Virtual Hydrogen Storage for Fuel Cells

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GE Global Research

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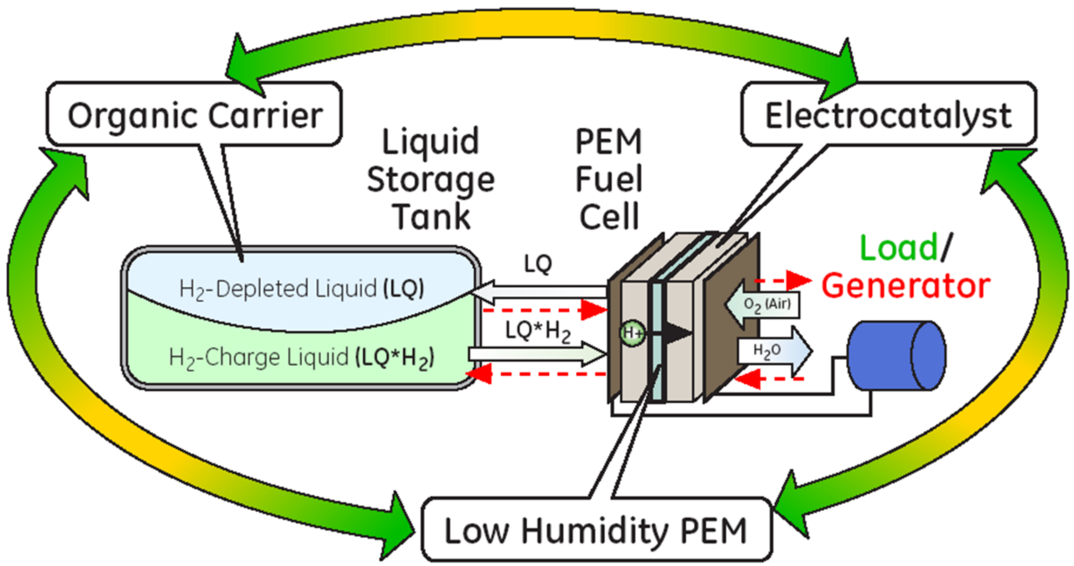
imagination at work

U.S. DEPARTMENT OF ENERGY

Center for Electrocatalysis, Transport Phenomena, and Materials for Innovative Energy Storage
Dr. Grigorii Soloveichik (GE Global Research)

Electrocatalysis, transport phenomena and membrane materials basic research aimed to three novel components of an entirely new high-density energy storage system combining the best properties of a fuel cell and a flow battery: organic carriers, electro(de)hydrogenation catalysts, and compatible PEM



Focus areas:
- C-H bond catalysis/
- Electro(de)hydrogenation catalyst
- Organic fuel
- Low humidity proton exchange membrane

Award DE-SC0001055

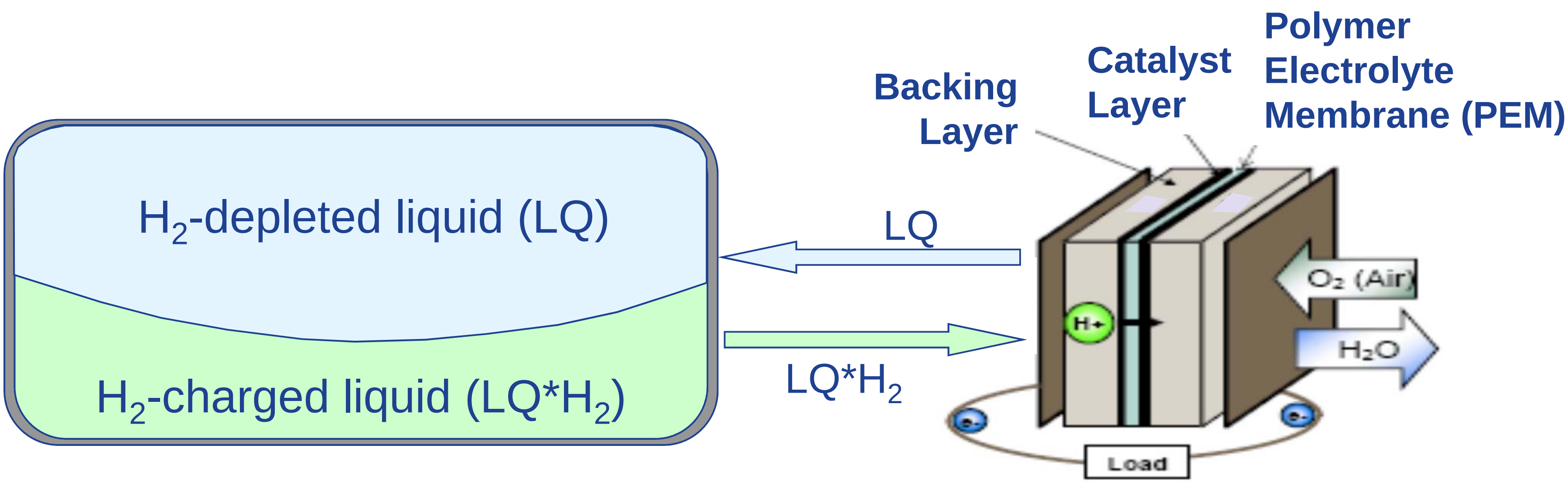
GE | Berkeley Lab | Yale University | Stanford University

an Office of Basic Energy Sciences
Energy Frontier Research Center

EFRC-CETM Vision

We are establishing a world class interdisciplinary research center enabling the reversible use of the liquid high energy density carriers in fuel cells for next generation of effective, flexible, and safe systems for mobile and stationary applications

Direct* organic *fuel cell/flow battery concept

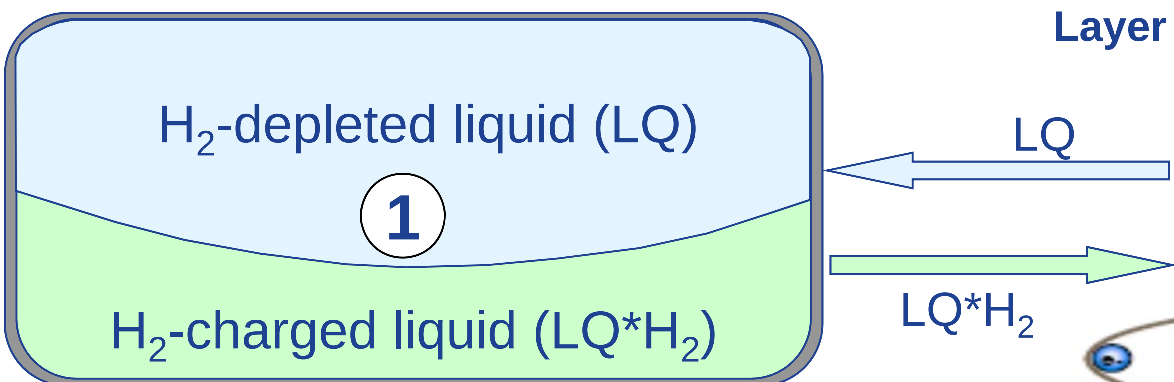


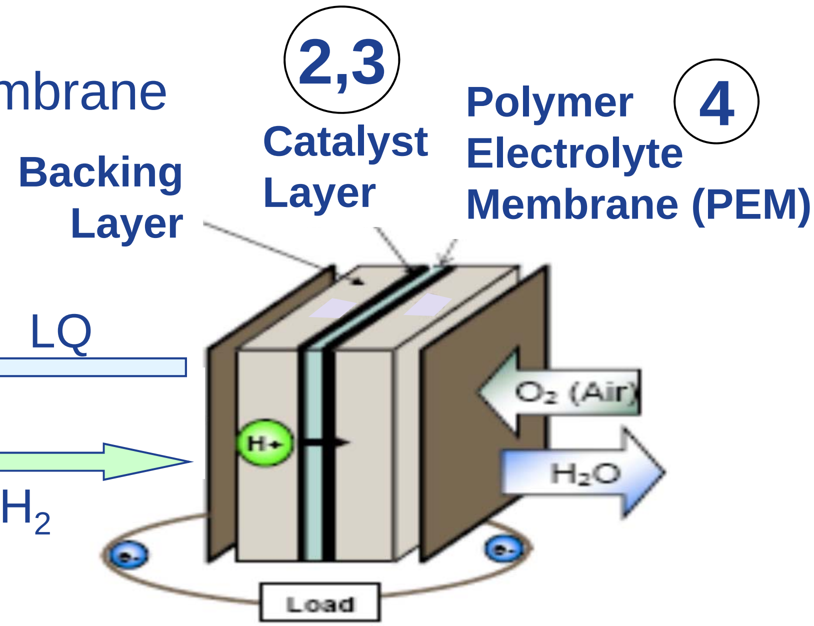
EFRC-CETM Strategy

The EFRC is pursuing **electrocatalysis and transport phenomena** in anode and membrane **materials** of the organic fuel cell/flow battery as the basis for an entirely new high density electrical energy storage

Focus areas:

1. Organic fuel
2. C-H bond catalysis
3. Electro(de)hydrogenation catalyst
4. Low humidity proton exchange membrane





EFRC-CETM long-term goals

Challenges and needs

- Electron level material processes
- Atom- and energy efficient synthesis
- Far from equilibrium processes control
- Electrical energy storage
- Catalysis for energy
- Hydrogen economy
- Solar energy utilization

Fundamental research

EFRC

Focus 1
Selection and synthesis of organic carriers

Focus 2
Discovery of electro(de)hydrogenation catalysts

Focus 3
Immobilization and characterization of electrocatalysts

Focus 4
Novel proton exchange membrane development

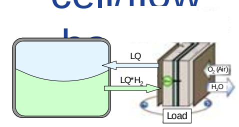
Focus 5
Modeling of interactions among components

Program management

System integra

Technology

High density energy storage organic fuel cell/flow



Applications

Solar energy

Plug-in hybrids

Wind energy

Load leveling

EFRC-CETM Team

Combined expertise in catalysis, electrochemistry, fuel cells, PEM membranes, electrocatalysts, batteries, hydrogen storage, computational modeling, and system integration

GE Global Research

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Megan Hoarfrost
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Oana Raluca Luca
Eduardo Sproviero

Stanford University

Chris Chidsey
Vadim Ziatdinov
Ali Hosseini

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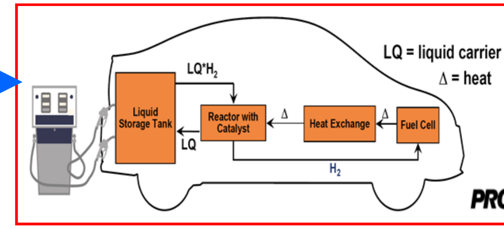
Fuel (organic carrier) focus

Traditional approach

$LQH_n \Leftrightarrow LQ + n/2\ H_2$

ΔH to be minimized



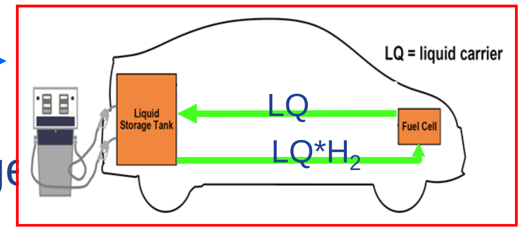
EFRC approach

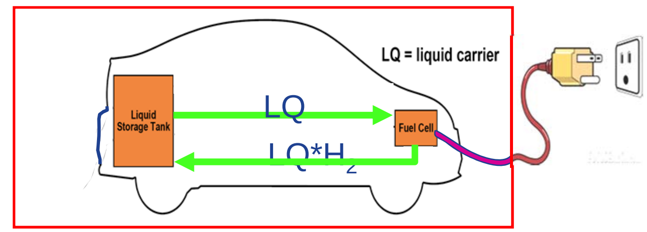
$LQH_n + n/4\ O_2 \Leftrightarrow LQ + n/2\ H_2O$

$\Delta(G_{LQHn} - G_{LQ})$ to be minimized to maximize cell voltage

Theoretical cell voltage 0.95 – 1.1 V

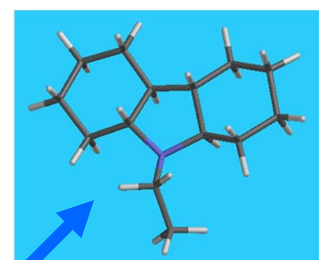
(depends on organic hydrogen carrier)

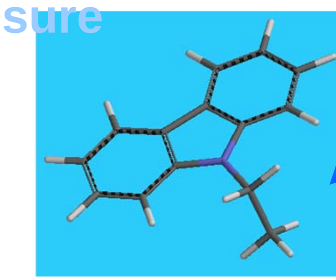




Organic fuel requirements

- **Minimal ΔG dehydrogenation of organic carriers via molecular modeling guidance**
- **Scalable synthesis of aromatic precursors and hydrogenation to saturated carriers (high pressure lab)**
- **Liquid at ambient conditions, low vapor pressure**





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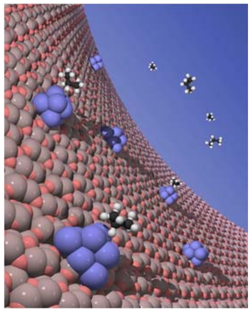
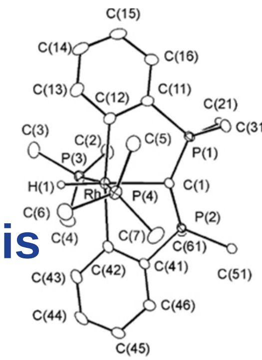
C-H Bond Catalysis Focus

Homogenous C-H bond activation AND electron transfer

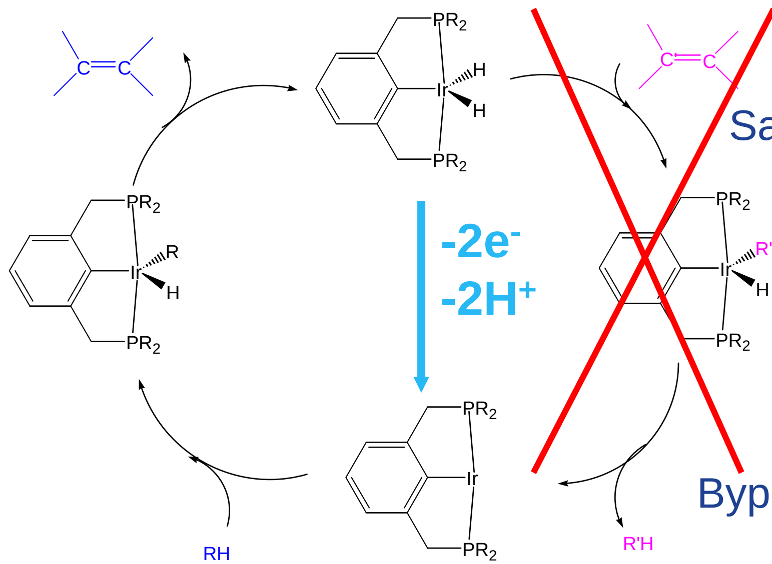


$$LQH_n \ - \ n\,e^- \ \overset{\text{catalyst}}{\Leftrightarrow} \ LQ + n\,H^+$$

From surface catalysis to defined center catalysis



- **Define the C-H bond activation preferable pathway (oxidative addition, electrophilic substitution, etc.)**
- **Factors controlling the catalyst's redox properties**
- **Mechanism of dehydrogenation/hydrogenation (first step the moist challen**
- **Multi-step activation/electron transfer on the same center**



Sacrificial olefin

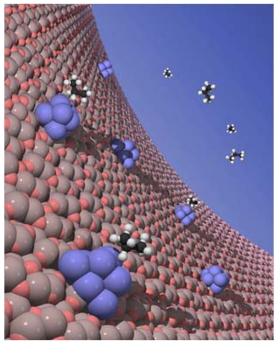
A.S.Goldman, 2003

Byproduct

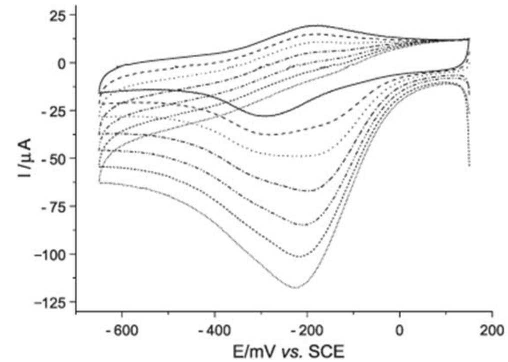
Thomas Miebach, GE Global Research
Tuesday, November 9, 2010

Electrocatalysis focus

Electrocatalysis for dehydrogenation and hydrogenation

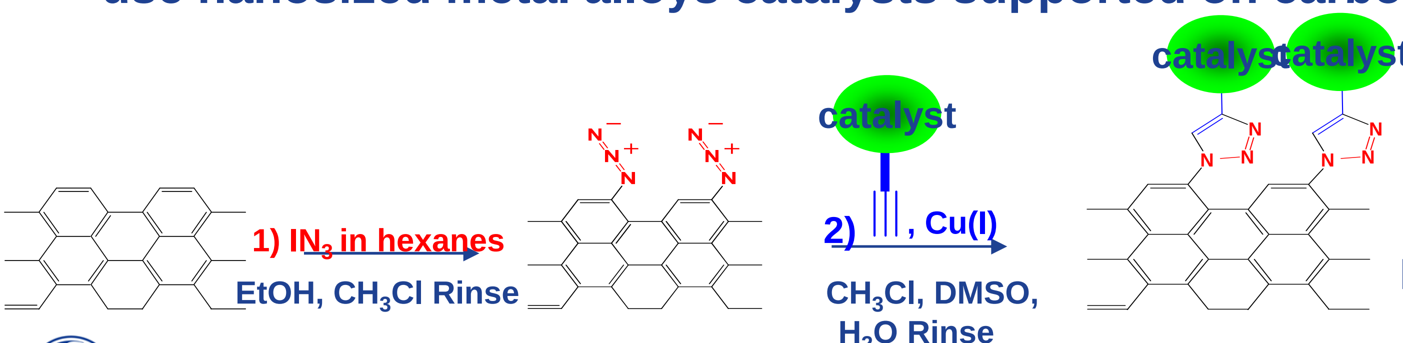


$$LH_n - n\,e^- \overset{\text{electrode}}{\Leftrightarrow} L + n\,H^+$$

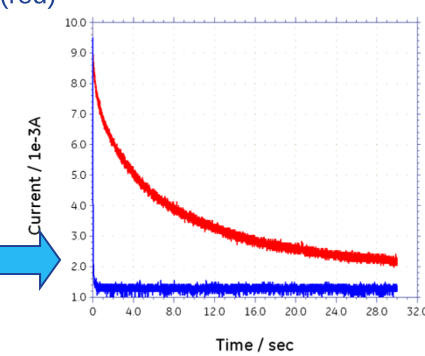


Electrocatalyst requirements

- **Fast electron transfer from metal centers through a linker to electrode via study of the transport mechanism and determination of controlling factors**
- **Fast proton transport to PEM via structured catalyst/support**
- **Robust catalyst that tolerant to impurities/reaction products**
  - **- design catalyst ligand environment for selectivity**
  - **- use nanosized metal alloys catalysts supported on carbon**



Chronoamperometry of baseline RVC (blue) and functionalized RVC (red)



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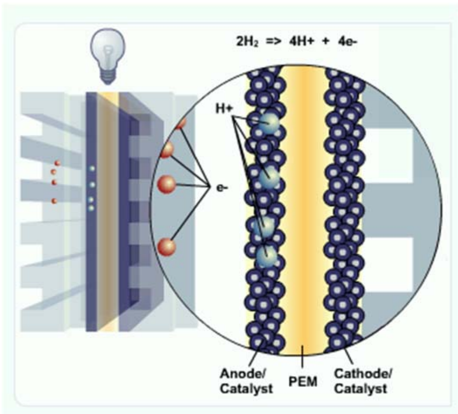
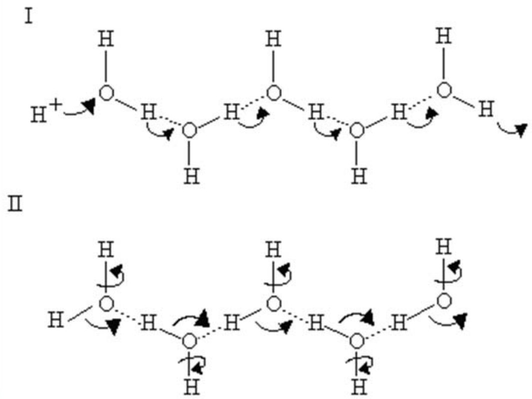
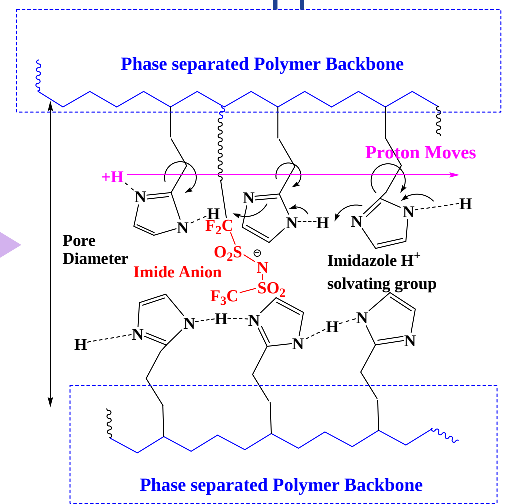
Proton exchange membrane focus

Traditional approach



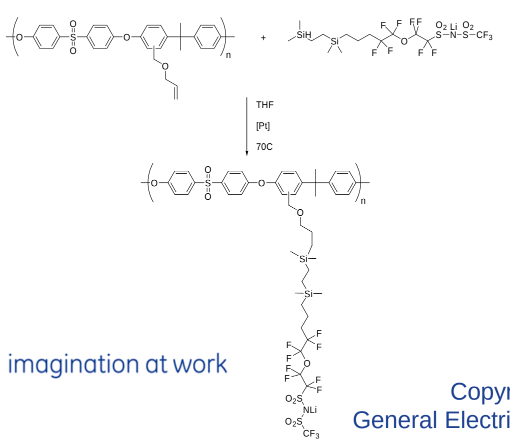


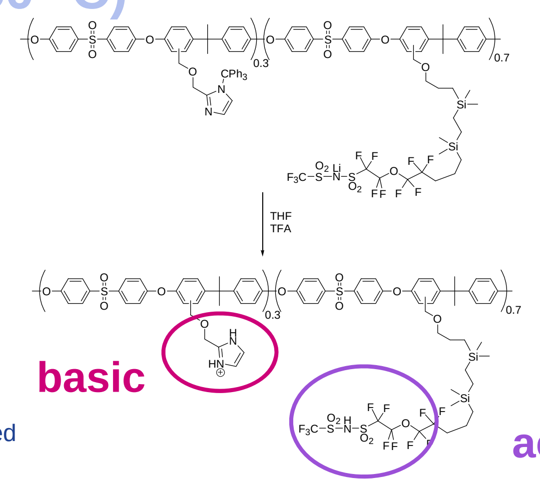
EFRC approach



Membrane requirements

- **Water free PEM (H_2O detrimental to anode chemistry)**
- **Low fuel and products solubility – mechanical integrity**
- **Proton conductivity 10^{-3} S/cm @ 120 ºC**
- **High oxidative stability at 120 ºC**
- **Thermal stability (> 150 ºC)**



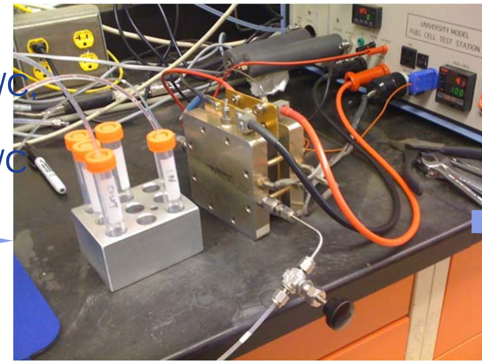


Direct organic hydride fuel cell testing

Membrane Electrode Assembly (MEA)

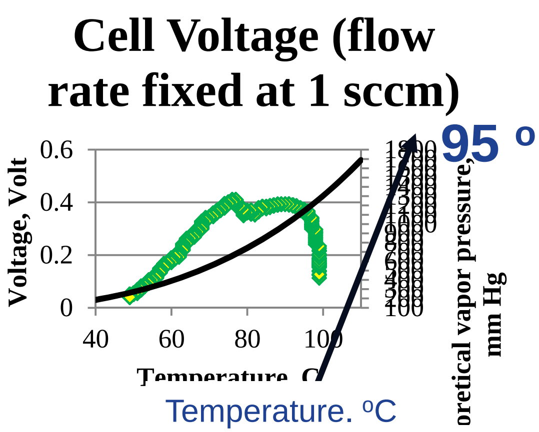
- 5 cm^2 active area
- Anode: 4mg/cm^2 60% PtRu/C, C-cloth anode GDL
- Cathode: 2 mg/cm^2 40% Pt/C
- 115 Nafion® membrane

Fuel Cell Assembly



Fuel Cell Testing

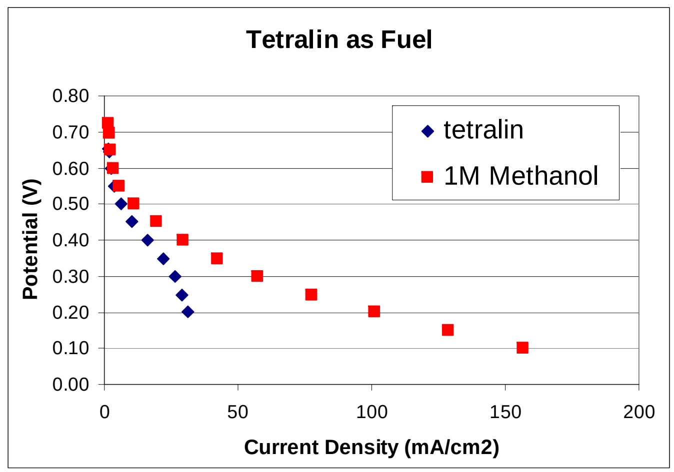
Cyclohexane/air cell



Temperature. ºC

Membrane dehydration, new membranes needed

Tetralin/air cell



Significant current observed for tetralin

Liquid fuel cells OCV, V

Fuel	Theory	Exp.
MeOH	1.21	0.73
Decalin	1.10	0.55
Tetralin	1.08	0.66

Use of liquid hydrocarbon fuel in fuel cell demonstrated

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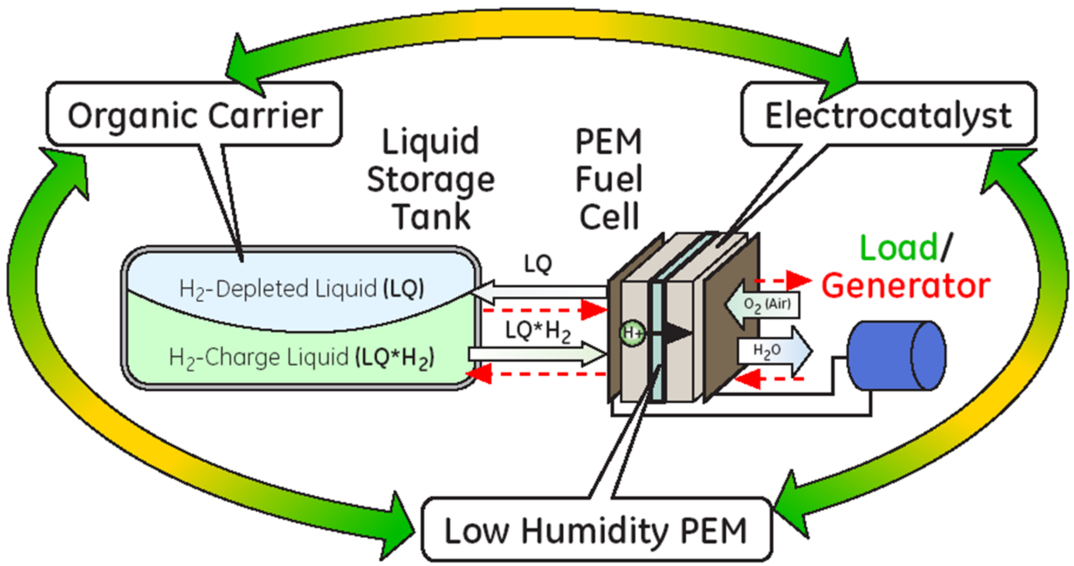

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