# Microstructured Electrodes and Diffusion Layers for Enhanced Transport in Reversible Fuel Cells

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Project ID FC181

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# Overview

Timeline:

- Project Start Date: January 1, 2018

Budget:

- FY18 Planned DOE Funding: $200K
- Total DOE Funds Received to Date: $200K

Barriers

A. Durability

B. Cost

C. Performance

Partners

- LANL (Jacob S. Spendelow, Siddharth Komini Babu, Zachary R. Brounstein)

# Relevance

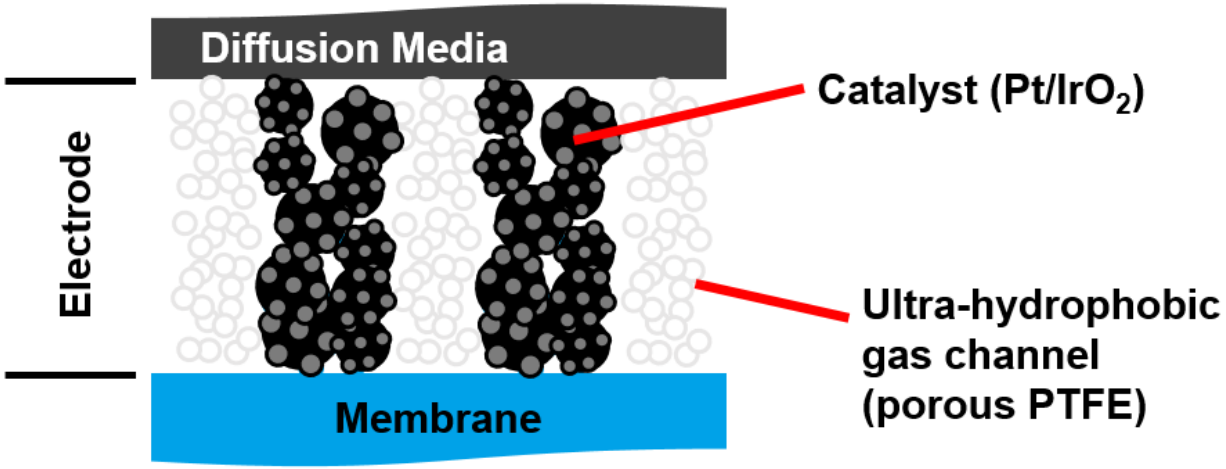
## Objectives

- **Enhance transport performance of unitized reversible fuel cells (URFCs) using arrays of interspersed hydrophobic and hydrophilic channels in electrodes, MPLs, and GDL substrates**
- **Fabricate, test, and validate URFCs with high performance and durability**

- URFCs could address energy storage challenges of intermittent renewable power sources and **could be instrumental in realizing the vision of H2@Scale**
- Achieving high performance in both fuel cell and electrolyzer mode is a critical challenge due to conflicting water management requirements:
  - Electrolyzers perform best with high liquid water saturation (rapid transport of $H_2O$ reactant to catalyst)
  - Fuel cells perform best with low liquid water saturation (rapid transport of $O_2$ reactant to catalyst)
- **Amphiphilic electrode structures and diffusion media are the key to overcome this $H_2O$ and $O_2$ transport challenge**

# Approach: Amphiphilic Catalyst Layers

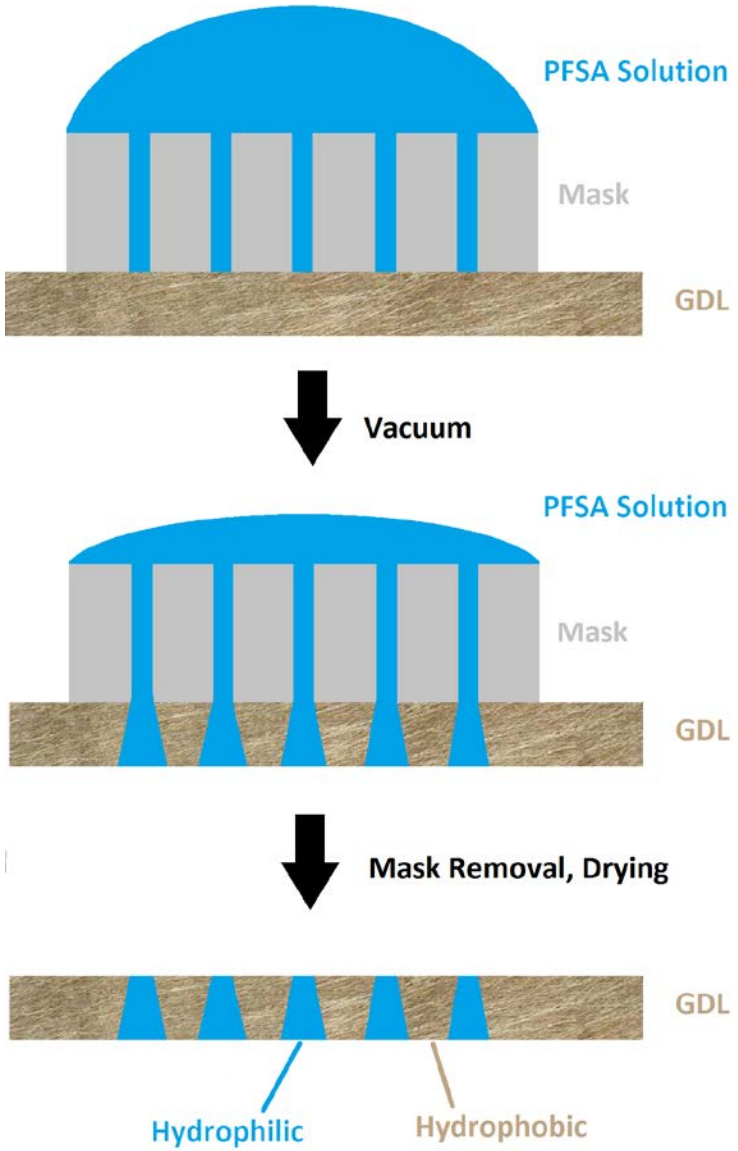
***Interspersed arrays of hydrophobic and hydrophilic through-plane channels provide enhanced $O_2$ and $H_2O$ transport, enabling high performance in both fuel cell and electrolyzer mode***



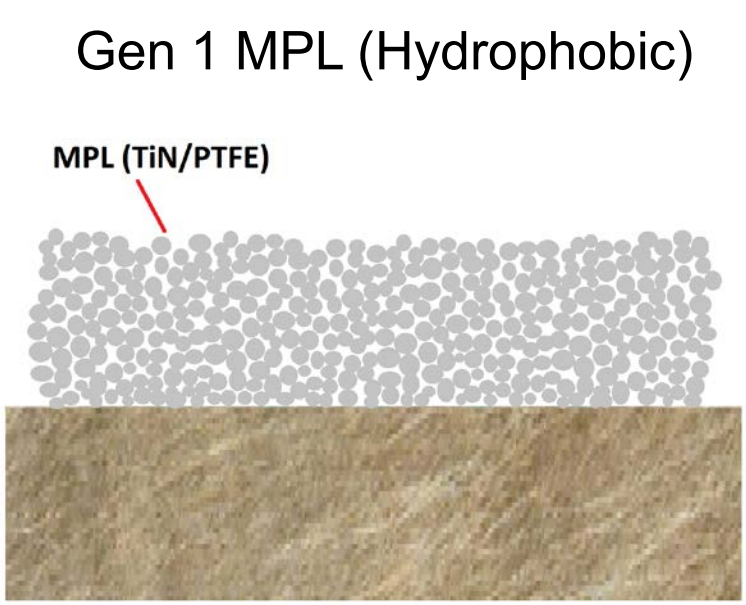

- Catalyst layer is composed of interspersed arrays of catalyst domains and gas transport domains
- Hydrophilic catalyst domains are flooded during normal operation, while hydrophobic gas transport domains serve as channels for $O_2$ transport
- Since hydration state of amphiphilic catalyst layer is similar in fuel cell and electrolyzer modes, rapid switching between fuel cell mode and electrolyzer mode without gas purging is possible

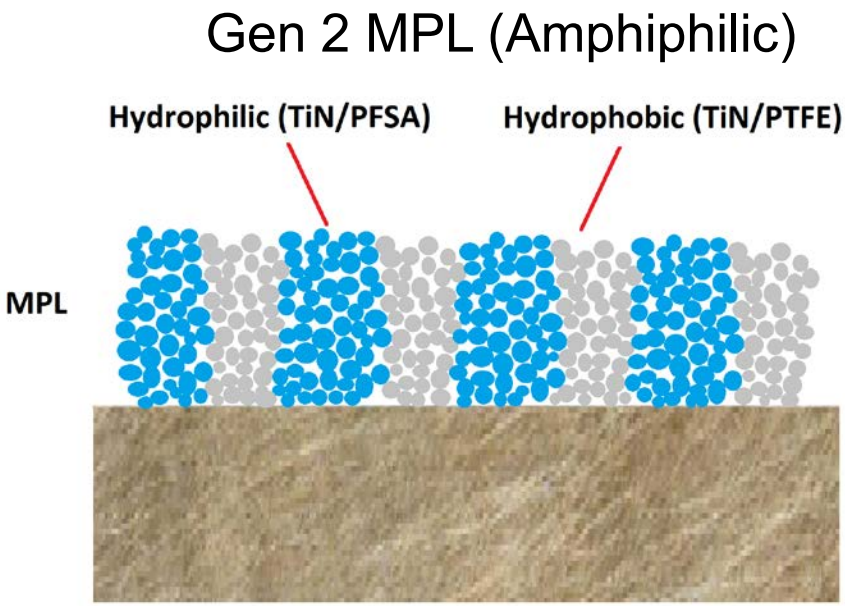
# Approach: Patterned GDL Substrates

GDL substrates (Ti fiber, Nb-doped Ti fiber, or Ti sinter) can be locally patterned with hydrophilic (PFSA) and hydrophobic (PTFE) agents to create channels for rapid transport of $H_2O$ and $O_2$



# Approach: Microporous Layers

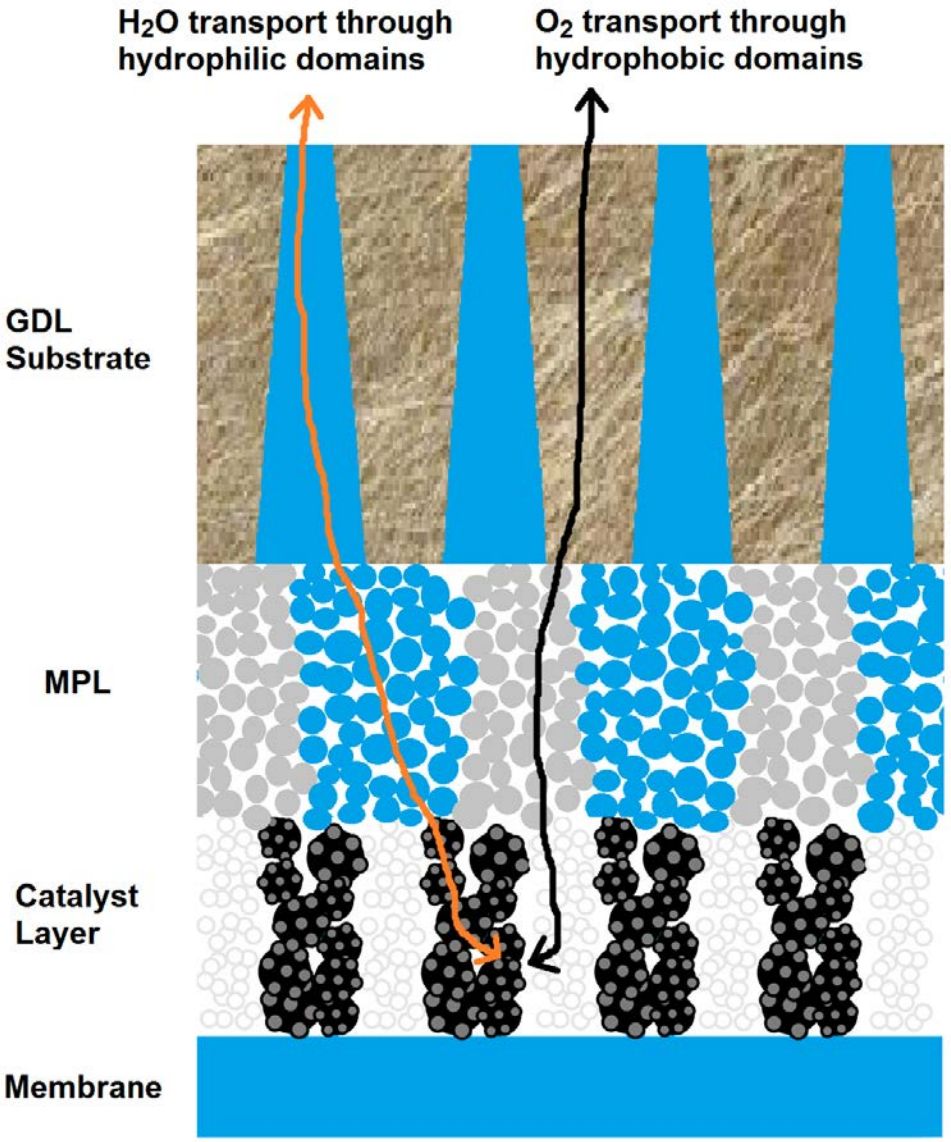


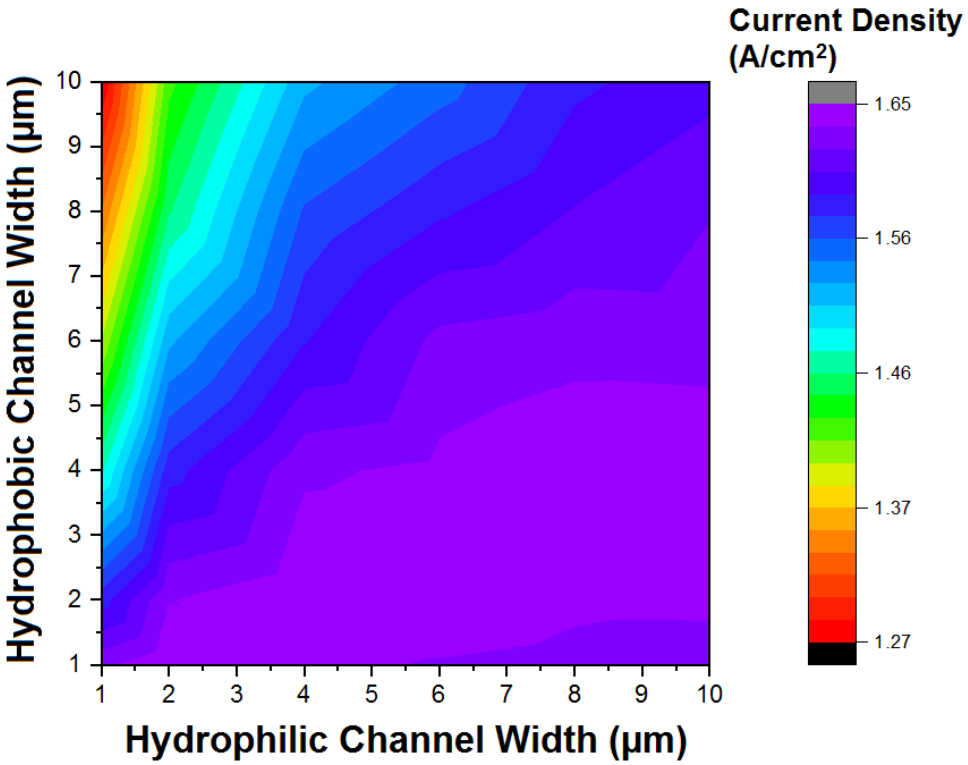

- Microporous layers (MPLs) are a critically important component of diffusion media in conventional fuel cells, but most URFC designs lack an MPL
- MPLs help with water management, keeping GDL substrate from flooding while catalyst layer stays well-hydrated
- MPLs will be fabricated using stable and conductive metal or ceramic powders (Ti, TiN, Nb-doped Ti) with PTFE binder (Gen 1)
- Patterned hydrophilic/hydrophobic MPLs will further enhance water management for effective transport in both fuel cell and electrolyzer modes (Gen 2)

# Approach: Patterned MEA

- Patterned hydrophilic/ hydrophobic GDL substrates, MPLs, and catalyst layers will be combined to produce a patterned MEA with enhanced $H_2O$ and $O_2$ transport characteristics
- This amphiphilic MEA is expected to enable:
  - Improved performance in fuel cell and electrolyzer modes
  - Rapid switching between modes

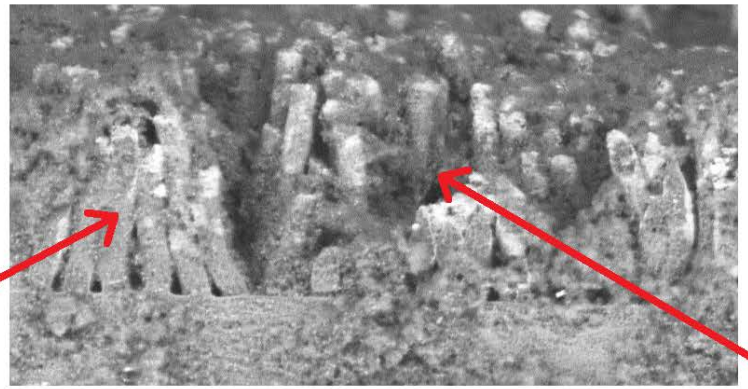


# Accomplishments and Progress: Transport Modeling




- Performance in fuel cell mode was modeled to determine the relationship between hydrophilic/hydrophobic channel dimensions and spacing on transport performance
- Highest performance predicted for relatively narrow hydrophobic channels

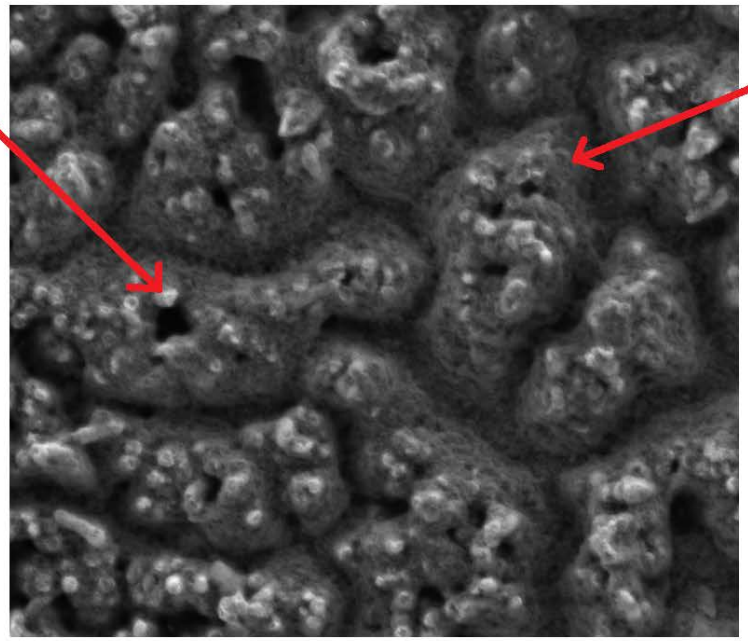
# Accomplishments and Progress: Amphiphilic Catalyst Layers



Side View

High PFSA content hydrophilic channels (bright due to PGM content)

High PTFE content hydrophobic channels (dark)

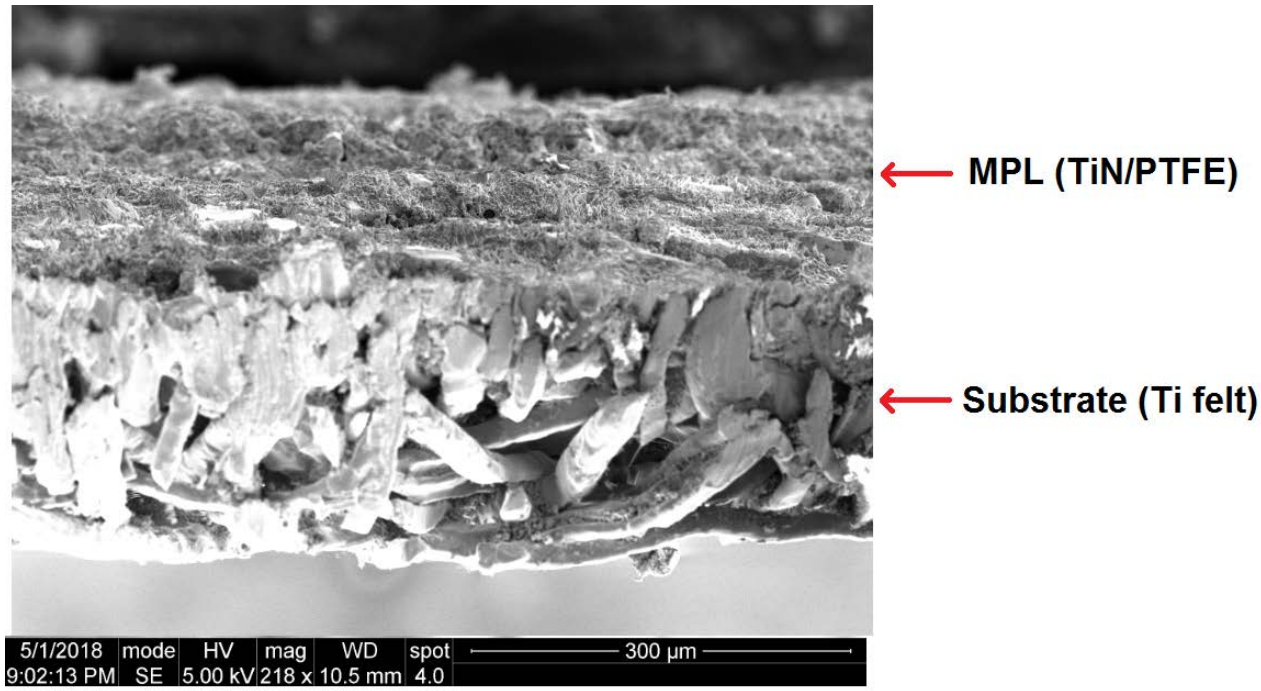


Top View

Two-step fabrication of amphiphilic catalyst layer:

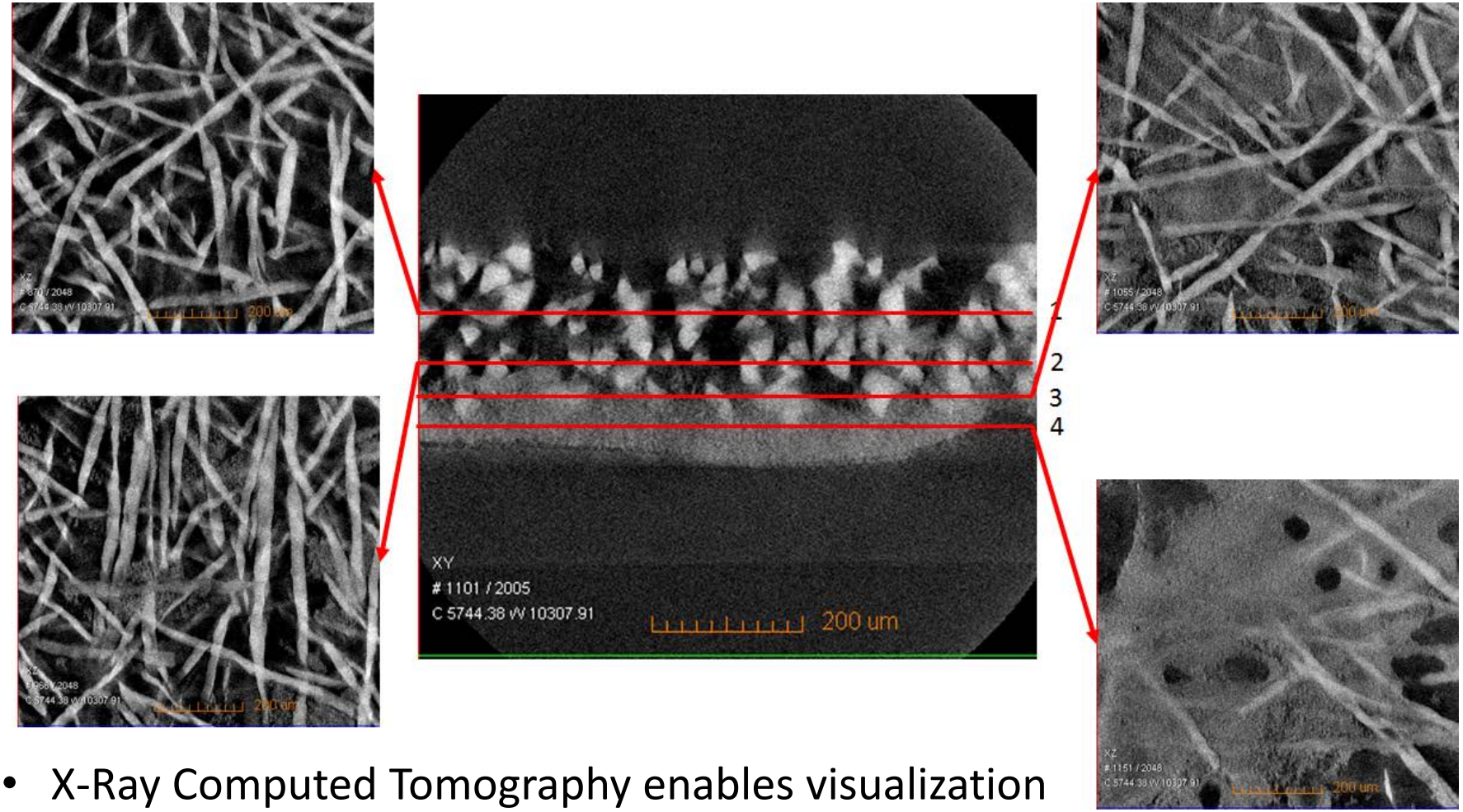
1. Deposition of microscale hydrophilic catalyst tubes
2. Deposition of PTFE-rich hydrophobic $O_2$ transport regions in voids between catalyst tubes

# Accomplishments and Progress: Fabrication of URFC MPLs




- TiN/PTFE MPLs have successfully been deposited on Ti felt GDL substrates
- Performance and durability will be tested under URFC conditions
- TiN is expected to offer significant corrosion resistance, but formation of $TiO_2$ surface layer may increase contact resistance over time
- Durability to be addressed by TiN sintering to reduce contact resistance, or Nb-doping to increase conductivity of surface oxide films

# Accomplishments and Progress: Fabrication of URFC MPLs




- X-Ray Computed Tomography enables visualization of internal structure within Ti felt substrate, TiN/PTFE MPL, and substrate-MPL interface

# Collaborations & Coordination

We are collaborating with multiple projects and organizations, including:

- Electrolysis Rocket Ignition System (LANL LDRD project)
- FC-PAD consortium (complementary efforts in electrode microstructure development for fuel cells)

# Milestones

| | |
|---|---|
| **3/18** | Perform modeling to determine optimal hydrophobic channel size and spacing for GDLs and electrodes |
| **6/18** | Prepare GDL templates and use them to demonstrate fabrication of local hydrophobic GDL microstructures |
| **9/18** | Prepare 4 different electrode templates and use them to demonstrate fabrication of local hydrophobic electrode microstructures with characteristic lengths of < 1 micron |
| **12/18** | Go/No-Go: Incorporate microstructured GDLs and electrodes into functional URFCs and demonstrate E-FC voltage difference at 0.6 A/cm$^2$ of < 1.4 V |
| **3/19** | Use characterization tools to determine effect of local microstructure on water management |
| **6/19** | Use diagnostics to determine effect of local microstructures on gas transport |
| **9/19** | Tailor URFC structures based on characterization and diagnostic results to achieve an E-FC voltage difference at 0.6 A/cm$^2$ respectively of < 1.1 V |
| **12/19** | Tailor URFC structures to limit the transport-related degradation to less than 50 mV after 1,000 E-FC mode cycles |

# Remaining Challenges and Barriers

- Improvement of fabrication techniques by:
  - Increasing control and quality of deposited structures
  - Improving positioning and alignment of transport channels
- Improvement of techniques for controlled and reproducible integration of multiple layers of controlled transport structures into an MEA
- Adaptation of fabrication techniques to low-cost and scalable processes compatible with high volume manufacturing

# Proposed Future Work

**FY18:**

- Further develop fabrication methods for patterned amphiphilic media
- Characterize fabricated structures
- Test MEAs containing patterned media under URFC operating conditions
- Use performance diagnostics (impedance, limiting current methods, helox measurements) to characterize transport resistances

**FY19:**

- Use characterization techniques including *in operando* X-ray computed tomography and neutron radiography to quantify effects of amphiphilic structures on water transport
- Demonstrate achievement of < 1.4 V difference between electrolyzer and fuel cell modes at 0.6 A/cm$^2$ (12/18 go/no-go point), and continue to optimize amphiphilic array structures to achieve project target of < 1.1 V difference at 0.6 A/cm$^2$
- Perform durability studies and characterize and mitigate degradation modes
- Initiate cost analysis, examine scalable fabrication techniques like self-assembly

Any proposed future work is subject to change based on funding levels.

# Technology Transfer Activities

- We are developing IP related to patterned amphiphilic structures for URFC applications
- If successful, we will pursue licensing of technology to URFC developers
- We will pursue tech transfer opportunities leveraging resources of LANL Feynman Center for Innovation

# Summary

**Objective:** Enhance transport performance of unitized reversible fuel cells (URFCs) using arrays of interspersed hydrophobic and hydrophilic channels in electrodes, MPLs, and GDL substrates.

**Relevance:** URFCs could address energy storage challenges of intermittent renewable power sources and could be instrumental in realizing the vision of H2@Scale, but achieving high performance in both fuel cell and electrolyzer mode is a critical challenge due to conflicting water management requirements. Amphiphilic electrode structures and diffusion media are the key to overcome this $H_2O$ and $O_2$ transport challenge.

**Approach:** Interspersed arrays of hydrophobic and hydrophilic through-plane channels provide enhanced $O_2$ and $H_2O$ transport, enabling high performance in both fuel cell and electrolyzer mode. Hydrophilic domains are flooded during normal operation, while hydrophobic domains serve as channels for $O_2$ transport. Since hydration state of amphiphilic catalyst layer is similar in fuel cell and electrolyzer modes, rapid switching between fuel cell mode and electrolyzer mode without gas purging is possible.

**Accomplishments:** Project just started. So far we have performed modeling work to guide design decisions and completed initial fabrication of amphiphilic electrode structures and TiN-based MPLs.

**Collaborations:** Coordination with Electrolysis Rocket Ignition System LDRD project and FC-PAD, as well as InRedox and Smart Membranes (microstructure fabrication)