# U.S. DEPARTMENT OF

Office of ENERGY EFFICIENCY & RENEWABLE ENERGY

# H2-AMP: A Workshop on Advanced Materials for Proton Exchange Membrane Electrolyzers

Summary Report - March 2022

Hydrogen and Fuel Cell Technologies Office

U.S. Department of Energy

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## Preface

Prepared by: U.S. Department of Energy/Office of Energy Efficiency and Renewable Energy/Hydrogen and Fuel Cell Technologies Office, with contributions from workshop moderators and scribes listed below.

## Acknowledgments

The Hydrogen and Fuel Cell Technologies Office (HFTO) acknowledges and thanks all of the presenters and panelists for presenting valuable information and sharing their knowledge. HFTO thanks the moderators and scribes for their preparation and leadership in breakout sessions, and the organizing team for their effort in planning and executing the meeting. HFTO also thanks the participants of the meeting for their engagement in valuable discussion and for providing informative feedback.

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## List of Acronyms

ANL	Argonne National Laboratory		
AST	Accelerated stress test		
BOP	Balance Of Plant		
BPP	Bipolar plate		
ССМ	Catalyst Coated Membrane		
CL	Catalyst Layer		
DOE	U.S. Department of Energy		
EERE	Office of Energy Efficiency and Renewable Energy		
EV	Electric Vehicle		
HER	Hydrogen Evolution Reaction		
HFTO	Hydrogen and Fuel Cell Technologies Office		
H2NEW	Hydrogen from Next-generation Electrolyzers of Water		
LANL	Los Alamos National Laboratory		
LBL	Lawrence Berkley National Laboratory		
MEA	Membrane Electrode Assembly		
MPL	Microporous Layer		
NREL	National Renewable Energy Laboratory		
OEM	Original Equipment Manufacturer		
OER	Oxygen Evolution Reaction		
ORNL	Oak Ridge National Laboratory		
PEM	Proton Exchange Membrane		
PFSA	Perfluorosulfonic acid		
PGM	Platinum Group Metal		
РТЕ	Porous Transport Electrodes		
PTL	Porous Transport Layer		
RDE	Rotating Disk Electrode		
R&D	Research and development		

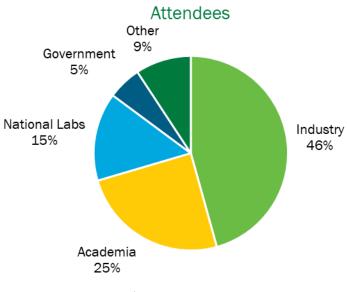
- TOF-SIMS Time-Of-Flight Secondary Ion Mass Spectroscopy
- UTK University of Tennessee, Knoxville

## **Executive Summary**

The U.S. Department of Energy (DOE) Hydrogen Program, led by the Hydrogen and Fuel Cell Technologies Office (HFTO) within the Office of Energy Efficiency and Renewable Energy (EERE) conducts research and development in hydrogen production, delivery, infrastructure, storage, and fuel cells. Hydrogen demonstrates major promise towards reducing  $CO_2$  emissions and increasing energy security through, for example, decarbonizing energy intensive industries and facilitating increased deployment of clean energy on the grid. To accelerate the production of clean hydrogen, DOE announced the Hydrogen Energy Earthshot, the first of several Energy Earthshots. The Hydrogen Shot sets an ambitious yet achievable cost target to accelerate innovations and spur demand of clean hydrogen by reducing its cost by 80% to \$1/kg of hydrogen by 2031.<sup>1</sup>

Production of clean hydrogen by proton exchange membrane (PEM) water electrolyzers is a promising pathway to achieve the Hydrogen Shot goal; however, research and development (R&D) is needed to bring electrolyzer costs down while maintaining or improving efficiency and lifetime. On March 30-31, 2022, HFTO co-hosted a workshop with the Hydrogen from Next-generation Electrolyzers of Water (H2NEW) consortium on Advanced Materials for PEM Electrolyzers. The primary goal of the workshop was to convene stakeholders in order to:

- Identify the status, challenges, and R&D opportunities of PEM electrolyzer materials
- Prioritize R&D opportunities that would yield significant electrolyzer cost reductions and commercialization



• Provide input to the Hydrogen Program's strategy for PEM electrolyzers

Figure 1. Attendance breakdown.

Nearly 700 participants attended the workshop to hear from expert speakers and engage in deep discussions on advanced PEM electrolyzer materials. A range of individuals attended from industry, national laboratories, academia, and government (Figure 1). The first day of the meeting featured expert presentations and a panel discussion to provide an overview of the status of PEM electrolyzer materials from an industrial and R&D perspective. The second day of the workshop involved a series of breakout discussions dedicated to materials for specific cell and stack components. For each session, the goal was to identify the status, challenges, and R&D opportunities for PEM electrolyzer components with a focus on reaching the Hydrogen Shot goal.

Throughout the workshop, attendees focused on the high costs of current materials and the lack of rigorous testing for novel materials. Platinum group metal (PGM) loading reductions for the PEM electrolyzer was the primary focus in multiple sessions. The decreased durability resulting from low PGM loadings and in using advanced materials was also a topic of discussion in many of the sessions. Overcoming these challenges will be key to cost reductions called for by the Hydrogen Shot. Lower costs will enable deployment of PEM electrolyzers at the scale needed to reach the Administration's decarbonization goals.

<sup>&</sup>lt;sup>1</sup> https://www.energy.gov/eere/fuelcells/hydrogen-shot

Key R&D opportunities to develop PEM electrolyzers are based on the challenges identified by participants. These opportunities include developing novel anode and cathode electrocatalysts with a focus on reducing or eliminating PGM content; thinner, more durable, membranes with perfluorosulfonic acid (PFSA) polymers or alternative hydrocarbon materials; new porous transport layer (PTL) structures and coatings and materials development; and novel bipolar plate (BPP) materials and coatings.

Fundamental diagnostic studies to correlate performance with material and interfacial properties and to understand degradation mechanisms are needed. Such studies will inform material development efforts for novel cell and stack components. Material durability is a key metric for determining the industrial potential of materials. Low PGM loadings is correlated with a decrease in durability for electrocatalysts, PTLs, and BPPs. For membrane materials, there is a strong push to develop standard accelerated stress tests (ASTs) to evaluate performance and durability over short times. Particularly for PFSA membranes, current ASTs and designs were developed for fuel cells and would benefit from evaluation from an electrolyzer perspective.

Discussions were also held on other R&D opportunities, such as recycling of materials, particularly BPPs, Ir, and PFSA membranes. Recyclable materials would lead to significant capital cost reductions, and in the case of PFSA membranes, a more environmentally beneficial choice. Along with recyclability, a pipeline of advanced materials to industry should be developed. This pipeline would heavily benefit from the development of standardized testing protocols, as mentioned above. Overall, the key to advanced PEM electrolyzer materials is reducing costs without sacrificing durability or performance.

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## **1** Introduction & Background

As part of the U.S. Department of Energy (DOE) and the Office of Energy Efficiency and Renewable Energy (EERE), the Hydrogen and Fuel Cell Technologies Office (HFTO) leads the Hydrogen Program which enables the development of advanced hydrogen and fuel cell technologies by funding research, development, and demonstration projects. Details on the Hydrogen Program can be found in the most recent Hydrogen Program Plan.<sup>2</sup> HFTO regularly engages with stakeholders to incorporate knowledge from research, industria l, and governmental entities into Hydrogen Program activities.

Proton exchange membrane (PEM) water electrolyzers are a promising pathway for clean hydrogen production. On March 30-31, 2022, HFTO co-hosted a workshop with the Hydrogen from Next-generation Electrolyzers of Water (H2NEW) consortium on Advanced Materials for PEM Electrolyzers. The primary goal of the workshop was to convene stakeholders in order to:

- Identify the status, challenges, and R&D opportunities of PEM electrolyzer materials
- Prioritize R&D opportunities that would yield significant electrolyzer cost reductions and lead to incorporation into commercial products
- Provide input to the Hydrogen Programs strategy for PEM electrolyzers

The input received from workshop participants will be used to help guide the R&D plan for the Hydrogen Program. This workshop included expert presentations and an industry panel followed by eight in depth breakout session discussions to identify the status and R&D opportunities for advanced PEM materials for various cell and stack components. This report summarizes the information gained from these engagements and the presentations and report are available to the public at: <u>https://www.energy.gov/eere/fuelcells/h2-amp-hydrogen-shot-workshop-advanced-materials-pem-electrolyzers</u>

### 1.1 Hydrogen Shot: Accelerating the H2@Scale Vision

The Biden-Harris Administration has made the call for the nation to combat the climate crisis and reach energy goals that accelerate the clean energy transition, with the aim of reducing carbon emissions by 50% by the end of the decade, producing 100% clean energy by 2035, and reaching net-zero carbon emissions by 2050.<sup>3</sup> Hydrogen is a versatile energy carrier that has the potential to help decarbonize many industrial sectors and address global climate issues. To unlock new markets for hydrogen, the cost of clean hydrogen production must be reduced. To address this issue and overall climate goals, DOE announced the Hydrogen Energy Earthshot, the first in a series of Energy Earthshots that set ambitious goals for clean energy technologies. The Hydrogen Shot calls for an 80% reduction in the cost of clean hydrogen production to \$1 for 1 kg in 1 decade.<sup>4</sup> To achieve this cost reduction, R&D efforts on clean hydrogen production technologies are needed.

<sup>&</sup>lt;sup>2</sup> https://www.hydrogen.energy.gov/roadmaps\_vision.html

<sup>&</sup>lt;sup>3</sup> https://www.whitehouse.gov/briefing-room/statements-releases/2021/04/22/fact-sheet-president-biden-sets-2030-greenhouse-gas-pollution-reduction-target-aimed-at-creating-good-paying-union-jobs-and-securing-u-s-leadership-on-clean-energy-technologies/

<sup>&</sup>lt;sup>4</sup> https://www.energy.gov/eere/fuelcells/hydrogen-shot

The Hydrogen Program's H2@Scale vision shown in Figure 2 supports the Hydrogen Shot goal. H2@Scale calls for advancing affordable hydrogen production, transport, storage, and utilization to enable decarbonization and revenue opportunities across multiple sectors. Water electrolysis is a key part of the H2@Scale vision and is a potential production pathway to reach the Hydrogen Shot goal.

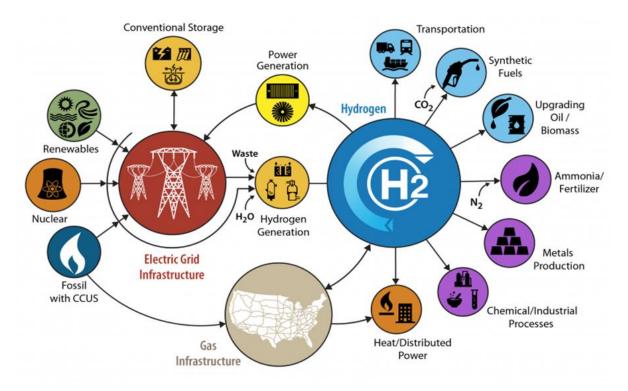


Figure 2. H2@Scale vision to enable decarbonization across multiple sectors of the economy.

### 1.2 Current Hydrogen Program: Electrolyzer Development

The current Hydrogen Program funds research, development, demonstration, and deployment of electrolyzer technologies, among other production pathways to achieve the Hydrogen Shot goal. Water electrolysis is the process of using electricity to electrochemically split water into hydrogen and oxygen. This technology is well known and can produce clean hydrogen when coupled with renewable or nuclear energy sources. Through the Bipartisan Infrastructure Law, \$1 billion in additional funding was announced for a Clean Hydrogen Electrolysis Program. This workshop is one in a series of stakeholder engagement activities to provide input to guide development of the Hydrogen Program's RD&D strategies.

The Hydrogen Program has established several national lab-led consortia to lead R&D on electrolyzer technologies. The H2NEW consortium focuses on R&D for implementation of large-scale electrolyzers, by making them more durable, efficient, and affordable. H2NEW addresses components, materials, integration, and manufacturing R&D to overcome technical barriers and enable manufacturable electrolyzers that meet required cost, durability, and performance targets, simultaneously, to meet the Hydrogen Shot goal. H2NEW focuses on low-temperature and high-temperature electrolyzers, including PEM electrolyzers.

### 1.3 PEM Electrolyzers

PEM electrolyzers use a solid polymer membrane electrolyte that enables high current densities and smaller footprints than commercially available liquid alkaline electrolyzers. The solid membrane also enables pressurized operation which mitigates the need for hydrogen pressurization equipment. The PEM electrolyzer

design is also amenable to fast, dynamic response making it ideal for integration with intermittent electricity production from renewables.

The challenges of this technology include the acidic operating environment which limits the materials and components that can be used. Platinum group metal (PGM) catalysts and coatings are currently used due to their stability in this environment. The currently developed membranes are also limited by the environment and operating requirements. The commercially available membrane used for PEM electrolyzers contains perfluorosulfonic acid (PFSA) polymers, which pose environmental risks at end-of-life. To achieve the Hydrogen Shot goal, significant cost reductions in the materials for PEM electrolyzers must be realized. Key areas for cost reduction are the reduction of PGM loading, new bipolar plate (BPP) and porous transport layer (PTL) materials and coatings, and thinner membranes, all while maintaining or improving durability and performance. This workshop intends to identify the status of PEM electrolyzer materials and identify focus areas for R&D to mitigate these challenges.

## **2** Expert Presentations

Dr. Ned Stetson, the Hydrogen Technologies Program Manager from HFTO, set the context for the workshop by introducing the DOE Hydrogen Program, the Hydrogen Energy Earthshot initiative, and the recent hydrogen-related provisions in the Bipartisan Infrastructure Law. Dr. Stetson covered the pathways to reduce the cost of hydrogen to \$2/kg by 2026, including capital cost reductions, efficiency improvements, and longer stack lifetime.

Dr. Bryan Pivovar is the Director of the H2NEW consortium and oversees NREL's electrolysis and fuel cell R&D. Dr. Pivovar presented technoeconomic analysis for PEM electrolyzer stack costs developed by H2NEW. Historically, federal funding for PEM fuel cells has successfully driven development and cost reduction s and some of these advances have been applied to electrolyzers; however, there is a need for materials designed specifically PEM electrolyzers. To decrease stack costs, R&D should focus on increased efficiency and current density, decreased PGM loading, and scale-up of manufacturing processes that can significantly reduce the stack capital cost. In addition, direct coupling of PEM electrolyzers to renewable energy sources, such as solar and wind, with an optimized operating strategy for the directly coupled system, can impact the cost of hydrogen production. Future systems will need to be designed to withstand the operating strategies required for renewable energy integration. Dr. Pivovar provided an overview of the needs for specific stack components, including catalysts, membranes, PTLs, and BPPs.

Presentation Title	Speaker	Affiliation
Introduction and Overview of Proton Exchange Membrane	Ned Stetson	HFTO
Electrolyzer	Bryan Pivovar	NREL
Overview of Proton Exchange Membrane Electrolyzer Electrocatalysis	Debbie Myers	ANL
Novel Membranes and Ionomers	Michael Hickner	Pennsylvania State University
Porous Transport Layers	Iryna Zenyuk	University of California, Irvine
Performance Coatings for Bipolar Plates	Ton Hurkmans	lonbond

#### Table 1. Expert presentations.

## 2.1 Overview of Proton Exchange Membrane Electrolyzer Electrocatalysis

Dr. Debbie Myers is Deputy Director of H2NEW and the Million Mile Fuel Cell Truck consortia and leads the Hydrogen and Fuel Cell Materials Group at Argonne National Laboratory. Dr. Myers began her talk by providing an overview of low-temperature PEM electrolyzers and discussed oxygen evolution reaction (OER) and hydrogen evolution reaction (HER) catalysts. She mainly focused on the anode catalysts, where the bigger challenges exist today, and where higher OER activity would lead to significant improvement in electrolyzer efficiency. Typically, the electrocatalysts used in PEM electrolyzers contain PGMs with Pt and Ir used for HER and OER, respectively. However, these materials are costly and not easily replaced.

An alternative to the state-of-the-art catalysts would be using low PGM loadings or non-PGM alternatives such as transition metals. For fuel cell applications, reducing the amount of Pt on the cathode oxygen reduction reaction electrocatalyst, either by incorporating supports or development of nanomaterials, has proven effective and should be applied to electrolyzers. Thrifting noble metals like Ir, can lead to diminished performance for OER. In addition, degradation of the anode appears to accelerate degradation in the stack overall, especially under intermittent operation. Performance losses in Ir catalysts are correlated with Ir dissolution. The use of PGM-free catalysts for OER in acidic conditions faces very substantial challenges, especially since transition metals are often oxidized and dissolve at high potentials in acidic conditions.

Research has shown that alloying Ir with metals such as Ru or other metals (e.g., Ti and Sn) can tune the binding energy gap between O<sup>-2</sup> and -OOH during OER, which can increase mass activity of catalysts in order to achieve higher efficiency. However, alloys must also be tested for stability as these materials tend to not be as stable as Ir. Supports for OER catalysts could yield higher performing catalyst layers owing to greater Ir utilization and/or higher electrochemical surface area. Nevertheless, OER catalyst supports must be conductive and stable under the reaction conditions. Ideally, these OER catalyst supports should have favorable electronic interactions with the catalyst itself. Thus far, R&D efforts are focusing on increasing the conductivity of stable transition metal oxides or increasing the stability of conductive supports such as nitrides and carbides.

For electrode structures, ohmic losses in the catalyst layer due to limited mass transport can be significant with thick or high loading electrodes. In contrast, low catalyst loadings and different coating methods can result in different conductivity of the electrode layer and catalyst utilization. Alternative electrode structures, such as the nanostructured thin film electrode developed by 3M, are promising approaches to decrease Ir loading and improve the mass transport within the electrode.

The design of enhanced electrodes relies on understanding how to improve catalyst characteristics, ionomer characteristics, ink properties, and deposition/drying methods. In general, catalysts and electrodes must balance electronic and ionic conductivity, catalytic activity, and wettability for high current density operation, while also being stable over 80,000 hours.

During the Q&A, there were questions about the general advantages of catalyst coated membranes (CCMs) as compared to porous transport electrodes (PTEs). Some advantages are a reduction in cell resistance and adaptability to roll-to-roll manufacturing. The trend of Ir prices was also discussed which included understanding whether the Ir price is cyclical or influenced by short-run inflationary pressures. Generally, it is a combination of factors, and due to being a commodity market, a number of factors are at play.

### 2.2 Novel Membrane and lonomers

Dr. Michael Hickner is a Professor of Material Science and Engineering at Pennsylvania State University, whose research focuses on molecular identity, nanophase structure, and the resulting transport properties in polymeric materials with applications in novel membranes and ionomers. Most PFSA and non-PFSA alternatives have been examined in detail for fuelcells, but limited research has been done for their application in electrolyzers. There are still some challenges to overcome for PEM electrolyzer membranes, which include

high gas crossover, limited fundamental studies around electrolyzer operation and degradation, cost, and improving conductivity. Addressing these limitations could help improve and advance PEM electrolyzers.

Generally, at high current densities, membrane ohmic losses are significant. Reducing membrane areal resistance can make a large impact on efficiency particularly at higher current densities. There is limited opportunity to improve the ionic conductivity of PFSA membranes; therefore, reducing the thickness of the membranes is a more realistic solution. This reduction will require additives, mechanical support, and/or gas recombination layers, in part, to accommodate high differential pressures across the membrane. Thinner membranes have shown high performance, but they also need to demonstrate long lifetimes, which is an active area of research. Measuring F ion release rate is a key metric for evaluating lifetime of the PFSA membranes. Testing of membranes can leverage any overlap with fuel cell development.

Gas recombination catalyst additives can reduce hydrogen crossover through the membrane from the cathode to the anode and can be integrated into the membranes without compromising the cell's performance. Extending the lifetime of thinner PFSA membranes can be addressed by incorporating additives. This method has proved effective for PEM fuel cells, but more studies are needed to identify degradation mechanisms in PEM electrolyzers.

Currently, R&D for non-PFSA membranes is motivated by growing environmental concerns about the manufacturing of fluorinated polymers. Gas crossover tends to be low in non-PFSA membrane. However, there are trade-offs in conductivity, mechanical properties, gas crossover, and water transport, which needs to be studied in-depth. In general, non-PFSA membranes must meet lifetime requirements in order to be implemented in PEM electrolyzers.

During the Q&A, participants discussed considerations for manufacturing in designing new membranes. Dr. Hickner stated that there is a huge manufacturing basis for non-PFSA membranes for water filtration. Therefore, scaling non-PFSA for manufacturing is not a concern. Other questions focused on techniques for ionomers and ionomer inks in the catalyst layer, which was mentioned to still be a challenging process.

## 2.3 Porous Transport Layers

Dr. Iryna Zenyuk is an associate Professor of Chemical and Biomolecular Engineering at University of California, Irvine, whose research focuses on fundamental understanding of coupled transport phenomena and reaction kinetics in electrochemical energy-storage and conversion technologies. Dr. Zenyuk began with an overview of PTLs. Typical PTL materials are Ti based, and come in many morphologies (sintered Ti powder, felts, meshes, etc.). Some of the manufacturing methods of PTLs presented were sintering of Ti, using titanium felt and incorporation of alternative materials. There are several morphological properties and functions that need consideration when designing a PTL. The thickness, porosity, tortuosity, pore-size distribution, and pore connectivity are all metrics that affect PTL performance. Some functions that the PTL serves are water transport, removal of evolved O<sub>2</sub>, electrical conductivity between BPP and the catalyst layer, heat removal, and mechanical support. Controlling the characteristics of PTLs to perform these functions while maintaining durability is key.

When comparing PTLs that are sintered vs. untreated Ti fiber, there is a more uniform in-plane porosity after sintering. Generally, PTLs with non-uniform pore size distribution can result in dead zones where oxygen cannot reach. Sintered PTLs have shown better performance at low currents, but worse or similar performance at higher current densities. It is important to optimize porosity to minimize interfacial contact resistance without limiting mass transport.

There are some advantages for using PTEs instead of CCMs, which include shelf-life and expanded membrane choices. However, some advantages of CCMs are the ease of low catalyst loading deposition and expanded PTL choices. Another method for improving PTLs is incorporating microporous layers (MPLs) to enhance the interface with the catalyst layer by decreasing feature sizes including pore space exposed catalyst layer surface

area. This improved interfacial contact can reduce kinetic overpotential losses of the cell. Overall, wettability can be improved in a cell by tuning MPL and PTL hydrophilicity/hydrophobicity to optimize performance. There is active area of research to optimize the PTL/MPL structure for wettability. Coated stainless steel or other metals can be further explored to replace Ti PTLs and reduce costs, but the coatings will need to be defect-free to avoid corrosion of the metal substrate. MPLs may be particularly useful here to improve performance and efficiency.

PTL degradation can cause an increase in interfacial resistance that results in high overpoten tials. Protective coatings are needed to extend lifetime. Decisions on the choice of material and coating methods affect performance. PGM coatings are commonly used today and are important, particularly with low catalyst loadings. However, PGM loadings of the PTL and catalyst layer need to be minimized to achieve cost reductions.

There has been development in characterizing PTLs, including ASTs for passivation and corrosion to quantify Ti leaching and oxidation rates. Water imaging using neutrons can provide high resolution imaging for inplane directions and low-resolution imaging in through-plane direction. Time-of-flight secondary ion mass spectroscopy (TOF-SIMS) has high sensitivity (up to ppm) and high surface specificity, which can provide depth profile thickness. TOF-SIMS is quicker, easier to analyze multiple regions, and provides 3-D data. It could also provide profiles of oxides species (which allow for differentiation of oxide species), can track evolution of oxide in degradation studies, and detects impurities and contaminants.

There are still challenges that need to be addressed in PTL design. Considerations for PTL designs includes inplane electric conductivity of catalyst layers as catalyst loading is reduced, durability, MPL incorporation to improve contact, and inhomogeneities in the layer. These considerations are based in challenges faced as a result of reducing PTL thickness. Thin membranes will require rigorous PTL design and precision in manufacturing.

During the Q&A, someone asked about the contact resistance due to Ti oxidation by the structure and porosity. It was explained that small increases in oxide thickness at the PTL surfaces can readily increase through-plane resistance 10-100 times. A similar amount of oxidation of the Ti within the bulk has a negligible impact on through-plane conductivity. Carbon PTLs were also addressed, stating that corrosion at anodic potentials made carbon an unsuitable material. A question was posed about identifying the contributions of MPLs. It is difficult to delineate the effect of MPL hydrophilicity in such a heterogenous and uncontrolled environment. There have been studies on the effect of MPL by stacking PTLs, but isolating testing requires free standing MPLs which are not commercially available. For characterizing the influence of the quality of PTL/catalyst layer (CL) interface, X-ray computed tomography can be used to quantify contact area and correlate it to electrochemical surface area.

### 2.4 Bipolar Plates

Ton Hurkmans is the Chief Technology Officer at Ionbond with extensive experience in the thin film coating industry and material science and engineering. Ionbond provides coating services for a wide variety of industries, including automotive, medical, and electrolyzer, using physical and chemical vapor deposition technologies. The motivation to provide coatings for PEM BPPs is in protection from corrosion and hydrogen embrittlement. BPPs represent a substantial fraction of the total cost of the stack and cost reductions in the BPP material or coating could yield significant stack cost reductions.

Ti is the main commercial material for PEM BPPs but is expensive and can suffer from hydrogen embrittlement. Coating BPPs can enhance corrosion resistance and maintain minimal contact resistance over the lifetime of the stack. These coatings must meet 80,000 hr lifetime expectations while withstanding challenging operating conditions, including low pH, oxidizing voltages, and elevated temperatures. The lifetime expectations far outpace requirements of coatings in other industries. In addition, there is a trade-off between high electrical conductivity and corrosion resistance that must be optimized. Dr. Hurkmans illustrated Ionbond coating technologies for BPPs, including one based on DOT<sup>TM</sup> technology that they have licensed, which is a method of sputtering Au and Pt onto a Ti BPP before oxidizing to form a thin TiO<sub>2</sub> layer. Coating development moving forward needs to maximize electrical conductivity while achieving long lifetimes and capital cost reductions.

## **3 Industry Panel**

The industry panel featured representatives from three leading PEM electrolyzer manufacturers: Nel Hydrogen, Plug Power, and Electric Hydrogen. Each panelist provided a brief overview of their company and discussed the status and needs for materials, manufacturing, recycling, and testing.

## 3.1 Nel Hydrogen

Nel Hydrogen is a global company providing solutions for the production, storage, and distribution of hydrogen. Today, they have delivered over 2,700 PEM systems, and have manufacturing production capacity of 150 MW/yr. Dr. Kathy Ayers is Vice President of Research and Development at Nel Hydrogen. She began by highlighting the importance of material design and development for manufacturing at scale with continuous and automated processes. In addition, materials such as membranes and PTLs have been adapted from other fields, and there is an opportunity to design these materials specifically for PEM electrolyzers. To accelerate materials development, electrolyzer original equipment manufacturers (OEMs) should be engaged early on in the development process to demonstrate that the novel material provides a substantial improvement and can be integrated into manufacturing processes. In addition, thrifting of Ir might be used to mitigate volatility in price.

### 3.2 Plug Power

Plug Power is developing hydrogen energy solutions for high growth markets around the world and has an extensive customer base for materials handling units. Dr. Corky Mittelsteadt is Vice President of Electrolyzer Technology at Plug Power, and he began by presenting their 1, 5, and 10 MW systems that are versatile and easily scaled. In addition, Plug Power just opened a GW-scale factory in Rochester, New York. Their 2<sup>nd</sup> generation stack was designed for manufacturability and has enhanced performance and capability with reduced waste generation. Still, electrodes continue to be a dominant cost for their current and projected developments. Plug Power's current baseline for Ir is 0.2 kg/MW. Expanding the supply chain is a challenge facing OEMs today, not just for catalyst material, but for other stack components as well.

### 3.3 Electric Hydrogen

Dr. Nemanja Danilovic is the Director of Cell Development at Electric Hydrogen, which is a rapidly growing company with over 60 employees. They are scaling towards their first demonstration system. Dr. Danilovic echoed the call to design materials, such as membranes, catalysts, catalyst layers, PTL/CL interface, PTLs, and BPPs, specific for electrolyzer operation. In design of these materials, they should be characterized under local operating environments. For components like PTLs, it is important to understand what critical length scales impact performance. In addition, operando characterization of interfaces is important. There is also a need to fundamentally understand the IrO<sub>2</sub> catalyst and determine what the ideal structure and composition is in the local environment of these devices.

### 3.4 Q&A with Industry Panelists

The Q&A session is an opportunity for participants to get the perspective of industry experts on PEM electrolyzer materials. Their answers can help shape material considerations and designs that are relevant for industrial use. The three invited panelists had the following Q&A discussion with participants.

#### What do you see as the most critical material innovations needed to get down to \$1/kg cost target?

For Nel Hydrogen, the CCM is one of the major areas with the potential for performance improvement and capital cost reductions, but the whole stack must be designed to work together effectively. For Plug Power, the catalyst is their priority. Especially when production scales and processing costs decline, raw materials will become most of the cost. However, Ir is projected to not be limiting in the near term. Electric Hydrogen thinks that there is a need to re-design the system without focusing on any specific material costs. Also, the re-design of energy conversion systems should be like electric vehicles (EV), where EVs were re-designed around the battery rather than to try to fit batteries into cars.

## How can we accelerate materials development to commercial implementation? What does industry need to see to have sufficient confidence to move forward with a new component?

Each panelist had different answers for these questions, which included catalyst durability (Plug Power), test development (Electric Hydrogen), and realistic testing (Nel Hydrogen). Catalytic durability is difficult to address due to long test times and highlights the importance of standardized ASTs. When considering new materials, understanding its durability and recyclability is important. This led to the discussion of testing developments, especially to provide confidence in the translation of materials into operating environments. For instance, rotating disk electrode (RDE) tests of new catalyst materials for activity and stability is not sufficient. Therefore, publications without membrane electrode assembly (MEA) testing are interesting but only of limited relevance. Involvement of OEMs early on is also crucial, especially before too much time and effort go into designing new materials.

## Given that future electrolyzers will need to operate dynamically, how do you think variable operation will impact material needs?

Dr. Danilovic stated that it is still important to understand the state of the catalyst under a range of applied voltages in a device. Intermittent duty cycles may depend on the renewables they are coupled with. Also, confirming that ASTs are capturing real degradation mechanisms is important. Dr. Mittelsteadt agreed and is optimistic about Plug Power's stacks' ability to operate dynamically. These stacks can handle cycling, and ASTs have shown that cycling does accelerate degradation. However, knowing how many cycles a stack will really face in its lifetime is crucial. Dr. Ayers also agreed the duty cycles will depend on the energy production it is coupled to, but there is still a need to understand the frequency and noise of that input power source. Modeling and sensitivity analysis is needed and determining whether this should be addressed at the cell or balance of plant (BOP) level in order to get higher power quality from power electronics.

## To what extent should manufacturability and end-of-life/recovery/reuse be thought about during material design?

Dr. Ayers thinks it would be beneficial to decouple manufacturing and recovery, and consider manufacturability upfront to avoid wasted development time and efforts. PGMs might be more straightforward to recover, whereas membranes might be trickier. Dr. Mittelsteadt suggested considering the lifetime of the materials from the very beginning. Plug Power is considering the cradle-to-cradle lifetime of materials. Currently, for Ir, there is not a supply problem, and as demand might increase in the future the supply problem could be addressed by recycling. However, membranes could be more difficult to recycle than Ir. For recovery of electrolyzer units, most customers of Plug Power want the hydrogen, so recovery of the stacks back to OEMs is likely not an issue. For Electric Hydrogen, they foresee an almost completely closed loop for Ir in their processes.

#### What are the most important challenges for DOE to focus PEM electrolyzer R&D on?

Recommendations for DOE for PEM electrolyzer R&D included the development of components at a GW scale, including manufacturing and design studies around how to build and integrate BOP in those systems. With scaling up, BOP starts to dominate the system capital costs. Therefore, it is crucial to work on BOP components too, such as power conditioning at much larger scales. DOE funding will be instrumental for

industry needs, particularly for noncompetitive areas such as hydrogen sensors and alignment of safety standards. Lifecycle of the materials is another area that could use funding. Before scaling is reached it is critical to know the ideal and optimal materials for PEM electrolyzer applications that are to be scaled. For recycling processes, more time and funding on methods, technique development, and modeling for characterization and diagnostics are needed.

## 4 Breakout Sessions

There was a total of 8 breakout sessions, with 4 running concurrently (Table 2). Some of the breakout sessions used MURAL boards<sup>5</sup> (digital whiteboards) to facilitate conversation. Each breakout session had one moderator to guide conversation and one scribe. The breakout sessions covered a range of topics on PEM electrolyzer materials.

Round 1 - Morning Track				
	Novel Low-PGM OER Catalysts	Novel PGM-free OER Catalysts	Advanced PFSA Membranes	Novel PTL and Interface Materials
Moderator	Shaun Alia, NREL	DJ Liu, ANL	Ahmet Kusoglu, LBL	Guido Bender, NREL
Scribe	Julie Forniciari, LBL Angela Macedo, HFTO	Ahmed Farghaly, ANL	Jake Wrubel, NREL	Jason (Keonhag) Lee, LBL
		Round 2 - Afternoon	Track	
	Cathode Improvements	Catalyst Material Discovery & Electrode Structures	PFSA Membrane Alternatives	Bipolar Plates and Coatings
Moderator	Alexey Serov, ORNL	Jacob Spendelow, LANL	Tom Zawodzinski, UTK	Rod Borup, LANL
Scribe	Leiming Hu, NREL	Elliot Padgett, NREL	Eun Joo (Sarah) Park, LANL	James Young, NREL

### 4.1 Novel Low-PGM OER Catalysts

Novel low PGM catalysts for PEM Electrolyzers are a key component in the scale-up and durability of these systems. Reducing the amount of PGMs in the catalyst while maintaining and extending the durability of these systems is key. PEM electrolyzers operate well, but at the expense of very rare and expensive catalysts. Finding ways to eliminate or at least reduce the PGMs is crucial.

Within the breakout session discussion, the aim was to understand the status of the low-PGM catalysts on the market today, the important challenges to address with the current technology, and R&D opportunities that

<sup>&</sup>lt;sup>5</sup> https://www.mural.co/

DOE could support. There were 65 participants with a range of backgrounds, with a large majority of participants being from national labs and industry. All participants were asked to comment on the status of these devices, the challenges, and the R&D opportunities. In general, participation from industry was most prevalent in this session.

#### Status

Low-PGM catalysts have a Ir loading of 0.25 mg/cm<sup>2</sup> in industry but suffers from poor durability in real-world systems. Activity at low loadings can be improved by adding dopants or alloys to Ir or using a support. The typical dopants used are Ru and Pt, among others, though the stability of these materials is not improved as compared to dopant-free catalysts. Many agreed that Ru is a potential Ir replacement exhibiting better activity than Ir for the oxygen evolution reaction, but unfortunately, Ru dissolution has not yet been solved.

Supporting Ir on some sort of metal oxide, like Ti, Sn, or V was discussed as an option that has been explored at the R&D level. Again, unfortunately, the stability suffers from dissolution at high overpotential, and reduced conductivity is seen due to further oxidation in acidic media. However, there are some metal oxide supports discussed from literature that have been shown to maintain or improve stability and conductivity. There was some discussion about the link between structure, geometry, and surface area in determining the conductivity, activity, and stability, but that work has not been translated to industry.

#### Challenges

The challenges with low-PGM catalysts are stability and durability for large, industrial systems and testing methodologies. Many of the participants shared their worries about the Ir supply. The Ir supply is limited, and with the Hydrogen Shot goal in mind, many worry the cost of Ir will keep the electrolyzer cost high. Additionally, recycling and recovery of Ir is a challenge that many participants from industry and academia agreed upon.

Stability and durability were major concerns from the start of the conversation. Many participants shared that there is no standard AST for large systems to help identify degradation mechanisms. Without a standard protocol, identifying the origins of the losses within these larger systems, and relating large system degradation with research scale experiments is a challenge. Additionally, there has yet to be a clear answer on how to overcome the stability issue when dopants or supports are used. This challenge has made it hard to continue the progress and commercialization of these catalysts.

Improving testing methodologies is another challenge. In addition to standardizing the durability tests, the way novel catalysts are tested has some inherent challenges. RDEs are one way to rapidly determine catalyst activity, but integration into MEAs brings additional challenges. Determining the best way to integrate catalysts into the CL, understanding the CL structure, and assuring the activity carries over from the RDE to the MEA is vital. Determining a standard CCM recipe, materials, and testing protocols could help compare these new catalysts more effectively.

#### **R&D** Opportunities

The R&D opportunities for novel low-PGM catalysts include testing standardization; fundamental understanding of the catalyst and supports used; and development of new, stable, and active materials. For standardized testing, it is important to establish ASTs to provide information on the lifetime of novel catalyst systems. Target PGM loadings should be reported as A/g at a high frequency resistance (HFR) free potential (e.g., X A/g @ 1.45 V HFR-free).

With lower PGM loadings, it is important to understand how contaminants effect durability, stability, and activity. It was stressed that advanced testing of catalysts at relevant current densities is crucial to determine conductivity and activity, especially for bridging RDE results to CL structure. Additionally, methods for decoupling voltage and current losses during degradation are needed to identify the origins of instability of new low-PGM catalysts.

For development of stable and active low PGM catalysts, different aspects of supports were discussed in applications to target lower loadings. This includes the use of metaloxides, dopants, and advancements of synthesis methods for coating and atomically dispersing PGM materials on supports, which can help mitigate issues with conductivity, wettability, and adhesion. Also discussed, was the importance of supporting projects for recycling using early technology readiness level (TRL) systems, including more end-of-life modeling of cost projections of recycling or mining Ir.

## 4.2 Novel PGM-free OER Catalysts

The objective of this discussion was to evaluate the current status of PGM-free OER catalysts for PEM electrolyzers and identify the key challenges and future development opportunities. There were 42 participants who attended this breakout session with nine from industry, nine from academia, nine from NationalLabs, and three from government, among those who identified themselves. The participants were asked to provide information from their own perspectives on PGM-free catalyst/material development, as well as projected research needs, given that the research field is nascent at present.

#### Status

The current PGM-free OER catalysts for PEM electrolyzers are mainly derived from metaloxide type materials including Co/Ni/Mn based spinels, oxygen-deficient perovskites, and Ni and Fe oxyhydroxides. The reported performances are limited to RDE experiments with the acidic electrolyte. However, a recent PGM-free OER catalyst developed by ANL has demonstrated a promising high current density of 2 A/cm<sup>2</sup> at 2.4 V in an operating PEM electrolyzer using Nafion 115 membrane.

#### Challenges

The challenges for PGM-free OER catalysts for PEM electrolyzers is multifaceted, including a) activity – PGM-free catalysts at present are less active compared to Ir in specific volumetric and gravimetric current densities; b) conductivity – most of the oxides are deemed non-conductive; c) stability – oxides are deemed soluble in acid and the corrosion at anode catalyst can lead to cross-over of cations to poison the membrane and cathode catalyst.

The slow progress in PGM-free OER catalysts development in recent years can be attributed to the following: a) lack of understanding of the most stable and active phase of materials; b) lack of the connection between fundamental science and applied material development in this space; c) lack of knowledge of the active sites for OER catalysts, and d) lack of demonstration of larger electrolyzers using catalysts that operate at low current density and high efficiency.

#### **R&D** Opportunities

There are opportunities to explore multiple-element novel oxide materials, which have recently shown promising activity and durability. Other high-entropy OER catalyst materials are also promising candidates. We need better understanding of activity and durability through computational studies on active sites and the structure of oxide-based PGM-free catalysts. Combining such studies with the catalyst design/synthesis will accelerate PGM-free OER catalyst deployment.

To accurately screen novel PGM-free materials, we should develop testing matrixes using both RDE and MEA based on performance, durability, and conductivity. High throughput testing will further accelerate development. Modeling of water transport in thick, porous electrodes and PTLs will help determine optimized structures. Development of multi-functional PTLs could maximize performance and durability of electrode structures.

### 4.3 Advanced PFSA Membranes

The objective of this discussion was to identify the greatest needs and gaps in advanced PFSA membranes. There were approximately 50 participants with a relatively even split between industry, academia, and national labs. Participants were asked to discuss the key membrane properties and design parameters leading to the identification of gaps and targets within membrane research for electrolyzers. The session was concluded with a discussion of the R&D needs and opportunities.

#### Status

Nafion, a commercially available PFSA, is the standard ionomer for PEM electrolyzers and is considered the benchmark material. Key membrane properties include conductivity, permeability (hy drogen crossover), morphology, chemical-mechanical durability, and manufacturability. The tunable design parameters which inform these key properties include thickness (directly relevant to crossover and ohmic losses), chemistry (equivalent weight, modifying sidechains, tuning phase-separation), additives (e.g., radical scavengers) or reinforcements for stability, recombination layers (for hydrogen crossover), and mechanical or thermal processing (e.g., heat treatment).

#### Challenges

The major identified challenge was the lack of standard tests and long-term degradation studies designed specifically for electrolyzers. Most tests have been adopted from the fuel cell industry despite the fundamental differences in device operation. The unique assembly techniques, cell architectures, operating conditions, and conditioning procedures need to be adjusted and standardized, especially for high pressure operation. Key topics in long-term degradation studies include the effects of water quality, the durability of recombination layers as well as the effect of other cell components on membrane durability. Other considerations for membrane durability are leaching from metal components, temperature/pressure/voltage cycling, membrane/CL interface degradation with adhesion characterization, and characterization of degradation mechanisms in thinner vs. thicker membranes. Related challenges include correlating fluoride release rate to actual degradation, identifying the role of long-term mechanical effects, and characterization under conditions that reflect operationally relevant temperature, pressure, and time.

There is also a need for designing and carrying out detailed sensitivity studies to probe which membrane properties have the largest impact on device and energy requirements. Moreover, optimization goals must be delineated more clearly, such as (i) selectivity-related objective function for maximizing conductivity while minimizing crossover or (ii) the tradeoff between thickness and hydrogen production efficiency when using recombination layers in thin membranes. Other areas of further research include the interfacial properties between ionomer and support, and other crossover mitigation strategies. In terms of developing new materials, creating new fluoropolymers is not trivial but can be done.

#### **R&D** Opportunities

There are opportunities to develop standardized tests with precise definitions and make use of a round robin process to validate the results. Long-term durability and ASTs are example of tests that should be standardized. Sensitivity studies at laboratory scale to determine which membrane properties have the biggest impacts. To the greatest extent possible, research should work with commercial polymers to mitigate costs. Research should involve new reinforcing strategies, crossover mitigation strategies, and composite materials development. There is an identified need to precisely characterize properties discussed above for novel materials and, to the greatest extent possible, use standardized testing methods. There are opportunities to understand degradation better from a chemistry/characterization perspective to develop mitigation strategies tailored for electrolyzer operation and stressors. Non-PFSA membranes, such as those using block copolymers, have the potential to reduce costs by enabling thinner membranes, lower crossover, and higher temperature operation. Non-PFSA membranes were discussed in more detail in another breakout session, summarized in Section 4.7.

### 4.4 Novel PTL and Interface Materials

A PTL is one of the key components of a PEM electrolyzer. It dictates performance and has the potential to reduce the manufacturing cost of the electrolyzer system. Currently PTLs are fabricated from Ti, one of the only materials that can withstand the oxidizing environment of a PEM electrolyzer. Furthermore, PTLs are

typically coated with a PGM material for effective interfacial contact with the catalyst layer. Cost reduction of PTLs is imperative to further curtail the cost of PEM electrolyzer systems.

The objective of this session was to identify R&D opportunities to advance PTLs with the Hydrogen Shot goal in mind. There were approximately 66 participants in the breakout session with about 1/3 actively participating in the discussion. Participants backgrounds were evenly distributed between industry, academia, and national labs. The discussion was structured into three main parts. First, the current status of PTLs were discussed, in terms of their structure, coating techniques, and manufacturing processes. Then, challenges for cost reduction and performance improvements were discussed. Lastly, participants discussed R&D opportunities on PTL materials and structures that may further improve performance and lower cost with two-time frames in mind: less than five years, and greater than five years.

#### Status

Ti-based PTLs are currently used in electrolyzers in the form either of sintered powder, fiber, or mesh.PTL properties typically range from 250-500  $\mu$ m in thickness, from 30-50% in porosity and from 10-200  $\mu$ m in particle size. Platinum is typically utilized as a protective PTL coating material that improves the contact resistance of the PTL and thus performance and durability. Two main coating techniques are used: (i) electroplating in industrial applications and (ii) physical vapor deposition in R&D applications. Most commercially used PTLs are a single layer with constant porosity and pore structure. Historically, PTLs are adapted from filtration materials, and therefore, architectures, material sizes, thicknesses, and pore structures are limited.

#### Challenges

The main challenges in advancing PTLs are in development of novel PTL structures and materials/coatings while improving electrolyzer performance and reducing cost. The high cost of PTLs stems from the Ti base material and the PGM coating required for high performance and longevity. Moreover, suppliers originate from the filtration industry and do not currently employ production processes at the scale necessary for electrolyzer production scale up. Potential solutions discussed within the group were to find alternatives to Ti as the base material, to identify cost-efficient coating materials and coating techniques, and to optimize mass-production methods. To improve the performance of the electrolyzer, novel PTL structures can be beneficial. Most participants agreed on the need to develop MPL structures that can provide improved interfacial contact and mass transport.

#### **R&D** Opportunities

R&D opportunities were discussed in two timelines, within five years and beyond five years. R&D within five years focused on alternative materials to Ti and PGM coatings; optimization of coating strategies; MPLs and porosity tuning; standardized test development; setting performance and cost targets for PTLs; and recyclability. Standardized test protocols are a common theme addressed in many breakout sessions. Overa ll, the R&D goals for PTLs target reducing the overall cost.

Beyond five years, R&D should focus on optimizing the PTL structure for stability and high electrolyzer activity. Considerations for the manufacturability of PTL materials and structures should also be considered, with high throughput processes, such as roll-to-roll manufacturing, in mind. Understanding of the effects the PTL has on other electrolyzer components, particularly next generation catalysts and electrodes, will be needed.

### 4.5 Cathode Improvements

Cathode improvements are focused on decreasing the amount of PGM loading and potentially implementing PGM-free materials. Considering the bulk of R&D for electrolyzers has focused on anode optimization, R&D on the cathode is critically important for achieving the Hydrogen Shot goal.

The main objective of this breakout session was to identify the status, challenges, and R&D needs for cathodic materials in PEM electrolyzers. In total 32 participants attended the session with a broad range of backgrounds, including catalyst development, design of catalyst layers, and testing protocol development. The participants represented a range of institutions, including national labs (four), academia (two), government (one), and industry (nine). The discussion began by establishing the status of cathodic materials, including catalysts and supports. There was also discussion on designing new cathodic materials for performance and durability, including PGM-free electrocatalysts.

#### Status

PEM electrolyzers use a commercially available Pt/C materials for the cathode, designed for fuel cell application. The participants indicated that there are no significant R&D in development of cathodic catalysts specifically designed for PEM electrolyzers. It was noted, that PGM loading on the cathode side varies in the range of 0.1 to 1 mg Pt/cm<sup>2</sup> and is most commonly supported on high surface area carbon. Non-PGM HER catalyst research effort does exist but needs more experimentation incorporated as part of MEAs. There was consensus that electrode structure and GDL morphology affect cathode quality. However, neither catalyst layer nor GDLs were optimized for electrolyzers. No specific characterization tools have been applied to deconvolute activity and durability losses of cathode from anode electrodes.

#### Challenges

The main challenge in understanding and designing improved catalysts stems from current MEA designs which are optimized for fuel cell operation, not for electrolyzers. An additional challenge is the lack of understanding of the degradation mechanisms on the cathode. Understanding degradation mechanisms guide the design of novel, improved cathodic catalysts. Considerations for catalyst design include, adjusting PGM catalyst particle size, changing the support material or design, and varying PGM loading on the support. Hydrogen crossover was identified as another challenge, which could be at least partially addressed by using new types of cathodic catalysts in combination with re-designed catalyst layers. Another challenge which can be resolved using improved cathodic catalyst structures is water removal from downstream hydrogen gas. By keeping water near the membrane interface, it is possible to produce a dry hydrogen stream and eliminate additional drying BOP components. The group discussed the challenges related to reuse and recycling the cathodic electrocatalysts and agreed that there is currently no significant ongoing effort in this topic area.

#### **R&D** opportunities

The R&D opportunities focused on the challenges discussed above. There is an opportunity to develop electrolyzer characterization methods to decouple cathodic catalyst activity and durability from anodic processes. Fundamental understandings of the degradation mechanism and factors that affect durability are areas that needs R&D. From degradation data, degradation stressors for AST and advanced diagnostics tools specifically for the cathode can be developed. New catalyst designs for high activity, durability, and low PGM content is an area of ongoing development to replace the current catalyst. This is of particular importance considering that current commercial catalysts have been designed for fuel cell operation.

From a stack perspective, understanding the effect of hydrogen crossover will determine CLs needed to improve system durability. GDL or CL optimization for better hydrogen removal, including gradient CL structures are materials to be developed. There is an opportunity to design novel supports with lower hydrogen transport resistance and tuned hydrophilic/hydrophobic properties.

There is a lack of effort to transition novel materials from lab synthesis to industry. This pipeline is also key to considering manufacturability in choosing materials. Along with manufacturability, there is an opportunity to develop novel methods for reuse and recycling of cathodic materials. This will be particularly important if PGM materials are used.

### 4.6 Catalyst Material Discovery & Electrode Structures

Slow OER kinetics are the largest source of overpotential in PEM electrolyzers under typical operating conditions. Additionally, Ir-based OER catalysts are a high-cost stack component due to scarcity. Limited durability of OER catalysts at low electrode loadings is a barrier to widespread deployment, while lack of effective catalyst supports and poor understanding of the role of electrode structure continue to limit development.

The objective of this session was to identify status, key challenges, critical knowledge gaps, and priority R&D areas for PEM electrolyzer anode catalysts and electrodes. The discussion covered Ir-based catalysts, as well as prospects for alternative PGM and PGM-free catalysts. There were approximately 80 participants in the breakout with representation from industry, academia, and national labs.

#### Status

Ir is currently the only viable OER catalyst for PEM electrolyzers. Most commercial OER catalysts are based on unsupported Ir or IrO<sub>2</sub>, although Ir-based catalysts with TiO<sub>2</sub> supports are available. The benefits of existing commercial OER catalyst supports beyond serving as a filler material have not been well established. While Ru-containing catalysts, including IrRu alloys, are a topic of investigation, current materials are unsuitable due to rapid leaching of Ru. Pt has similar or superior stability compared to Ir under PEM electrolyzer anodic conditions, although relatively poor OER activity. For this reason, Pt is currently used for coating anodic PTLs and BPPs. In a scenario in which clean electricity becomes extremely inexpensive, such that capital cost becomes much more important than energy efficiency, Pt could potentially become a lower-cost and more abundant replacement for Ir, However, in the timeframe considered by the Hydrogen Shot, such a scenario is unlikely, although using Pt as a support with Ir is likely viable. Current PGM-free catalysts for OER are severely limited in their stability and can cause degradation of other cell components through dissolution. Current PGM-free catalysts also have OER kinetic overpotentials several hundred mV higher than those of Irbased catalysts.

Current electrode structures are typically fabricated by deposition of catalyst inks (Ir or IrO<sub>2</sub>) and PFSA ionomer. Understanding of the relationship between ink properties, deposition methods, and the resulting electrode structure is limited. In particular, the role of ionomer is not well understood. The ionomer serves as a binder and facilitates proton transport but may also have deleterious effects associated with blockage of active sites or obstruction of electron transport. The role of electrode structure in controlling transport, including two-phase transport in the presence of oxygen bubbles, is poorly understood, as is the severity of the various transport limitations (protons, electrons, water, oxygen, heat). The role of electrode porosity and pore size distribution, as well as effects of catalyst and support morphology on these properties, are also poorly understood. Alternative electrode structures including nanostructured thin films and coaxial nanowire electrodes have been demonstrated to be competitive with existing structures, but rigorous analysis and comparison of these alternative structures is needed.

#### Challenges

The key challenges are associated with durability, performance, and cost. Current viable catalysts are limited to Ir, creating vulnerability to Ir price shocks and posing potential problems due to the low earth abundance of Ir. High Ir loadings (typically >0.4 mg/cm<sup>2</sup>) are required to provide sufficient performance and durability. Low loadings lead to Ir degradation and affect CL continuity and conductivity which limit catalyst utilization and performance. Intermittent and dynamic operation accelerates catalyst and electrode degradation, presenting a challenge for use of low-cost renewable power. OER kinetic overpotentials are a major factor limiting electrolyzer performance and efficiency. Ru is known to have higher OER kinetics than Ir, but Ru has extremely poor durability.

A lack of suitable supports and limited understanding of how to design and manufacture effective electrode's performance continues to limit progress. The understanding of degradation mechanisms, and of understanding of how catalyst composition, morphology, and electrode structure control OER kinetics and degradation rates,

are insufficient. QA/QC in catalyst synthesis for both novel catalysts and batch-to-batch variation in commercial catalysts is poor. Standardization and reproducibility of testing between laboratories has not been firmly established. Testing is limited by a lack of harmonized ASTs and other test protocols. Validation of ASTs to verify that they accurately represent real-world degradation mechanisms and can effectively predict lifetime will be critical.

#### **R&D** Opportunities

For catalysts, there is an opportunity to improve durability of Ir and IrO<sub>2</sub> by control of morphology, size, and doping/alloying, particularly for catalysts with low PGM loading. Development of strategies for stabilization of Ru is a high-risk research area as a potential replacement for Ir. Pt-based materials may also be a candidate either as a catalyst or electrode additive. The relatively poor OER activity of Pt may lim it the applications to those that do not prioritize efficiency. However, the high stability and conductivity of Pt may present opportunities to develop Pt-based supports or electrode additives. Some participants felt that IrO<sub>2</sub> is the only material with suitable activity/durability for OER in PEM electrolyzers, while other participants thought that further work on improving OER kinetics using non-Ir components should be pursued. If stable/active PGM-free catalysts can be identified, a realistic timeframe for R&D leading to deployment is >10 years. One comment from the discussion was that this would not be relevant to 2030 targets but may be relevant for 2050 targets.

While working to improve catalyst materials, improvement in understanding of IrO<sub>2</sub> degradation mechanisms (including theory-based), with development of validated ASTs can create a feedback loop to further improve catalyst and support designs. For supports research focus areas include improved electronic conductivity, catalyst utilization, electrode pore structure, Ir dispersion, and catalyst-support interactions.

There are opportunities to develop alternative electrode architectures that could transcend current limitations on transport, performance, and durability. Understanding how ink properties and deposition methods control electrode structure and catalyst utilization and how electrode structure controls mass, charge, and heat transport are areas that would benefit from research. There is limited understanding of bubble formation, removal, and development of electrodes that are resistant to bubble entrapment. Improvement in understanding local electrode conditions at relevant testing conditions and how those conditions impact durability will help elucidate degradation mechanisms. This research requires development of characterization capabilities to understand the local environment, including lifetime/degradation changes. As discussed above, the role of ionomers in electrodes is not well understood and will be important for developing PFSA membrane alternatives. Studies of the PTL-electrode interface controls performance and durability, and there is research needed on how this interface can be improved.

## 4.7 **PFSA Membrane Alternatives**

The objective of the session was to discuss the status and challenges of PFSA membrane alternatives and identify the research needs and directions. There were 43 participants with a broad range of backgrounds with even representation from national laboratories, academia, and industry. Participants were asked to discuss the advantages and drawbacks of non-PFSA alternative membranes, the most promising alternative materials and structures known today, their potential to meet demands of high current density and intermittent operation, and the research efforts needed and possible R&D opportunities to overcome the current challenges.

#### Status

The commercially available membranes for PEM electrolyzers are PFSAs, but given their environmental impact at the production stage, during device operations, and at end-of-life, the need for non-PFSA alternatives is rapidly growing. The advantages of hydrocarbon-based alternative membranes include low gas permeability (gas recombination layers may not be required), high mechanical stability (less membrane creep than PFSA membranes), better sustainability, increased processing options, and cost-effectiveness. Their reusability and recyclability have not been well investigated.

Non-PFSA membranes cover a broad range of polymer structures, designs, and construction possibilities. We note that there is a near total lack of detailed study of the durability of such materials, even in the context of fuel cells. Thus, what follows are to be taken as intuitive guesses rather than evaluations based on data. A few known materials that may be promising for PEM electrolyzers include polyaromatics, copolymers, aliphatic polymers, and hybrid hydrocarbon-fluoropolymers. Polyaromatics and hybrid hydrocarbon-fluoropolymers have the potential to form thin membranes with high modulus, low gas crossover, and decent proton conductivity, but their oxidative stability varies depending on the backbone structure. Aliphatic polymers have high oxidative stability and high elongation properties, but their thermal stability is questionable. In addition to the base polymer, the reinforced or composite membranes are also of significant interest given the pressure differentials in the cells. Due to the limited experimental data available for the use of these materials in PEM electrolyzers, no down selection was made during the discussion.

#### Challenges

The biggest challenge with PFSA membrane alternatives is the lack of investigation to determine their potential. There is no information on the fundamental understanding of the chemical and mechanical membrane degradation mechanisms. There was no discussion on chemical degradation of membranes, due to lack of membrane durability and lifetime testing at high current density and high voltage operation in cells. In addition to chemical stability, mechanical stability, while broadly more understood, still requires significant work. Hydrocarbon-based ionomers and their interaction with electrocatalysts is also unstudied and needs to be addressed to assess MEA performance and durability. Other research gaps include, membrane dry out, mass transport, interface/adhesion characterization, and interaction with other MEA components. In summary, the non-PFSA membrane area for electrolyzers is essentially a blank slate.

#### **R&D** Opportunities

As stated above, non-PFSA membranes are an area where very little research has been conducted, which leaves room for many R&D opportunities. Understanding the membrane environment in an electrolyzer so that appropriate testing protocols are developed is a need. The conductivity, gas permeability, transport properties, and mechanical properties in both a baseline and compressed state, of membranes at relevant operating conditions are membrane properties that are important to determine their potential for PEM electrolyzers. There was consensus that a pipeline from R&D to scaled up synthesis capacity would be useful for getting new membranes into industry.

Any membrane or polymer that is considered needs to be practical, scalable, and cost-effective to synthesize. To understand the synthesis, detailed studies on reinforcement, composite formation, high molecular weight polymer synthesis, flexible cross-linking, and grafting are required. The MEA should be designed with the PEM electrolyzer in mind, while current designs were developed primarily for fuel cells. This includes, characterization of ionomers, MEA fabrication methods, electrode-membrane adhesion, sealing properties, and cell durability.

Fundamental understanding of the underlying chemistry of degradation in electrolyzer-specific conditions is required for novel membrane incorporation. Full cell testing would elucidate the degradation mechanism and allow for development of AST protocols. Once the degradation mechanisms are determined, efforts in MEA, membrane, or electrode design can be made to mitigate degradation. Lastly, the recyclability and processing of any identified novel membranes should be considered.

### 4.8 Bipolar Plates and Coatings

The objective of this session was to discuss the status, challenges, and future developments related to BPPs for PEM electrolyzers. The discussion was similar to discussions of BPPs for fuel cells; however, fuel cells can consider carbon plates and coatings which do not work for electrolyzers due to the electrochemical potential experienced in electrolyzers. The attendees were overwhelmingly from industry.

#### Status

Current, commercial BPPs use a Ti substrate with a thin noble metal coating (either Au or Pt) to maintain low contact resistance, but it should be noted that the costs considered for PEM electrolyzers assume a stainless-steel substrate, which results in a substantially different cost compared to the current commercial reality. There was consensus that baseline costs should consider coated Ti. Current commercial BPPs use a 1-5 mm thick Ti base with Au/Pt coating. BPP flowfield/manifold designs are largely proprietary, and no information was given on their current effectiveness.

#### Challenges

The challenges related to BPPs are primarily related to the cost of the materials and processing/coating costs. The material needs are related to the corrosive electrochemical environment required for PEM electrolyzers. Current metrics for BPPs include resistance, conductivity, corrosion, hydrogen embrittlement, mechanical properties, and cost. The limitations on size for BPPs are based on the availability of companies with equipment to handle coating large parts and the speed at which they can coat them. There is room for improvement in BPP design to improve cell performance. Lowering BPP costs will likely require low-cost materials and processing. Improved designs for BPPs should consider recyclability and thinner plates to decrease cradle-to-cradle costs.

#### **R&D** Opportunities

The R&D opportunities were primarily related to reducing cost of BPP base materials and coatings. The group agreed that there is a lack of understanding of degradation mechanisms, testing protocols, and well-defined targets. R&D needs were categorized under short-term and long-term goals.

Near Term R&D should focus on reducing noble metal requirements for coatings and developing non-noble metal coating alternatives. Additionally, coatings that would enable the use of stainless-steel would allow for significant cost reduction. The degradation mechanisms of BPPs are not well understood. Understating these mechanisms would allow for coating designs to mitigate degradation, particularly in intermittent operation.

Standard ASTs for BPPs and coatings would help screen coating candidate materials for quick integration into industry. Information on flowfield designs is extremely limited due its proprietary nature, but they need to be improved to minimize transport losses. Long-term R&D goals include development of pore-free coatings to enable lower-cost plate materials. New BPP materials could also be developed to avoid coating requirements entirely. Advancement of recycling technologies to allow for direct re-use of BPP would cut costs dramatically. Of these focus areas lowering coating and substrate material costs were considered the highest priority for DOE funding. AST development and manufacturing technique research were lower on the priority list.

## **5** Conclusion

Closing remarks were given by Ned Stetson, HFTO. He thanked presenters, attendees, organizers, moderators, and scribes for their valuable contributions. Participants gave positive feedback on the workshop and were appreciative of the opportunity to participate in the informative and engaging event.

The workshop achieved its objective to identify the status of PEM electrolyzer materials and identify focus areas for R&D to mitigate these challenges. There were high level and valuable discussions on the status, challenges, and R&D opportunities for novel low-PGM and PGM-free electrocatalysts; PFSA and PFSA alternative membranes; BPPs and coatings; PTLs; and interface materials. Topics that encouraged the most discussion were the need for standardization of characterization and measurements, development of joint facilities for ASTs, the development of recycling for PGM materials, and the importance of working together to reach everyone's common goals. Together, the presentations and breakout discussions will allow DOE to better understand the various challenges and opportunities to achieve the Hydrogen Shot goal.

## Appendix: Meeting Agenda

# **Day 1:** Expert Presentations & Panels (*Q&A to follow each individual session*)

11:00 AM	Welcome, Context, & Overview of Workshop Goals Speaker: Dr. Sunita Satyapal & Dr. Ned Stetson, DOE HFTO		
11:15 AM	Component/System Overview & Technoeconomic Analysis Speaker: Dr. Bryan Pivovar, H2NEW		
12:00 PM	Current Status and Needs: Advanced PEM Materials (Industry Panel) Dr. Kathy Ayers, Nel Hydrogen Dr. Corky Mittelsteadt, Plug Power Dr. Nemanja Danilovic, Electric Hydrogen		
1:00 PM	Networking Break		
1:45 PM	Low-PGM/PGM-free Catalysts and Novel Supports Speaker: Dr. Debbie Myers, Argonne National Lab		
2:30 PM	Novel Membranes & Ionomers Speaker: Prof. Mike Hickner, Pennsylvania State University		
3:15 PM	Porous Transport Layers Speaker: Prof. Iryna Zenyuk, University of California, Irvine		
3:45 PM	<b>Bipolar Plates</b> Speaker: Dr. Ton Hurkmans, Ionbond		
4:15 PM	Wrap-up and Adjourn		

11:00 AM	Welcome			
Round 1 11:15 AM - 12:45 PM	Novel Low-PGM OER Catalysts	Novel PGM-free OER Catalysts	Advanced PFSA Membranes	Novel PTL and Interface Materials
12:45-1:15 PM	Break			
1:15-2:00 PM	Report-Out			
Round 2 2:00-3:30 PM	Cathode Improvements	Catalyst Material Discovery & Electrode Structures	PFSA Membrane Alternatives	Bipolar Plates and Coatings
3:30-4:00 PM	Break			
4:00-4:45 PM	Report-Out			
4:45 PM	Wrap-Up and Adjourn			

## Day 2: Break-out Discussions

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