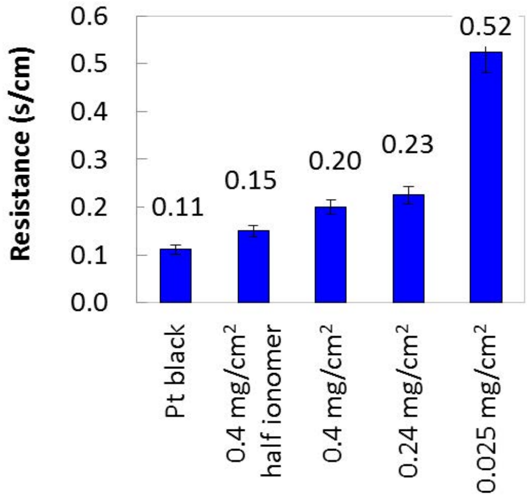
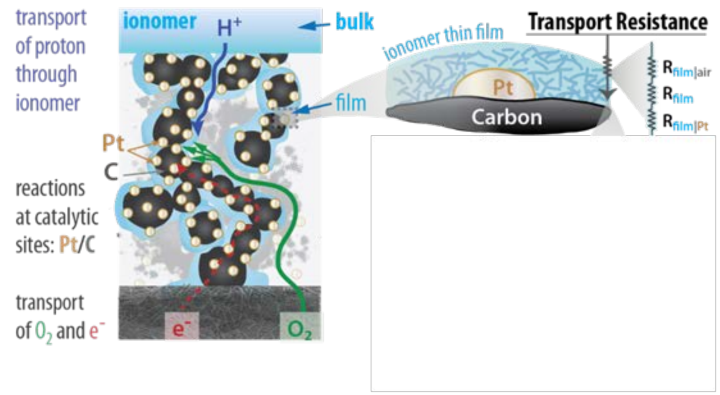
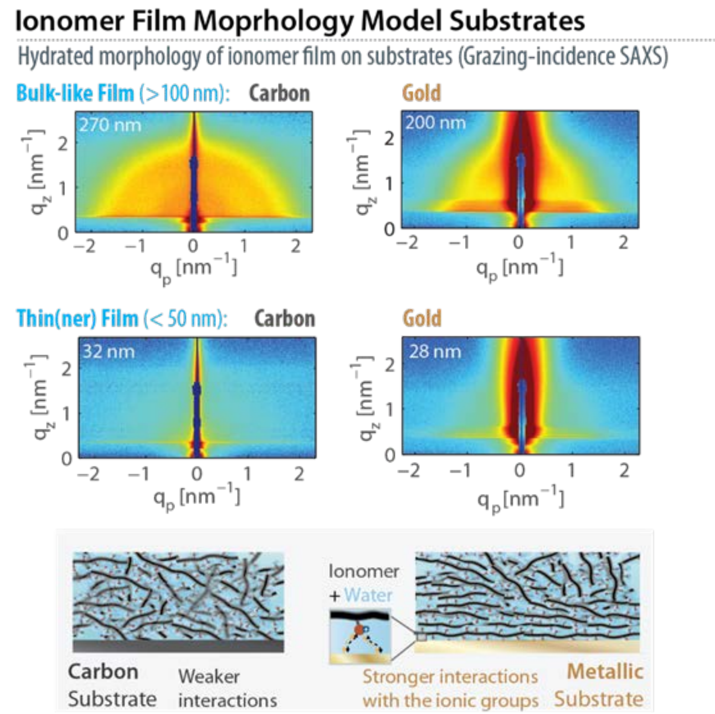


  - Correlating resistance to ionomer thin-film structure on model substrates
    - Elucidate limiting phenomena
    - Measure critical transport properties
- **Insights will allow for novel strategies and materials to overcome limitations**





Related Publications

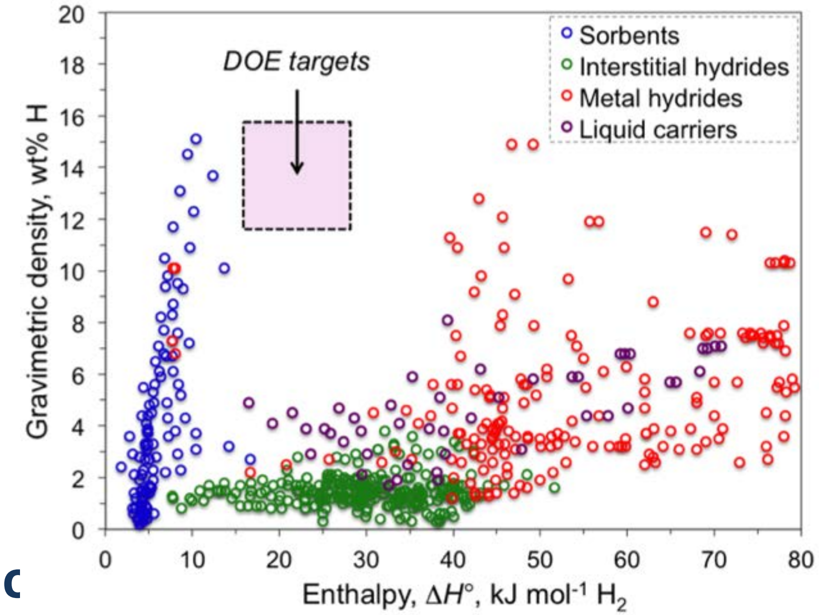
A.Z. Weber and A. Kusoglu, *J. Mater. Chem. A* (2014) | DOI: 10.1039/c4ta02952f

A. Kusoglu *et al.*, *Adv. Functional Materials* (2014) | DOI: 10.1002/adfm.201304311

H_2 Storage

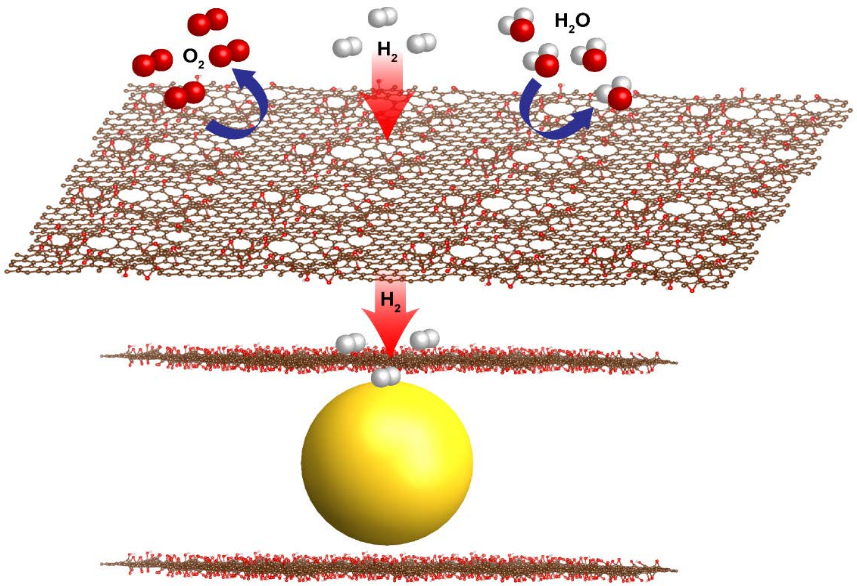
Critical Scientific Challenges

- **Sorbents: Eng. COE target: 15 – 20 kJ/mol**
- **Volumetric capacity at operating temp.**
- **Increased usable hydrogen capacity needed**
- **Distribution of H_2 binding sites and ΔH at ambient temperature not optimized**



- **Metal hydrides: Eng. COE target: ≤27 kJ/mol H_2**
- **Poor understanding of limited reversibility and kinetics**
- **Role of interfaces and interfacial reactic**
  - Solid-solid
  - Surfaces
- **Importance and potential of nanostructures**

Hybrid Graphene Oxide-Metal Hydrides



This work pioneers the use of atomically-thin sheets of reduced graphene oxide to encapsulate Mg metal hydride nanocrystals

System is robust to oxygen, moisture with no aging, oxidation, or degradation in performance

System provides dense storage (6.5 wt% total composite and 0.105 kg H_2/L) at low P, T

Want to have pristine hydride model systems to enable fundamental understanding

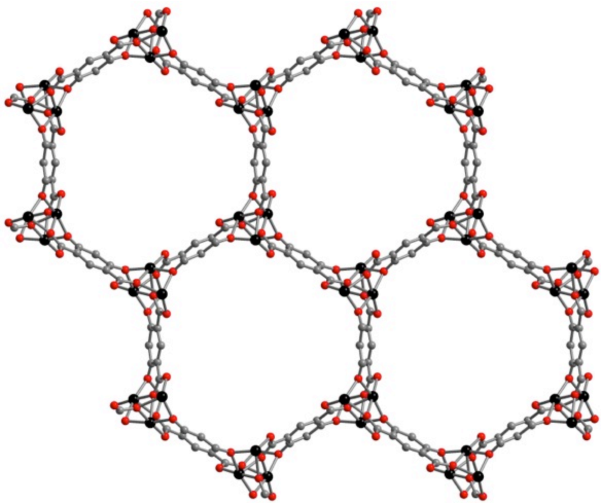
Provides platform for development of advanced materials: from Mg and Al to complex hydrides such as $LiNH_2$, $Mg(BH_4)_2$

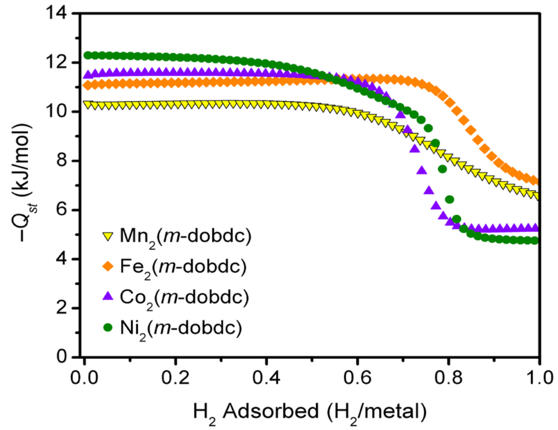
Cho, E., Urban, J. J. et al. *Adv. Mater.* (2015)

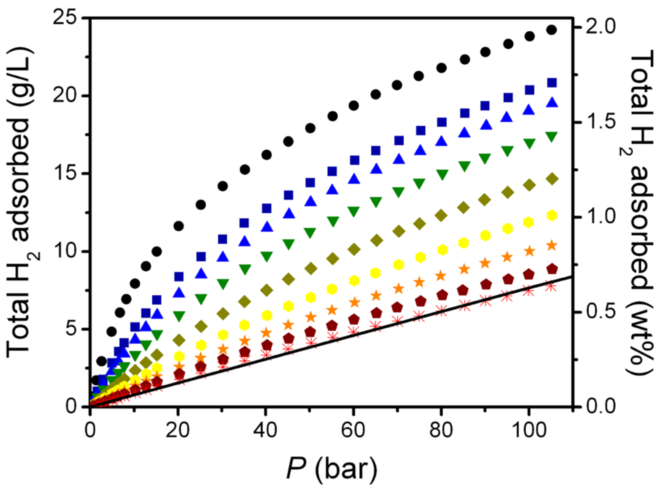
Cho, E. et al, *Nature Communications* (2016)

H2 Storage in Metal-Organic Frameworks

- **Metal-organic frameworks (MOFs) are promising materials for H_2 storage in transportation applications at lower pressures than currently used**
- **Strong H_2 binding sites in metal-organic frameworks are targeted in order to store H_2 at high volumetric energy densities**
  - Guided by *ab-initio* modeling







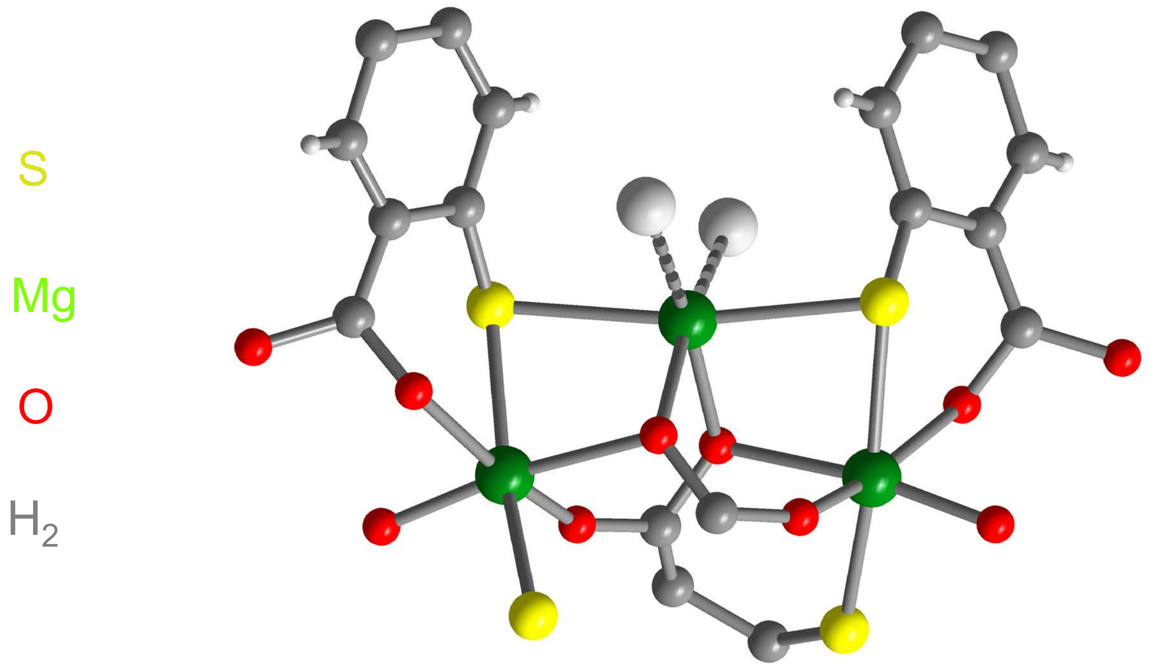
M_2(*m*-dobdc)
(M = Mg, Mn, Fe, Co, Ni)

M_2(*m*-dobdc) isosteric heat of adsorption plots, among the highest H_2 binding enthalpies known in MOFs

Kapelewski, M. T. *et al. J. Am. Chem. Soc.* 2014, *136*, 12119.

H2 Storage in Metal-Organic Frameworks

- Multiple H_2 molecules binding to each metal is necessary to increase H_2 density
  - Improved volumetric capacity
  - First experimental example of binding two H_2 molecules (white spheres) to a single metal center (Mn^{2+}) in a MOF



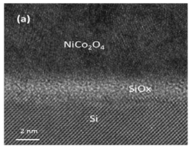
Runčevski, Kapelewski, Torres-Gavosto, Brown, Long. *Submitted*.

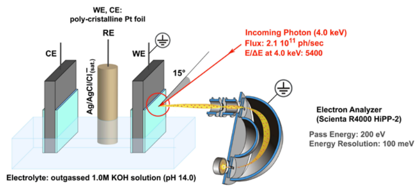
Tsivion, Long, Head-Gordon. *J. Am. Chem. Soc.* **2014**, *136*, 17827.

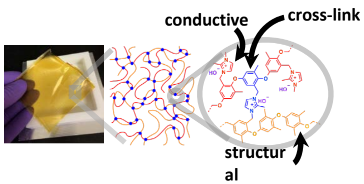
H_2 Production

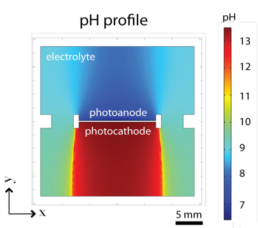
JCAP's Core Expertise and Accomplishments to Date

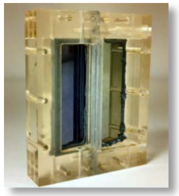
LBNL strengths

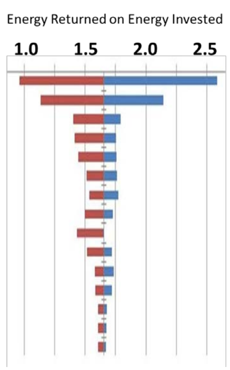


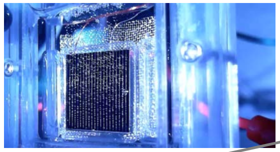








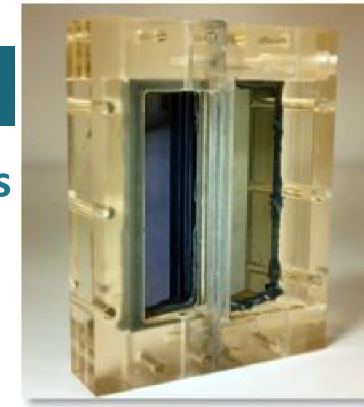




- Protective coatings for photoelectrodes
- High throughput materials discovery Theory
- New electrocatalysts with benchmarked performance
- Operando and in-situ characterization of materials and related theory
- Optimal separator membrane properties and synthetic platform
- Multi-physics modeling and simulation tools
- Robust prototype designs and fabrication experience
- Fully integrated prototype with unassisted water splitting
- Energy and life-cycle analysis of GW solar H2 facility

JCAP
JOINT CENTER FOR ARTIFICIAL PHOTOSYNTHESIS

INTEGRATED DEVICE FOR EFFICIENT, SAFE H_2 GENERATION USING SUNLIGHT

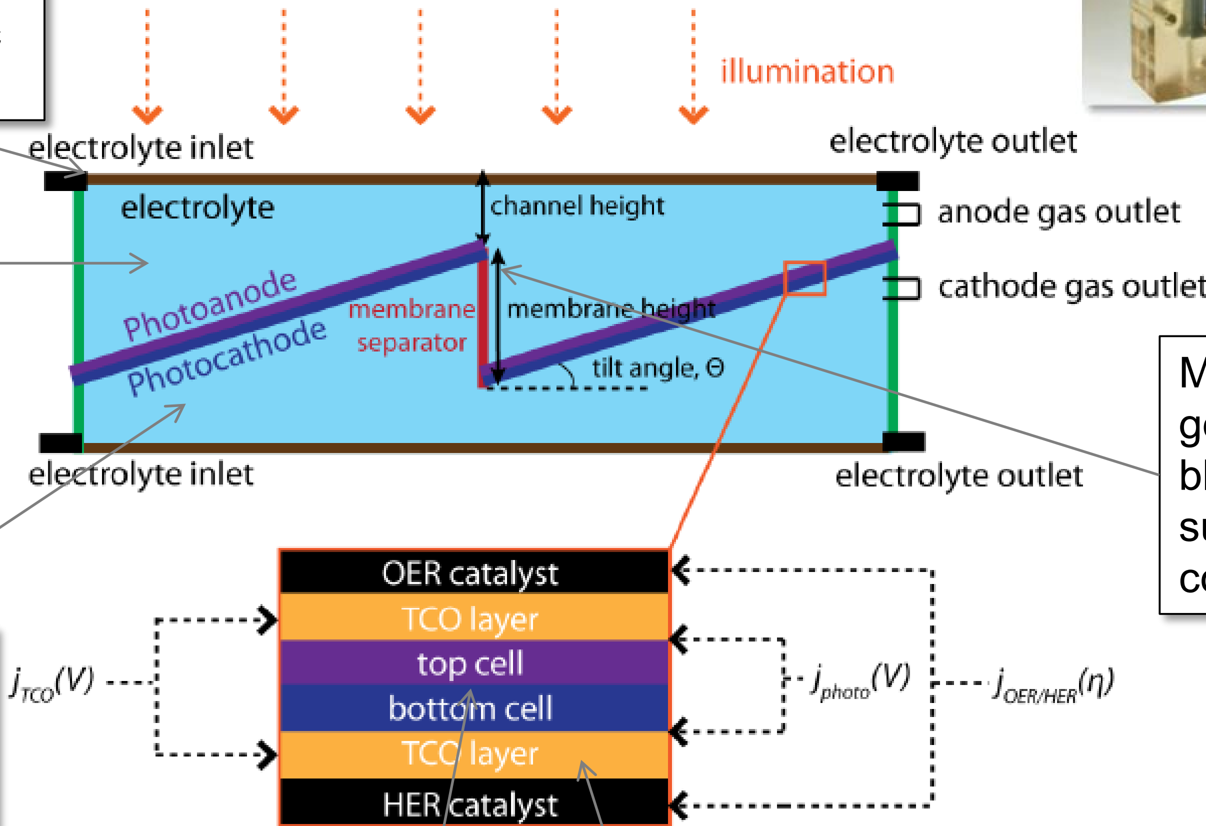


Louvered configuration optimized through multiphysics calculations

Electrolyte: highly acidic or basic

Water converted to oxygen by oxygen evolution reaction (OER)

Protons converted to hydrogen by hydrogen evolution reaction (HER)



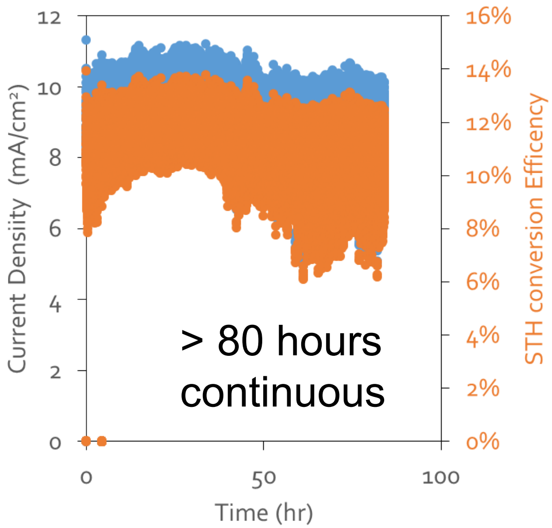
Membrane: good gas blocking, sufficient conductivity

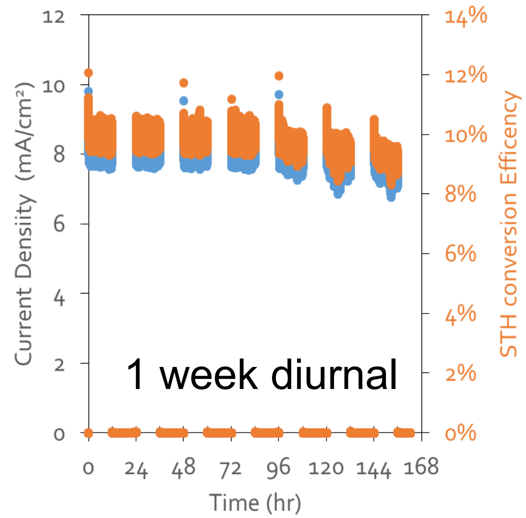
Semiconductors for electron and hole generation

Transparent conducting oxide

IMPROVEMENT: PEC EFFICIENCY AND LIFETIME, PHOTOCATHODE DEVICE

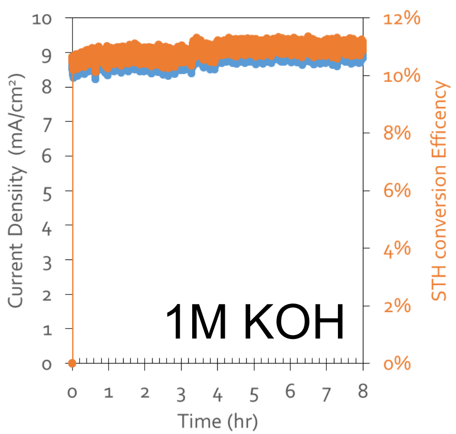
New catalyst-protection layer system for III-V devices with full product separation has >10% efficiency, days lifetime under a range of conditions

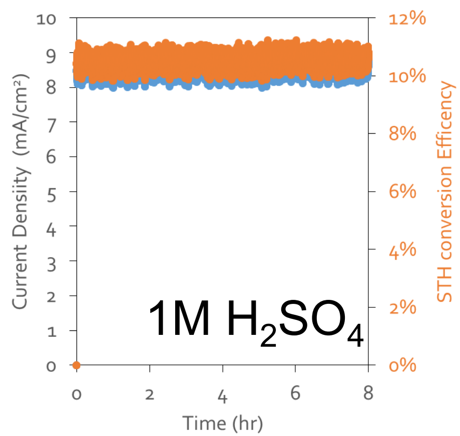




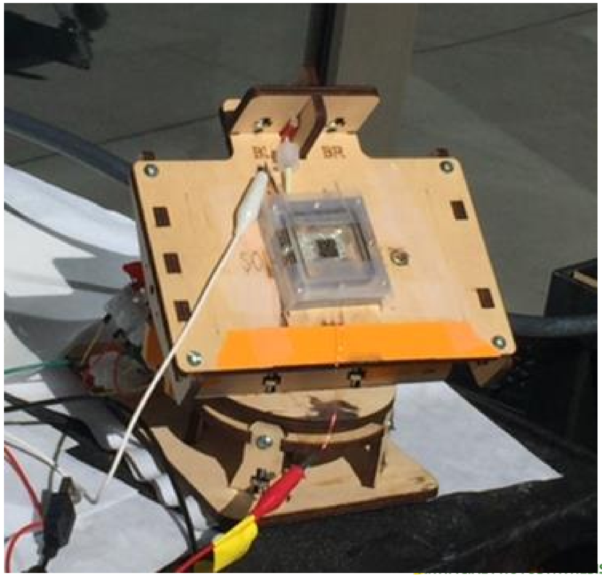
AM 1.5 G simulator, 1 sun
Materials:
1M H_2SO_4
III-V Spectrolabs cell
Pt HER, IrOx OER
Nafion

Same device functions in acid and base





Outdoor testing with tracker (2 tests so far): >13% efficiency



Karl Walczak, Jeff Beeman, David Larson, Rui Liu, CX Xiang, Frances Houle, Ian Sharp, in preparation 2016

Questions?

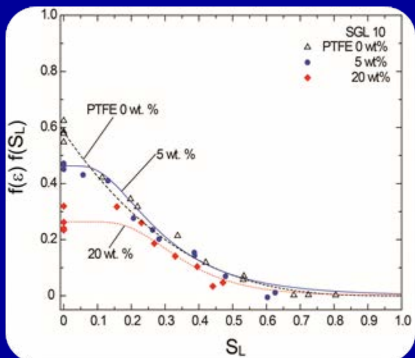
Fuel-Cell-Technologies Programmatic Vision

- **LBNL seeks to understand and optimize the next generation fuel-cell and related energy-conversion and energy-storage components and materials mainly through physics-based multi-scale modeling of cell behavior, advanced diagnostics of cell properties, and synthesis of novel key materials**
  - Utilize core team of electrochemists, chemical engineers, mechanical engineers, theorists, material scientists, and organic chemists
  - Leverage LBNL facilities and core competences
  - Collaborate extensively with labs, industry, and academia

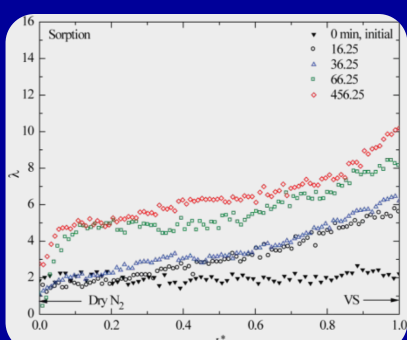
Analyzing Fuel-Cell Transport Phenomena

In/ex-situ Diagnostics

Component properties

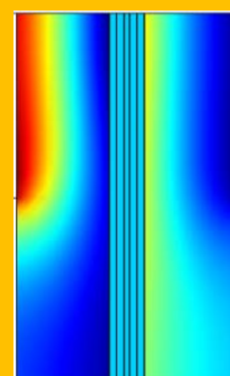


Component phenomena



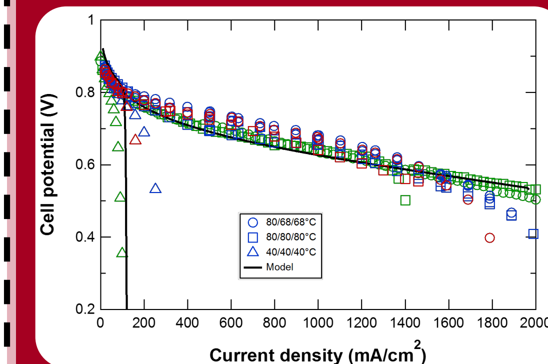
FUEL CELL FCPAD PERFORMANCE & DURABILITY

Cell Model



Operando Studies

Cell performance



Cell diagnostics