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Advanced Water Splitting Materials Workshop Report

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HydroGEN Advanced Water Splitting Materials

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Preface

This report serves as the proceedings of the Advanced Water Splitting Materials (AWSM) Workshop held by the U.S. Department of Energy's (DOE's) Fuel Cell Technologies Office (FCTO) on April 14-15, 2016 at Stanford University in Palo Alto, CA. More than 120 experts and stakeholders from academia, government, and industry met at the workshop to share up-to-date information on advanced technologies for producing hydrogen from water using renewable energy sources, including the pathways of high- and low-temperature electrolysis, direct photoelectrochemical (PEC) water splitting, and solar thermochemical (STCH) water splitting. Workshop participants were asked to assess the current status of these promising water-splitting approaches, identify the key materials-related research challenges and knowledge gaps associated with each, and propose pathways forward for critical materials RD&D to accelerate progress toward commercially-viable, industrial-scale renewable hydrogen production. This report offers a summary of the diverse perspectives and constructive ideas generated by the dedicated individuals who attended the workshop.

Acknowledgements

Special thanks are extended to DOE's Deputy Assistant Secretary for Transportation Reuben Sarkar, FCTO Director Sunita Satyapal, and Arun Majumdar of Stanford University for delivering the opening remarks that inspired and helped frame this workshop.

The workshop organizers also wish to thank Brian James, Amgad Elgowainy, Bryan Pivovar, Frances Houle, and Tony McDaniel who presented informative briefings at the workshop on the status of relevant technologies and key challenges. Organizers further extend their great appreciation to the many individuals who volunteered time and effort to moderate the breakout sessions and prepare breakout session summary reports.

FCTO gratefully acknowledges the valuable ideas and insights contributed by all of the stakeholders who participated in the Advanced Water Splitting Materials Workshop. The willingness of these experts to share their time and knowledge has helped to identify current and emerging opportunities to accelerate the development and deployment of advanced water splitting technologies. These individuals are listed in Appendix A of this report.

Workshop planning and execution were conducted under the organization of Eric Miller, Katie Randolph, David Peterson, and Neha Rustagi (FCTO Federal employees); as well as Benjamin Klahr and Max Lyubovsky (FCTO Research Fellows). Other esteemed members of the workshop organizing committee included Katherine Britton, Maya Minamihara and Adam Weber of the Lawrence Berkeley National Laboratory; Amita Gupta, Olayinka Popoola, and Thomas Jaramillo of Stanford University; and Carlos Gomez of Redhorse Corporation.

DISCLAIMER

Executive Summary

Workshop Overview

On April 14-15, 2016 the U.S. Department of Energy's (DOE's) Fuel Cell Technologies Office (FCTO) conducted a workshop on Advanced Water Splitting Materials for hydrogen production from renewable energy sources. The Workshop was hosted by Lawrence Berkeley National Laboratory, and held on the campus of Stanford University in Palo Alto, CA. More than 120 experts and stakeholders came together in the fields of advanced high-temperature (High-T) and low-temperature (Low-T) electrolysis, as well as photoelectrochemical (PEC) and solar thermochemical (STCH) hydrogen production. The workshop participants were charged with evaluating the current status of these technologies, identifying the most relevant metrics for technology evaluation, and discussing common cross-cutting needs and opportunities in accelerated materials research, development, and deployment (RD&D) that could enable the wide-scale production of renewable hydrogen through advanced water splitting processes. The important stakeholder information gathered at this workshop was compiled by DOE to provide critical guidance in the establishment the HydroGEN Energy Materials Network (EMN) consortium on Advanced Water Splitting Materials for hydrogen production, which is being launched in 2016.

Introductory plenary presentations at the workshop given by Reuben Sarkar, Sunita Satyapal and Eric Miller from DOE, and Arun Majumdar from Stanford University emphasized the importance of renewable hydrogen to improving the sustainability and accelerating deep decarbonization of the global energy sector, and stressed the need for accelerated materials RD&D in advanced water splitting technologies. Additional plenary presentations by Brian James from Strategic Analysis Inc. and Amgad Elgowainy from the Argonne National Laboratory further highlighted challenges and opportunities framed by technoeconomic and lifecycle analyses of different renewable hydrogen production pathways.

Following the plenary session, the remainder of the two day workshop featured four breakout sessions during which experts in Low-T electrolysis, High-T electrolysis, PEC, and STCH independently discussed the current status of their specific technologies along with their most pressing materials RD&D challenges. Each of the breakout sessions was followed by a report-out session which included open discussions of crosscutting challenges and opportunities led by interdisciplinary panels comprised of spokespersons for each of the water-splitting technologies. Specific topic areas of the four breakout sessions were:

- Metrics to characterize and compare system- and component-level performance framed by technoeconomic analysis (TEA) and life cycle analysis (LCA) of each technology;
- Performance, parameters, and metrics for critical functional- and balance-of-plant materials;
- Requirements and design options for benchmarking / demonstration platforms;
- Resource availability and needs for effective EMN consortium in advanced water splitting.

The format and content of the Advanced Water Splitting Materials Workshop, including the plenary sessions, the breakout sessions and the interdisciplinary panel discussion sessions, were specifically designed to spark vigorous engagement among workshop participants and encourage synergistic, cross-technology interactions focused on the future of critical materials RD&D for accelerated development of viable technologies for industrial-scale renewable hydrogen production.

Major Outcomes

Participation among the workshop attendees was considered highly productive. Formal discussions at technology-specific breakouts and cross-cutting panels, as well as informal dialogue throughout the course of the two day event, culminated in positive outcomes with recognition of common goals and priorities, and with paths forward that include expanded collaborative opportunities across all the advanced water splitting research communities. Specific important outcomes included:

- Detailed technoeconomic and greenhouse gas (GHG) emission analyses were highlighted as an important prerequisite for market and industry acceptance.
- Participants stressed that accurate technoeconomic analysis requires a strong understanding of full system requirements for each water-splitting technology, both for specific active components as well as for the overall balance-of-plant (BOP). Materials research needs should be informed by technoeconomic analyses of full systems.
- There was strong consensus on the importance of well-defined materials metrics which are clearly connected to device- and system-level metrics. Progress was made defining new and refining current relevant metrics at the systems and materials level for all technologies.
- Workshop participants emphasized the importance of standardized testing and benchmarking platforms for all of the water splitting technologies. Such platforms are needed at appropriate scales for qualifying materials innovations operating under real-world water-splitting conditions, with standardized measurement and reporting protocols.
- Participants identified numerous opportunities for cross technology collaboration. As examples: common materials challenges and opportunities exist between High-T electrolysis and STCH, including active- and BOP-materials operating under extreme temperatures; catalyst discovery and development needs and opportunities are common to PEC and Low-T electrolysis; and membranes/separations materials research is needed for all technologies.
- Participants appreciated the broad range of technology readiness levels (TRLs) in the water-splitting technologies and embraced opportunities for cross-technology collaboration and knowledge sharing. Critical commercialization experience shared by the higher-TRL technologies and innovative materials research from the lower-TRL technologies, are all necessary for accelerating development and deployment of practical renewable hydrogen production from advanced water-splitting.
- There was widespread consensus that forums are needed which encourage and support collaborative interaction among the materials research efforts in all the advanced water-splitting technologies. An accessible platform facilitating collaboration and information sharing was highly recommended.

The workshop outcomes represent an important step in the necessary coordination of experts across all the water splitting technologies toward the common goal of commercialized large-scale renewable hydrogen production. The insightful feedback gathered from the workshop is providing critical guidance to DOE in its establishment of the HydroGEN EMN consortium on Advanced Water Splitting Materials.

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Introduction

The Advanced Water Splitting Materials (AWSM) Workshop, held at Stanford University in Palo Alto, California on April 14th and 15th, 2016, was organized by the Fuel Cell Technologies Office (FCTO) at the Department of Energy's (DOE) Office of Energy Efficiency and Renewable Energy (EERE). The workshop goal was to foster stakeholder engagement in materials research, development, and demonstration (RD&D) relevant to renewable hydrogen production technologies based on water splitting. The broad FCTO mission includes a critical focus on renewable hydrogen, with a renewable hydrogen production RD&D portfolio that is informed by industry, academia, and national laboratory stakeholder input and feedback. Workshops such as the AWSM Workshop are routinely held by FCTO to provide a convenient venue for collecting such input and feedback.

The ASM Workshop was specifically held to elicit stakeholder feedback that could guide FCTO in its development of an Energy Materials Network[1] (EMN) consortium on advanced water splitting materials (the HydroGEN consortium). More than 120 experts and stakeholders from academia, government, and industry met at the workshop to share up-to-date information on advanced technologies for producing hydrogen from water using renewable energy sources, including the pathways of high- and low-temperature electrolysis, direct photoelectrochemical (PEC) water splitting, and solar thermochemical (STCH) water splitting. Workshop participants were asked to assess the current status of these promising water-splitting approaches, identify the key materials-related research challenges and knowledge gaps associated with each, and propose pathways forward for critical materials RD&D to accelerate progress toward commercially-viable, industrial-scale renewable hydrogen production.

Introductory plenary presentations at the workshop emphasized the importance of renewable hydrogen to improving the sustainability and accelerating deep de-carbonization of the global energy sector, and stressed the need for accelerated materials RD&D in advanced water splitting technologies. Following the plenary session, the remainder of the two day workshop featured four breakout sessions where experts in Low-T electrolysis, High-T electrolysis, PEC, and STCH independently discussed the current status of their specific technologies along with their most pressing materials RD&D challenges. Each of the breakout sessions was followed by a report-out session which included open discussions of crosscutting challenges and opportunities led by interdisciplinary panels comprised of spokespersons for each of the water-splitting technology disciplines.

The complete AWSM Workshop agenda is included in Appendix B of this report, and the workshop attendee list is included in Appendix C. The aim of the report is to capture the larger themes discussed by the entire group of participants while also providing details on specific technical findings and recommendations. Included in the report are overviews of the plenary session presentations; documentation of discussions and feedback generated during the breakout and report-out sessions; and a summary of major outcomes, recommendations, and envisioned pathways forward in the deployment of the HydroGEN consortium to accelerate materials RD&D in advanced water splitting technologies.

[1] The overarching goal of the DOE EMN initiative is to dramatically decrease the time-to-market for advanced materials that are critical to manufacturing clean energy technologies. Additional information is available at the EMN website: http://energy.gov/eere/energy-materials-network/energy-materials-network.

Plenary Presentations

Plenary presentations were given at the beginning of the AWSM Workshop to highlight the importance of renewable hydrogen and motivate the need for continued fundamental and applied materials research to advance water splitting technologies for clean and sustainable hydrogen production. The full presentations are available at the workshop website.[2] Summaries are included below:

Advanced Water Splitting Materials Workshop Overview

Eric Miller, Program Manager— Hydrogen Production & Delivery, Fuel Cell Technologies Office, EERE, U.S. Department of Energy

Dr. Eric Miller called on workshop attendees to appreciate the importance of establishing a nexus of scientific resources to address the overarching materials-, device-, and system-level research needs in renewable hydrogen production through all the water-splitting pathways. Dr. Miller encouraged stakeholders to engage in open and honest discussion about the current opportunities and challenges in their own work, and to consider the broader benefits of cross-cutting collaboration among experts in all facets of hydrogen production based on advanced water-splitting technologies. He offered the AWSM Workshop as a venue in which experts and stakeholders could openly discuss fundamental materials challenges in the context of practical and scalable systems for renewable hydrogen production, learn from each other, and contribute invaluable feedback to FCTO's efforts to establish the HydroGEN EMN consortium on advanced water splitting materials.

Fuel Cell Technologies Office Overview

Sunita Satyapal, Director, Fuel Cell Technologies Office, EERE, U.S. Department of Energy

Dr. Sunita Satyapal provided an overview of the FCTO portfolio in the research, development and demonstration of hydrogen and fuel cell technologies. She highlighted the significant progress in fuel cell stacks, which have seen a 50% cost reduction since 2006 due to ongoing research efforts; and reported on the recent growth in the fuel cell industry, which has been consistent at ~30% annually since 2010. While much of this growth has been in the stationary power market, the transportation sector is also starting to take off, as evidenced in the commercial fuel cell electrical vehicles on the market today. She emphasized that large-scale renewable hydrogen would be key for meeting long-term greenhouse gas emission reduction goals, and noted that while FCTO investments have reduced the costs of many renewable hydrogen production technologies, such as electrolysis, further performance enhancements and cost reductions are still necessary for renewable pathways to be cost-competitive with the non-renewable reforming of low-cost natural gas. She stressed that fundamental and applied scientific advances are still needed, particularly in the discovery and development of innovative materials systems to improve efficiency and durability while reducing costs; and that establishment of an EMN consortium on advanced water splitting materials would accelerate the necessary RD&D.

[2] http://energy.gov/eere/fuelcells/downloads/advanced-water-splitting-materials-workshop

Technoeconomics of Decarbonization

Arun Majumdar, Stanford University

Dr. Arun Majumdar's presentation delved into the global challenges associated with decarbonizing our energy systems while maintaining economic growth. He highlighted that the global conversation is increasingly focused on the critical need for deep decarbonization, but stressed the importance of economic viability of any emerging technology being introduced for large-scale reduction of CO_2 emissions. He made a compelling case that a growing portfolio of technoeconomically viable alternative energy pathways, which will be needed for reducing atmospheric CO_2, will also inevitably lead to job creation and improved standards of living. In this context, Dr. Majumdar explained that the large-scale production of clean and renewable hydrogen can be a key enabler for significantly reducing carbon emissions across several important energy sectors, including industrial chemicals, transportation fuels, and stationary power. Using fundamental thermodynamic arguments along with technoeconomic reasoning, he presented illustrative case studies detailing how current trends in the cost reduction of renewable electricity coupled with the emergence of new water-splitting technologies could offer cost-competitive solutions for decarbonization through renewable hydrogen in the near future. However, Dr. Majumdar stressed that continued RD&D is still needed, particularly in advanced materials research, to enable efficient, durable and cost-effective water splitting at necessary scales.

The Energy Materials Network: Vision and Deployment

Reuben Sarkar, Deputy Assistant Secretary for Transportation, EERE, U.S. Department of Energy

Deputy Assistant Secretary Sarkar, who has been one of DOE's main champions in establishing the Energy Materials Network (EMN), offered a portrait of the EMN overarching vision to dramatically decrease the time-to-market for advanced materials that are critical to many clean energy technologies. The Deputy Assistant Secretary described his work with FCTO and other EERE Offices over the past year and a half to develop the EMN concept, leveraging founding principles of the 2011 Presidential "Materials Genome Initiative" along with additional guiding pillars based on establishing a network of world-class materials RD&D capabilities with clear points of stakeholder engagement, comprehensive data management resources, and streamlined access facilitated by rapid agreement processes. He detailed how DOE's initial set of EMN pilot consortia are focusing on targeted materials tracks aligned with some of industry's most pressing clean energy materials challenges, including light-weighting, catalysis, and thermal management. He further highlighted the EMN's innovative and comprehensive approach to materials RD&D, which spans materials design and discovery to full scale manufacturing and qualification, and which is laser-focused on addressing market deployment barriers and getting new technologies to market faster. In concluding his enthusiastically-received plenary talk, the Deputy Assistant Secretary unveiled the establishment of the new HydroGEN EMN consortium on advanced water splitting materials for renewable hydrogen production.

Technoeconomic Studies and Cost of Water Splitting

Brian James, Strategic Analysis, Inc.

Mr. Brian James presented an informative overview focused on standard technoeconomic methodologies for analyzing hydrogen production technologies. He described in detail the H2A analysis tool developed by DOE at the National Renewable Energy Lab (NREL), which is a standard discounted cash flow analysis tool for projecting hydrogen costs for a specified production technology based on technology-specific parameters and standardized economic inputs. The presentation highlighted that the advanced water splitting technologies span a range of technology readiness levels (TRLs), which impacts the interpretation of technoeconomic case study results. Mr. James explained that H2A offered a standardized, transparent approach for the analysis and reporting of projected hydrogen production costs, but warned that results from a given technology case study need to be sufficiently qualified by the TRL to avoid inappropriate comparisons of technologies with different TRLs. He emphasized that materials RD&D is needed to accelerate progress in all advanced water splitting technologies, and that cost projections and sensitivity studies are invaluable for identifying and quantifying system-, component- and materials-level metrics to guide research toward meeting long-term cost targets for hydrogen production.

Lifecycle Analysis and GHG Emissions of Water Splitting

Amgad Elgowainy, Argonne National Lab.

Mr. Amgad Elgowainy delivered a thought-provoking presentation spotlighting the importance of lifecycle analysis to assess greenhouse gas emissions, energy use, water use and criteria pollutants as critical factors in addition to technoeconomic costs in energy and vehicle systems, including hydrogen and fuel cell electrical vehicle systems. He provided a comprehensive overview of the publically-available GREET (Greenhouse gases, Regulated Emissions, and Energy use in Transportation) Model, which has been used to analyze the life cycle emissions of many hydrogen production and delivery pathways, specifically in the context of fuel cell electric vehicle applications. The baseline reference he cites is the current incumbent technology for hydrogen production based on steam methane reforming of natural gas which produces on average of 11 kg CO_2 emissions per kg of H_2 produced. Alternative hydrogen production technologies, including advanced water-splitting technologies, have the potential to significantly reduce the CO_2 emissions, but the actual decarbonization benefits need to take into account the full life analysis that includes energy requirements for production as well as the means for delivery to the point of use, for example via gaseous or liquid delivery. The presentation spotlighted the frequent neglect of important life-cycle figures of merit and the need for continued RD&D to address these.

Technical Breakout Sessions

Following the introductory and plenary presentations, four technical breakout sessions were held over the course of the two day AWSM Workshop. Breakout session topics included:

1. *Analytical frameworks for deriving system and component level metrics*
2. *Performance metrics of critical water-splitting materials*
3. *Demonstration platforms for benchmarking innovations in advanced materials*
4. *Capabilities resources for an Advanced Water Splitting Materials EMN consortium*

During each breakout session, workshop participants separated into four sub-groups, each focusing on one of the four technology thrusts: Low-T Electrolysis, High-T Electrolysis, PEC, and STCH. A Moderator and Co-moderator was designated in each sub-group to motivate discussions and document outcomes. Following the breakout sessions, the workshop participants re-assembled in report-out sessions where the Moderators and Co-moderators from each sub-group presented summaries of the major outcomes and discussions from their sessions. Each report-out session was followed by a 'fire side chat' where all the Moderators and Co-moderators formed an interdisciplinary panel which engaged the audience in a brainstorming session on opportunities for technology cross-cutting synergies.

Below are summaries of the outcomes from the four technical breakout sessions, including the main points from each of the report-out presentations and from the follow-on discussions during the cross-technology panel sessions. The full report-out presentation materials have been reformatted for this report, and are included in the tables found in Appendix D.

Breakout session I: Analytical Framework: System and Components Metrics

The *Analytical Framework* breakout session focused on system- and component-level parameters and metrics that can be directly tied to the cost and carbon-emission projections from technoeconomic and lifecycle analyses of the advanced water-splitting hydrogen production technologies. As a motivation for the session, the system- and component- level assessments are seen as providing a useful framework for further determination of advanced materials requirements in each of the technology thrusts. In this breakout session, participants in each technology sub-group were specifically asked to:

- Share information about existing technoeconomic analysis (TEA) and life cycle analysis (LCA) case studies
- Identify standardized processes for technical and economic inputs and assumptions
- Recommend refinements to FCTO Multi Year Research, Development and Demonstration (MYRD&D) plan metrics
- Identify needs for further studies and improved analysis

The overarching discussion question posed to workshop participants for this topic was: *What are the major issues in framing analysis and in system and component metrics?* Summaries of the breakout session outcomes and discussions are included below for each of the technology-specific sub-groups:

Low-T Electrolysis Summary

The Low-T Electrolysis group discussed system and component metrics issues associated with manufacturing and scale up costs. Questions on how TEA can account for supply chain issues, as well as system size and production volume were considered. Metrics related to the transient operation properties of Low-T electrolysis were also discussed, such as dynamic electricity pricing and how to monetize electrolyzer function in electricity grid stabilization. Additionally, metrics related to utilities requirements (water and air purity, electricity quality, etc.) were found to be important.

Major issues in system level technoeconomic and life cycle analysis were identified as:

- Need for improved Design for Manufacturing and Assembly (DFMA) Analysis
- Valuation of TRL and Maturity levels and better understanding of scaling factors used in LCA
- How to quantify costs to increased readiness and scale up size kW → MW → GW
- How to handle dynamic energy pricing? How to quantify benefits like grid stabilization?
- How to quantify value of hydrogen pressure, purity, etc. for varying end users? Value of storage?
- Need to consider Energy return on investment (EROI) metric
- Importance of quantifying CO_2 footprint
- Water implications/availability
- General agreement that as long as low-cost natural gas is a primary energy source, Low-T electrolysis will have difficulties competing economically

Important system metrics that were identified include:

- Unification of system definitions and goals
- Durability characteristics
- Recyclability of parts
- Metrics related to energy intermittency: Slew rate, Start-up-shutdown characteristics, Turn-down ratio
- Metrics for water purity and consumption
- Metrics related to electricity quality and power electronics

Important components metrics that were identified include:

- Metrics related to the cell and stack: Stack efficiency vs. stack costs, open circuit voltage, EIS standards, voltage stability, membrane mechanical strength, diffusion media cost, % H_2O uptake of membranes, PGM loading per hydrogen production rate, and strategic value of non-PGM catalysts, cell voltage drop broken down by component, membrane crossover metrics
- Metrics related to auxiliary system components: separator durability, drier metrics, power rectifying efficiency as a function of duty cycle, hydrogen embrittlement tolerance for components, cycling durability targets

High-T Electrolysis Summary

The High-T Electrolysis group discussed strategies and metrics for integrating the electrolysis systems with heat and power sources, particularly, when using intermittent renewable power sources. How the TEA analysis captures the benefits of providing reversible electrolyzer / fuel cell operating regimes for grid stabilization when operating with intermittent renewable sources was considered important. Also, the critical importance of capital cost and components durability vs. electricity cost in determining cost of hydrogen was discussed.

Major issues in system level technoeconomic and life cycle analyses were identified as:

- Need for H2A analysis for different scenarios for high-T electrolysis, such as nuclear coupled /distributed / industrial, etc.
- Implications of reversible SOEC + SOFC operation / thermal storage / Co-electrolysis

- Critical importance of capital cost analysis in determining levelized cost of hydrogen
- Analysis of current density vs. degradation rate in TEA
- Developing metrics that capture benefits of Hybrid / intermittent operation

Important system metrics that were identified include:

- Cost as a function of performance
- Electricity usage, electricity price vs. efficiency
- CAPEX vs durability
- Intermittent duty cycles characteristics: turn down ramp rate
- Metrics addressing degradation, corrosion, and contaminants
- Metrics should be normalized to operation at 1.5A/cm^2 @ 1.3V, and at pressure,
- System scale, minimum operating pressure
- Maintenance schedule

Important components metrics that were identified include:

- Characterizing thermal gradient, interfaces, mechanical properties, seals
- Developing a standard testing protocol, standard configuration, accelerated testing protocol
- ASR 0.2; 1.5A/cm^2 @1.3V, 3mbar, 0.005 sccm/cm^2-psi, water purity

PEC Summary

The PEC group discussed several studies which examined the viability of PEC using technoeconomic analysis and energy return on investment (EROI) analysis. While preliminary analyses suggest that PEC has the potential to offer financial and energy returns, discussion participants recognized that assumptions with large uncertainties are still used due to the low TRL of the technology and the conceptual nature of system-level designs. It was discussed that standard metrics in stability and performance will aid future analysis, and ensure that researchers are working towards the same goal of pushing the TRL forward. The following specific high-level metrics in need of development and improvement were discussed:

- Product hydrogen purity and pressure for different applications
- Efficiency in terms of KWh/kg-H_2 (in addition to solar-to-hydrogen efficiency)
- Stability testing including accelerated stress testing (AST)
- GHG targets and assessments for PEC
- Protocols for materials compatibility and performance benchmarking

The need for a well-defined hydrogen product was heavily discussed among participants. For example it is important to define hydrogen purity and pressure for any stability or performance metric to be accurately compared between materials and technologies. The required purity and pressure will vary depending on the application. The group discussed that well-defined standardization is needed for system benchmarking with a focus on efficiency and stability. A standardized efficiency metric in terms of KWh of sunlight per kg of H_2 was considered to be useful, since it would allow PEC systems to be easily compared to advanced electrolysis and photovoltaic-electrolysis systems. It was felt that the kWh/kg-H_2 metric would provide added value to the solar-to-hydrogen (STH) metric commonly employed to date.

It was stressed that standards are particularly needed for stability testing and benchmarking. For example, in systems measured with a reference electrode (a 3-electrode configuration), only half of the system can be analyzed and functions as if paired with an ideal counter electrode. This is not representative of how the system would work under real-world conditions since the counter will likely be an imperfect photoanode or photocathode. The community must decide if measurements made with a 3-electrode configuration are valid, or if a 2-electrode system configuration must be used for durability benchmarking. It was also suggested that a standard stability test should simulate diurnal energy source. Standards should also be developed for accelerated stress testing (AST). It was mentioned that the PEC community could learn from the electrolysis community on AST. Standardization efforts were considered relevant for both fundamental research and commercialization purposes.

The group felt that there has not been a thorough study of GHG emissions of the PEC on a grams of GHG per kg H_2 basis. It was acknowledged that this is an important metric that must be analyzed so that the technology can be compared to other technologies including a likely low carbon competitor - steam methane reforming (SMR) with carbon capture, utilization and storage (CCUS).

STCH Summary

As discussed by the STCH group, solar thermochemical hydrogen production involves the use of extremely high temperatures to reduce metal oxides, followed by oxidation with water, which generates hydrogen. STCH cycles that have been studied to date include high-temperature 2-step cycles where high temperature heat (T_{red}>1400˚C) drives an endothermic reaction to reduce a metal oxide, followed by a lower temperature exothermic reaction with steam to re-oxidize the metal and release hydrogen, as well as "hybrid" cycles that use lower temperatures (~850˚C) to reduce materials, followed by an electrolysis step to produce hydrogen and re-oxidize the material.

One of the main challenges identified by the STCH group was the low technology readiness level (TRL) of the field, particularly for high-temperature cycles. Due to the low TRL of high-temperature cycles, it is difficult to predict system-level design and balance-of-plant (BOP) requirements, and accordingly also difficult to estimate the total cost of the system with technoeconomic analysis. Recommended needs for developing better system-level models and metrics include:

- Development of detailed processes, component-level understandings, and component flowsheets
- Better defined system designs (including definition of operating conditions and all balance of plant components)
    - *Moving particle systems*
    - *Fixed bed systems*
    - *Peripherals to reactor and concentrated solar power (CSP) systems (e.g. vacuum pumps, inert gas management, heat exchangers, separations, condensers)*
- Techniques to measure oxygen production accurately and reliably at the pressures expected in STCH cycles ($< 10^{-20}$ atm)
- Practicality of a system operating at oxygen pressures < 10 MPa

The group expressed that solar to hydrogen (STH) efficiency may not be the best metric for this technology, as it may not adequately capture overall cost and the many tradeoffs that occur in different system designs. Additionally, total GHG emissions may not be adequately captured in an efficiency metric, leaving the true energy intensity impact of the technology incompletely characterized. Stakeholders suggested that metrics should be filtered into a handful of overarching parameters which are tied directly to cost and GHG emissions. These parameters should also include the land footprint and water accounting, given the use of the resource as a feedstock.

The group identified a number of other inputs needed in determining total (lifecycle) cost of a plant, including embedded energy (e.g. kg CO_2 required to build plant), consideration of ancillary value (e.g. grid stability), ancillary equipment (e.g. heat pumps), and characterization of production rate over time. Theoretical thermodynamic efficiency, reaction kinetics, and durability of materials need to be understood and measured consistently.

Participants identified several overarching needs for effective research in this field. Foremost, a technology roadmap is necessary to define key areas of research that should be explored. Additionally, standard test protocols need to be established to ensure that the impact of relevant environmental factors, such as sudden cloud cover, are accounted for. Finally, participants recommended that a working group of STCH researchers be established to collaborate on research, and that a computational center be established to enable efficient sharing of research results.

Breakout Session II: Critical Materials: Performance Parameters and Metrics

The system- and component-level parameters and metrics discussed in Breakout Session I provided a framework for developing performance requirements for the key functional- and supporting-materials for the water-splitting technologies. Of particular interest are the thermodynamic, kinetic and structural properties of the crucial active materials, structures and interfaces essential to water splitting; and structural stability, corrosion resistance and cost of key balance-of-system materials. Breakout Session II focused on identification of the critical technology-specific materials necessary to high-efficiency, sustained water splitting, and the most appropriate corresponding performance parameters and metrics for these materials. In this session, participants in each technology sub-group were specifically asked to:

- Identify pathway-specific critical materials (e.g., catalysts, separators, absorbers, heat-transfer media, functional interfaces, balance-of-system materials, etc.)
- Identify appropriate materials metrics and targets tied to overarching TEA and LCA requirements
- Identify critical resource needs in benchmarking materials against metrics

The overarching discussion question posed for this topic was: *What are key issues and needs in improving critical functional and structural materials and performance metrics?* Summaries of the breakout session outcomes and main discussion topics are included below for each technology thrust followed by a summary of the panel discussions that covered topics in both Breakout Session I and Breakout Session II:

Low-T Electrolysis Summary

The Low-T Electrolysis group had vigorous discussions on the details of materials requirements, gaps and R&D required for stack and system improvements. The discussion focused on specific metrics and targets for materials development associated with individual components of PEM electrolysis cells, stacks and systems. It was emphasized that meaningful materials metrics for electrolysis need to include specific details of operating conditions, and that standardization would offer critical benefits.

Major functional materials issues and need were identified as:

- Membrane: Need for a standard tests for conductivity, permeability (<1% product loss, 100 mV at 2 A/cm^2)
- Catalyst: Need standards for: Catalyst activity (2 A/cm^2 <1.6 V IR corrected), Mechanical durability/delamination (<2mV/1000h), RDE standard, Cycling protocol (1.4-2.0 V, < 1mV/5000 cycles).
- MEA: Need for full cell benchmarking; Improved carbon stability on cathode side; Stability on reversal; Freeze tolerance
- Support Materials (Gas Diffusion Layers): Need improved: Pressure drops, Porosity, Hydrophilicity, Conductivity, Interfacial resistances
- Separators/Frames: Need better metrics for: Durability in terms of hydrogen uptake as a function of conditions, Resistance targets, Strength targets, Cost targets, Embrittlement, Oxidation resistance, Traceability
- End Plates: Need for better coatings development to improved durability

Major balance-of-system materials issues and need were identified as:

- Pumps: Efficiency, lifetime, ion shedding
- Rectifiers: Wide band gap power convertor
- Deionizer: Developing in line DI systems
- Drier: Regeneration efficiency, High pressure cyclability
- H_2 Separator: Need for high pressure operation, Mist removal is important
- H_2 in O_2 sensors
- Plastic O_2 resistance
- Replacing 316 SS with lower cost materials
- Standards for materials corrosion measurements
- Standards for inorganic and non-ionic contaminants, way to measure online, and know their impact.

High-T Electrolysis Summary

The High-T Electrolysis group identified a broad range of materials needs associated with all major components of the electrolyzer and the balance of plant. They stressed that due to high-temperature operation requirements particular attention should be paid to material properties and characteristics related to high temperature stability, thermal stress and corrosion resistance for both electrolyzer stack and balance of plant components. Related to the balance of plant, they expressed that advances in power electronic materials are important for lowering overall cost of the electrolysis systems; and advances in thermal storage materials are needed to improve High-T electrolysis operation with intermittent power sources.

Major functional materials issues and need were identified as:

- Electrolyte: superionic conductors, intermediate-temperature ionic conductors, durability under pressure operation
- Electrode: microstructure, catalytic, thermochemical stability, steam stability, microstructure stability, interface, 3D characterization
- Interconnect: coating, corrosion
- Seals: leakage, steam stability
- Operation: pressurized, life time (3-5-10 years)
- Manufacturing: capability, QA/QC
- Benchmark: protocol, ASR, degradation (11mv/1000h @ 1.5A/cm^2)

Major balance-of-system materials issues and need were identified as:

- Heat exchangers, recuperater, steam generator, water treatment, HT tubing, corrosion, sensors, controllers, seals, insulation
- Water purity, AC/DC inverters, power electronics
- High-temperature thermal storage
- System controller / integration

PEC Summary

The PEC group discussion focused on the specific material metrics needs for major functional components of the PEC system. A recurring topics was the challenge of finding materials which were compatible with each other under solar water splitting conditions. An extensive list of absorbers, catalysts, membranes, interfacial layers and back contacts were developed. In the context of compatibility, it was noted that high performance materials of each category were rarely stable under the same conditions (e.g. acidic vs basic, compatible band gaps and positions for tandem absorbers, etc.). New metrics will need to be developed to better identify and design compatible PEC components.

Discussion focused on the following components in need of protocols and benchmarking standards:

- Absorbers (III-V, silicon, earth abundant nitrides, etc.)
- Catalysts (e.g. Oxygen evolution and hydrogen evolution catalysts)
- Membranes (e.g. Nafion, bipolar, block copolymer, etc.)
- Back Contacts (e.g. gold, indium, transparent conducting oxides)
- Balance of Plant (e.g. electrolyte circulation, compression, piping, thermal management, etc.)

There was significant discussion on the challenges of finding suitable catalysts. Specific issues plaguing most catalysts include poisoning, interfacial issues, low pH stability, transparency, photo-corrosion, and low turnover frequencies. It was also noted that there is not a standard method or metric used in the PEC community that defines catalyst performance and stability. Standard catalyst performance and stability metrics will need to be developed in order to advance the TRL of this technology.

Membranes/separators were also a topic of significant discussion. It was expressed that stability metrics for membranes are not well developed to include diurnal solar cycles. Membranes may take hours to achieve a stable concentration gradient throughout, making transient operation a large potential challenge. The tradeoff between H_2 and O_2 gas cross over while maintaining high conductivity is common and may be worth developing a parameter to capture these issues together. Attention and research is still required to develop productive and compatible membranes and separators.

STCH Summary

The STCH discussion identified a number of material characterization needs that should be completed to help identify those materials worth utilizing in future experimentation and small-scale demonstration. It was also suggested that separate targets be set for high-temperature and hybrid-cycle systems, since the two technologies are very different. Parameters they suggested developing standardized metrics and baselines for included:

- Oxidation temperature (e.g. max temperature or delta) to help guide system design
- H_2 yield per mole of H_2O (e.g. < 10 mol H_2O and metal per mol H_2)
- Practical limit for P_{O2}
- Maximum feasible oxidation temperature to consider a material/design (e.g. 1400°C)
- Electrolyzer cell voltage (for hybrid cycle STCH)
- Material durability metrics that account for morphological changes with cycling and are quantified in a configuration that is structurally relevant (e.g. particle, monolith, RPC, etc.).
- Material phase stability
- Oxygen vacancy formation enthalpy

Specific material challenges that were identified during this breakout included:

- Improve the reliability of reliable measurements of thermodynamics and kinetics under high flux conditions.
- Develop PEM membranes that are able to withstand highly acidic environments for the hybrid STCH cycles (hybrid STCH cycles)
- Development of durable catalysts for hybrid sulfuric acid cycles
- Develop materials (e.g. advanced ceramics) that can be used in heat exchangers and are resistant to high-temperature creep

The group also discussed the need to reevaluate the underlying assumptions in the analyses of the STCH technologies and material systems. Suggestions they made included:

- Standardizing the assumptions for embedded energy in the solar concentrators used for STCH cycles; production of these concentrators is also greenhouse gas intensive
- Standardizing assumptions for solar energy production (e.g. global horizontal irradiation and concentration factor)
- Exploring the potential for heat sources other than solar energy.

Panel Discussion following Breakout Sessions I and II:

Following Breakout Sessions I and II the workshop participants reconvened for a report-out session where subgroup Moderators and Co-moderators reported on their main session outcomes, and then formed a cross-technology panel to lead a general discussion on synergies and collaborative opportunities among the advanced water splitting approaches. The panelists were specifically asked to provide thoughts on the following questions:

- *How can we better work across disciplines (analysis, materials research, investment and commercialization) to develop more industrially relevant critical materials metrics?*
- *How can we develop critical materials metrics that can be leveraged across water splitting technologies (Low-T and High-T Electrolysis, PEC, STCH)?*

The panel generally noted that Low-T Electrolysis, High-T Electrolysis, PEC and STCH represent a range of technologies with a wide spectrum of TRL status; and that lower TRL technologies, such as PEC and STCH, can adopt and benefit from system-level developments in the higher TRL electrolysis technologies, and conversely that the higher TRL technologies continue to benefit from fundamental scientific advances being made in across all the water-splitting technology thrusts.

According to the group discussions, general metrics across technologies that should be better defined and quantified include:

- Capital cost per unit of hydrogen produced
- GHG emissions per unit hydrogen
- Efficiency definitions
- Effect of component and system durability on hydrogen cost
- Common hydrogen safety codes and standards
- Development of and assessment of efficacy of education and outreach programs

The panel discussions also suggested that analysis be performed of how new hydrogen production technologies may build into existing hydrogen markets and /or find specific niche applications utilizing advantages of the specific technology. Workshop participants noted that there were common issues affecting the different technologies, and that these issues could provide opportunities for collaboration across hydrogen production technology disciplines. These issues included:

- Catalyst development—lowering PGM loadings and developing PGM free catalysts
- Water purity and water availability issues
- Hydrogen safety and public education issues
- Development of high-T auxiliary materials (e.g. for heat exchangers, insulation) may be common for High-T electrolysis and STCH
- Ways to utilize O_2 to improve process economics may be common between the water splitting technologies

Breakout Session III: Innovative Benchmarking and Demonstration Platforms

Breakout Session III focused on the importance of establishing standardized testing procedures and protocols for each of the advanced water splitting technologies to serve as a benchmarking platform for innovative materials operating under technology-specific water-splitting conditions, and provide a demonstration platform for advancing TRL and MRL to attract potential industry investors. Example features of a viable benchmarking/demonstration platform include:

- Be versatile to accommodate quantification and benchmarking of a wide spectrum of materials innovations
- Be viable in construction, operation & maintenance costs
- Produce hydrogen safely and quantifiably on different demonstration scales of interest to the research community as well as industry stakeholders and potential investors

Prior to Breakout session III, Drs. Bryan Pivovar of NREL, Frances Houle of LBNL and Tony McDaniel of SNL gave short presentations highlighting some current demonstration-platform work in electrolysis, PEC, and STCH, respectively.[3] After the presentations, workshop participants broke out into their technology sub-groups, and they were specifically asked to consider realistic near-term demonstration platforms for advancing TRL and MRL, while also serving as a useful materials benchmarking tool under technology-specific operating conditions. The overarching discussion question posed for this breakout session was: *What are the promising platforms for technology qualification, benchmarking and demonstration?*

Summaries of the breakout session outcomes and main discussion topics are included below for each technology thrust, followed by a summary of the cross-technology panel discussion following this session:

Low-T Electrolysis Summary

Many participants in Low-T Electrolysis group were from the companies commercializing PEM electrolysis systems and were intimately familiar with the needs for technology benchmarking and demonstration. The group identified a progression of three different benchmarking platforms needed to demonstrate performance of various components and subsystems. Initial testing should be done at the bench top scale where fast turnaround tests of the individual materials and components can be performed. Then subscale stacks and systems should be tested at a lab / pilot scale units under realistic operating conditions and integrating the BOP components. Then large, commercial scale demonstration projects would demonstrate full scale stack, integration with full scale power electronics and operation under real world operating environment. The sizes and details of the three benchmarking platforms were identified as follows.

[3] Presentations are available at the Workshop website: http://energy.gov/eere/fuelcells/downloads/advanced-water-splitting-materials-workshop.

Bench top, individual cell platform - 25-100 cm^2

- Example test conditions: Ambient pressure, 80 C, 2 A/cm^2. Need to define standard porous anode materials.
- Catalyst, electrodes, membrane, bi-plates, and porous materials can be evaluated at this level
- Durability: 100's of hour range
- Membrane- in situ testing: Crossover, F- release
- BOP: Sensors

Subscale stacks/systems (1- 10kW)

- Durability: single vs multi-cell, 100-5000 hour
- Delta P : 300 psi
- BOP/Materials: Hydrogen dryers, Gas-phase separators, Pumps
- Power electronics: Size, Input requirements (3-phase 480 VAC)

MW/Sub-MW or Large Format (0.1-1 MW)

- Power Electronics
- Large format cell –stack area

The group also emphasized the importance of developing improved accelerated stress testing (AST) protocols for facilitating the demonstration and qualification of materials innovations that could have major impact on electrolyzer technologies. The AST protocols needs to take into account:

- Catalyst cycling test example: 1.4-2.2 V, 30s @ each 10,000 cycle
- Cell degradation
- Impact of uncontrolled shutdown
- Need understanding of failure mechanism (example: membrane under various operating pressure and temperature)
- Impact of intermittent operation

High-T Electrolysis Summary

The Low-T Electrolysis group, similarly to the High-T Electrolysis group, identified a progression of scale-up steps necessary for verification and demonstration of the technology viability at different scales. Specific relevant scales for demonstration and benchmarking platforms that they identified include:

Component Qualification Platform will include laboratory qualification of the materials and components of the SOEC systems using button cells, short stacks and appropriate BOP components testing set ups. Component qualification platform should prove stack materials, contacts, integration and early manufacture methods. The metrics assessed at Component Qualification scale should include:

- Area Specific Resistance (ASR)
- Components Degradation rates (minimum 2000h testing under realistic duty cycles)
- Polarization curves
- Electrochemical Impedance Spectroscopy (EIS)
- Stack Seal Protocols

Participants felt that more studies were needed to identify and establish standard platform specs and metrics for component qualification scale.

Stack Benchmarking platform will include operating full SOEC stack at ~ 6 kW (4 kg/day H_2 production). The metrics assessed at Stack Benchmarking scale should include:

- Operating SOEC stack under real duty cycles
- Monitoring voltage and temperature distribution
- Proving cells and stack integration/design and seal protocol
- Measuring effective Area Specific Resistance (ASR)
- Demonstrating lifetime (at least 4000 Durability with <1.0%/1000h degradation)
- Scoping manufacturability
- Examining impact of thermal cycling

Demonstration Scale platform should be operating an integrated SOEC system at ~ 60 kW (42 kg/day H_2 production rate). The metrics assessed at demonstration platform should include:

- Demonstrating hydrogen production rate and system efficiency under real duty cycles
- Performance of all subsystems needed at large scale
- Evaluating operation and maintenance requirements
- System durability evaluation
- System cost metric verifications

The tables included in Appendix D shows which different SOEC system attributes can be verified / demonstrated at these 3 different scale demonstration platforms.

Commercial scale installations. There was general agreement in the group that the initial reasonable commercial entry system would be at about 600 kW SOEC (~200kW SOFC), 420 kg H_2/day production scale.

PEC Summary

For the topic of demonstration and demonstration platforms, the PEC group decided it would be instructive to consider two separate categories: (1) platforms for the demonstration and benchmarking of PEC photoelectrode systems based on PV-grade semiconductor materials which have been the focus of considerable recent research activities and have demonstrated the highest solar-to-hydrogen conversion efficiencies to date; and (2) platforms for demonstrating and benchmarking less-developed, potentially lower-cost approaches based for example on new materials, particle reactors, and other innovations. Summaries of discussions on each of these categories are included below:

PV-grade semiconductor material systems

The PEC group discussed a potential platform which could be developed for demonstration. To be significant enough to gain public and investor interest, the PV-grade semiconductor based PEC system should contain the following characteristics:

- 1 m^2 size panel
- >10% efficiency (24 grams H_2/day)
- Operation of at least the order of days

- Able to separate H_2 and O_2
- Able to integrate several types of PEC systems
- Simple design and description

This demonstration has the potential to establish and enhance expectations for PEC in the near to longer term. It was discussed that while high durability will ultimately be needed for investor interest, initial demonstrations which are stable on the order of days, would still be useful to gain public and government support for the technology. Participants also discussed platforms that could be developed for qualification and benchmarking of panel PEC materials systems. Participants discussed that instruments and protocols will need to be developed to analyze the following characteristics of PEC components:

- Reproducibility
- Operation under realistic lighting conditions (spectra, intensity, orientation, diurnal, etc.)
- Quality and quantity of H_2 and O_2
- Durability and degradation
- Capable of accelerated wear testing, different water feeds

New materials and particle-based systems

For Particle PEC Systems, it was acknowledged that a demonstration of a type 1 and type 2 reactor[4] would be extremely useful to generate industry interest. However, since the TRL is lower than panel systems (type 3 and 4), the following issues will likely need to be addressed before a large scale demonstration is developed:

- Successful gas separation for type 1 reaction which by design co-evolves H_2/O_2
- Eliminate back reactions for both type 1 and type 2 reactors
- Continuous evolution of stoichiometric H_2/O_2 under varying pressures and illumination
- Analysis of mass transport for type 2 system

STCH Summary

The STCH group emphasized that test systems needed for STCH cycles differ between high-temperature 2-step cycles and hybrid technologies. Materials for high-temperature 2 step cycles are at a lower TRL, and therefore require platforms to assess durability and thermodynamics and kinetics of the materials themselves, rather than assessing their ability to integrate with balance-of-plant. Relevant aspects that should be captured in a test system include: thermogravimetric analysis, impedance spectroscopy, rapid measurements of oxygen production at extremely low pressures, and performance under high rate of solar flux. Additionally, standard procedures should be developed to assess durability under cycling, and to characterize material structures before and after cycling. The test platform needs to be flexible since the materials and system designs are diverse. The STCH community should consider leveraging testing procedures as well as materials data from the catalyst community. The breakout group suggested the development of user facilities to address these needs. Once the community can demonstrate that the technology can be scaled to megawatt capacities, industry may have an interest in getting involved. The difficulty is what the focus should be on to get to this scale of a demonstration (i.e., can the STCH community focus on a demonstration without considering the requirements of the peripheral components as a way to expedite the time to demonstration?). With this in mind, it was discussed that a virtual platform that used material characterization data combined with engineering models as another way to engage industry.

[4] Reactor Types 1, 2, 3 and 4 nomenclature from the 2009 PEC Technoeconomic Study Report found at: https://www1.eere.energy.gov/hydrogenandfuelcells/pdfs/pec_technoeconomic_analysis.pdf

The hybrid sulfur STCH cycle is at a higher TRL than high-temperature STCH, and several facilities have therefore already been developed to assess the performance of components in this cycle. Existing facilities include:

- Pressurized button cell test facility (PBCTF) to evaluate the performance of catalysts and membranes in electrolyzers
- Bayonet acid reactor to enable decomposition of sulfuric acid and drive electrolysis

These facilities could be valuable to the research community if they are maintained and/or upgraded, and integrated with high-temperature solar receivers and electrolyzers to enable a fully functional system. Remaining challenges with these systems include the susceptibility of PBCTF electrodes to corrosion, and heat transfer within the bayonet acid reactor.

Panel Discussion following Breakout Session III:

The overarching question posed to the panel in the report-out session following the Breakout Session III was: *What general attributes of a scale-up and characterization platform would best engage industry stakeholders for investment and development of water splitting technologies?*

The panel generally noted the cross cutting benefit of lower TRL technologies adopting and incorporating many components and system characterization platforms, practices and performance metrics developed in higher TRL technologies. Also, serious efforts should be taken establish standard performance benchmarking protocols and capabilities which would be invaluable to verification of results prior publicizing or over-selling to the RD&D community.

Panel discussions emphasized that the demonstration and characterization platforms should operate under conditions similar to what would be expected in commercial applications, and stakeholders should work closely with industry to ensure the interests of both parties align to expedite transition to commercially viable products. One of the main goals should be the production of pressurized hydrogen under intermittent operating conditions pertinent to the relevant renewable energy source (e.g. solar, wind) providing the power. Many auxiliary and BOP components can be shared between the technologies and verified in common system characterization platforms.

It was discussed that characterization of new materials should determine early on if achieving durable operation consistent with system durability requirements is likely, before spending significant additional RD&D resources. Several stakeholders expressed that it was important to avoid spending significant sums of funding on systems and materials that result in poor outcomes, suggesting that funding could be redirected toward more promising technologies. There was broad consensus that institutional knowledge gained through RD&D and benchmarking activities is more widely-shared, allowing researchers to understand what has and has not already been explored.

All agreed that system safety issues should be considered early in the design and deployment of any technology characterization platform.

Breakout Session IV: Energy Materials Network Gap and Resource Mapping

The AWSM Workshop was held in preparation for establishment of the DOE HydroGEN EMN Consortium on Advanced Water Splitting Materials to accelerate RD&D of advanced materials and technologies for sustainable production of hydrogen from renewable energy sources. Prior to the breakout sessions on the second day of the workshop, Neha Rustagi from DOE gave an overview of DOE's EMN Initiative, including the general requirements and guiding principles essential to an Energy Materials Network Consortium.[5] Consistent with

[5] Presentations are available at the Workshop website: http://energy.gov/eere/fuelcells/downloads/advanced-water-splitting-materials-workshop.

EMN framework, the HydroGEN Consortium will encompass world-class scientific and technological resources in materials RD&D for the water-splitting technologies, including:

- Theory and computation
- Synthesis and fabrication scale-up
- Screening and characterization
- Data and informatics
- Manufacturing and commercialization

The focus of Breakout Session IV was to survey some of the existing resources that might be appropriate for incorporation into and Advanced Water Splitting Materials EMN Consortium and to identify key gaps in essential capabilities for all of the water-splitting technology thrusts. In this breakout session, the participants in each of the technology sub-group were specifically asked to:

- Populate a resource map of state-of-the-art tools in materials theory, computation, synthesis, characterization, analysis and benchmarking relevant to establishing an advanced water splitting EMN consortium, and developing related FOA topics
- Perform gap analysis of important resources for the EMN consortium

The overarching discussion question posed to participants for this session was: *What are the essential resources for an advanced water splitting materials EMN consortium?* Summaries of the breakout session outcomes and main discussion topics are included below for each technology thrust, followed by a summary of the panel discussions on cross-cutting opportunities:

Low-T Electrolysis Summary

Generally the group concluded that the technology was at higher TRL so resources were needed in developing high volume manufacturing and cost reduction tools. Particular needs were identified as:

- Developing proper tooling database for manufacturing
- Rapid prototyping – additive manufacturing to make a repeatable manufacturing process; Advanced manufacturing for mass production
- Better information around different plastics for BOP, techniques to better characterize compatibility with DI water and pure O_2, Direct Mechanical Testing (DMT) at operating conditions (specific to plastics).
- Capability to manufacturer electrodes at scale (at least sheet size, method translatable)
- Detailed characterization/analysis of components
- Large scale polymer fabrication (membranes and dryers)
- Characterization of membrane material mechanical properties at operating conditions (fully hydrated, relevant pressures and temperatures)
- Hydrogen embrittlement databases
- Electrolysis hardware: standardized hardware available (flow field, gas diffusion media)
- AST protocol, fast paced way to identify materials
- How to measure crossover, what condition?
- Standard test methods for components (corrosion rate in bi-polar plates)

- In-situ characterization capabilities (neutron imaging, x-ray…)
- Quality control in volume manufacturing
- Leveraging fuel cell industry and academia in materials work, creating database for material compatibility, effective contamination, reversible contaminates
- Flow modeling on the anode (fits in CFD modeling)
- Better understanding of degradation mechanisms, e.g., alkaline exchange membrane (AEM)
- More opportunities for scientific exchange/meetings focused on H_20 splitting
- Developing Codes and Standards

High-T Electrolysis Summary

The High-T Electrolysis group identified present day resources available in National Labs and Industry which could be leveraged in an EMN consortia as:

- Materials theory, computational modeling and design (Atomic modeling, CFD modeling, System modeling, Stack microstructure modeling, etc.)
- Materials/Cell/Stack Fabrication and Development (Combinatorial material discovery, Multiple fabrication methods for cells and stacks fabrication, Seals and protective coatings development)
- Button Cell / Single Cell / Short Stack testing (extensive capabilities at INL, PNNL)
- Stack testing / Demonstration / BOP (extensive capabilities at INL, PNNL, Ceramatec)
- Broad range of techniques available in materials characterization.

During the breakout session, the group prepare a more detailed and comprehensive list of potential resources that could be developed into useful EMN resource capabilities. This detailed list is available in the tables included in Appendix D.

Specific gaps in available resources were identified as:

- Database of SOA materials performance
- Computational predictive modeling for SOEC type materials particularly operating at lower temperatures
- Models to predict corrosion at high temperature, including the impact of contaminants.
- High throughput testing for screening (current capabilities are limited, or they're available but have not been applied them to solid oxide)
- Preventive coating- effectiveness, long term, other contaminants
- Microstructure evolution with time.
- In-situ analysis under high temperature operation conditions.

PEC Summary

The PEC group identified resources that could be leveraged in an EMN consortia as well as a number of capabilities that could be developed as useful EMN resources:

Theory and Computation:

Resources	Needs
• Band Mapping • Computational spectroscopy • Structure and mechanism (JCAP) • Multi-physics modeling (LLNL, JCAP) • TEA and LCA (NREL, LBL) • Supercomputing infrastructure • Computational spectroscopy	• Ability to predict kinetic and thermodynamic stability (Chemical, mechanical) of materials

Synthesis and scaled up fabrication:

Resources	Needs
• combinatorial synthesis (inkjet - JCAP) • combinatorial thin films (NREL) • plasma spray oxidation • micro plasma jets • spray pyrolysis • sputtering • Process development integration lab (NREL) • methodologies for materials scale up and integration	• spatial ALD (large format) • high throughput process development • high throughput device development

Screening and characterization:

Resources	Needs
• X-ray (SLAC, LBL, ANL) • high throughput characterization • in situ and operando characterization (SLAC, LBL) • Thin film characterization (e.g. TEM, SEM, AFM, etc.) (national labs)	• Quantitative degradation testing (QCM, ICP-MS, X-ray) • Photoelectrode imaging

Data and informatics:

Resources	Needs
• Data and informatics infrastructure • Demonstrated machine learning capabilities for materials optimization	• Network Database (materials, metrics) • Automated data collection (barcodes?) • connecting theory to real work experiments • incorporating historical data

Manufacturing and Commercial:

Resources	Needs
• Roll to roll • High pressure hydrogen experience (SNL) • Risk assessment from hydrogen refueling could be used in PEC systems.	• Leaking/safety testing • sensor systems • commercial advisory board

STCH Summary

The STCH group identified a number of resources and capabilities that are currently available for researchers in solar thermochemical hydrogen production:

Theory and Computation:

Resources	Needs
• System-level design, detailed process modeling to guide materials selection (SNL, NREL, SRNL) • Detailed physics-based and dynamic systems integration modeling of design boundaries, performance, thermal cycling, and stresses	• Models of deactivation of HT decomposition reaction catalysts in sulfurous environment • Validation of DFT for high temperature applications

Synthesis:

Resources	Needs
• PEM membrane industry/community • Bulk material synthesis scale-up	• Application-specific membrane fabrication

Screening and characterization:

Resources	Needs
• National Solar Test Facility (heliostat, falling particle receiver) (SNL) • High flux solar furnace (NREL) • Pressurized button cell test facility for PEM/catalyst characterization and screening (SRNL) • Temporal, chemical, physical testing in H_2SO_4 (SRNL) • Post-mortem analysis; lab-wide characterization (e.g. TEM, SEM, AFM, etc) (national labs) • BOP high-temperature materials qualification • Stagnation flow reactor for cycling and kinetics characterization (SNL)	• Understanding of impact of impurities on catalysts • Thermal cycling of mixed materials in relevant environments

Scale Up and Manufacturing:

Resources	Needs
• Bayonet reactor experience	• Solar process interface design • Commercial perspective for system definition • Joining technologies (mixed materials; ceramics + metals) • Pilot-scale demonstration/testing

The STCH breakout group also identified several resources that may also be accessed through industry and academia, including:

- Synthesis and fabrication of advanced ceramics
- Screening and characterization of advanced material
- Advanced data analytics

Panel Discussion following Breakout session IV:

The overarching question posed to the panel in the report-out session following the Breakout Session IV was: *How can we best create an EMN/MGI "innovation ecosystem" (encompassing theory, experimentation, benchmarking and data analytics) to accelerate commercialization of advanced water splitting technologies for renewable hydrogen production?*

Workshop stakeholders enthusiastically discussed and considered potential resource availabilities for an EMN consortium on Advanced Water Splitting Technologies, weighing both the advantages and challenges of leveraging these resources within such a consortium framework. It was felt that significant appropriate capabilities could be made available at the National Laboratories to facilitate materials RD&D in the primary water splitting technology thrusts, covering a broad spectrum of materials theory, synthesis, characterization, benchmarking, analysis and data management. It was also suggested, though, that there are numerous resources and experts at non-lab institutions that could be extremely useful to the EMN; and there was a lack of clarity on how they could be integrated in the proposed framework.

There was general consensus that forums are needed which encourage and support collaborative interaction among the materials research efforts in all the advanced water-splitting technologies, and that an accessible platform facilitating collaboration and information sharing would offer great benefit. In this context, there was clear support for the establishment and future growth of the EMN Consortium on Advanced Water Splitting Materials.

Major Outcomes

Participation among the workshop attendees was enthusiastic and productive. Formal discussions at technology specific breakouts and cross-cutting panels as well as informal intercommunications throughout the course of the two day event culminated in positive outcomes, with recognition of common goals and priorities, and with paths forward that include expanded collaborative opportunities across all the advanced water splitting research communities. Specific important outcomes included:

- Detailed technoeconomic and greenhouse gas (GHG) emission analyses were highlighted as an important prerequisite for market and industry acceptance.
- Participants stressed that accurate technoeconomic analysis requires a strong understanding of full system requirements for each water-splitting technology, including active components as well as the balance of plant (BOP). Materials research needs should be informed by technoeconomic analyses of full systems including BOP.
- There was strong consensus on the importance of well-defined materials metrics which are clearly connected to device- and system-level metrics. Progress was made defining new and refining current relevant metrics at the systems and materials level for all technologies.
- Workshop participants emphasized the importance of standardized testing and benchmarking platforms for all of the water splitting technologies. Such platforms are needed at appropriate scales for qualifying materials innovations operating under real-world water-splitting conditions, with standardized measurement and reporting protocols.
- Participants identified numerous opportunities for cross technology collaboration. As examples: common materials challenges and opportunities exist between High-T electrolysis and STCH, including active- and BOP materials operating under extreme temperatures; catalyst discovery and development needs and opportunities are common to PEC and Low-T electrolysis; and membranes/separations materials research is needed for all technologies.
- Participants appreciated the broad range technology readiness levels (TRLs) in the water-splitting technologies (with Low-T electrolysis at the highest TRL followed by High-T electrolysis, then PEC and STCH), and embraced the opportunities for cross-technology collaboration and knowledge sharing. Critical commercialization experience shared by the higher-TRL technologies and innovative materials research from the lower-TRL are all necessary for accelerating development and deployment of practical renewable hydrogen production from advanced water-splitting.
- There was widespread consensus that forums are needed which encourage and support collaborative interaction among the materials research efforts in all the advanced water-splitting technologies. An accessible platform facilitating collaboration and information sharing was highly recommended.

The workshop outcomes represent an important step in the necessary coordination and collaboration of experts across all the water splitting technologies toward the common goal of commercialized large-scale renewable hydrogen production. The insightful feedback gathered from the workshop is providing critical guidance to DOE in its establishment of the HydroGEN EMN consortium on Advanced Water Splitting Materials.

Path Forward: the HydroGEN EMN Consortium

The insightful feedback gathered from the workshop is providing critical guidance to DOE in its establishment of an EMN consortium on Advanced Water Splitting Materials. At the end of the AWSM Workshop, "HydroGEN" was unveiled as the name for this consortium. The broad DOE EMN initiative is focused on tackling major barriers to widespread commercialization of clean energy technologies through design, testing, and production of advanced materials. Within the DOE EMN network, the mission of the HydroGEN Consortium will be to accelerate research, development, and deployment of materials for advanced water splitting technologies for sustainable production of hydrogen from renewable energy sources. The main technology thrusts of Low-Temp Electrolysis, High-Temp Electrolysis, PEC and STCH will the core technologies covered by the HydroGEN consortium materials RD&D. An integrated approach including state-of-the-art capabilities in materials theory, synthesis, characterization, benchmarking, analysis and data management, coupled with facilitated access for industry, academia and the national laboratories is expected to be critical to the HydroGEN success.

Appendix A: Acronyms

AE	Advanced electrolysis
AST	Accelerated stress testing
AWSM	Advanced Water Splitting Materials
BOP	Balance of plant
CCUS	Carbon capture, utilization and storage
CO_2	Carbon dioxide
CSP	Concentrated solar power
DFMA	Design for manufacture and assembly
DOE	U.S. Department of Energy
EROI	Energy return on investment
FCEV	Fuel cell electric vehicle
FCTO	Fuel Cell Technologies Office
FOA	Funding opportunity announcement
GDP	Gross domestic product
GHG	Greenhouse gas
GREET	Greenhouse gases, regulated emissions and energy use in transportation
h	hour
H_2	Hydrogen (diatomic)
ICE	Internal combustion engine
IRR	Internal rate of return
kg	Kilogram(s)
kWh	Kilowatt hour
LCA	Life-cycle analysis
LH_2	Liquid hydrogen (diatomic)
MEA	Membrane electrode assembly
MYRD&D	Multi-year research, development and demonstration
NG	Natural gas
O&M	Operations and maintenance

PEC	photoelectrochemisty/photoelectrochemical
PGM	Platinum group metal
PPA	Power purchase agreement
RD&D	Research, development, and demonstration
SMR	Steam methane reforming
SOEC	Solid oxide electrolyzer cell
SOFC	solid oxide fuel cell
STCH	Solar-thermochemical hydrogen
T	Temperature
TEA	Technoeconomic analysis
TRL	Technology readiness level
W (kW, MW,GW)	Watt (kilowatt, megawatt, gigawatt)

Appendix B: Workshop Agenda

Thursday, April 14, 2016		Room
8:00 am	Check-in	Clubhouse Ballroom
Renewable H_2 Production and the Advanced Water Splitting EMN		
8:30 am	Welcome and Mission Overview, Eric Miller, *DOE*	Clubhouse Ballroom
8:40 am	The DOE Hydrogen and Fuel Cells Program, Sunita Satyapal, *DOE*	
8:55 am	Motivational Talk on Renewable Fuels: Former Acting Under Secretary of Energy, Arun Majumdar, *Stanford University*	
9:25 am	Motivational Talk on the Energy Materials Network (EMN): Deputy Assistant Secretary for Transportation, Reuben Sarkar, *DOE*	
9:50 am	Coffee Break	
Framing Analysis for Applied Materials RD&D in Advanced Water Splitting		
10:05 am	Technoeconomic Studies & Overarching H_2 Cost Targets Brian James, *Strategic Analysis Inc.*	Clubhouse Ballroom
10:25 am	Lifecycle Analysis & Overarching GHG Emission Targets Amgad Elgowainy, *Argonne National Lab*	
Breakout Sessions on Framing Analysis and Critical Materials Metrics		
10:45 am	Breakout Sessions Instructions for AE, PEC and STCH Groups	Clubhouse Ballroom
11:00 am	Lunch Pickup / Assemble into AE, PEC & STCH Breakout Groups	
11:30 am	Breakout Session I: Analytical Framework: System and Components Metrics • *Share information about existing TEA and LCA case studies* • *Identify standardized processes for technical and economic inputs and assumptions* • *Recommend refinements to FCTO MYRD&D PLAN metrics* • *Identify needs for further studies and analysis*	Electrolysis: Clubhouse Ballroom PEC: Cardinal Room STCH: Oak East
1:15 pm	Coffee Break	
1:30 pm	Breakout Session II: Critical Materials: Performance Parameters and Metrics • *Identify pathway-specific critical materials (e.g., catalysts, separators, absorbers, heat-transfer media, functional interfaces...)* • *Identify appropriate materials RD&D metrics and targets tied to overarching TEA and LCA requirements* • *Identify critical resource needs in benchmarking materials against metrics*	Electrolysis: Clubhouse Ballroom PEC: Cardinal Room STCH: Oak East
Group Re-assembly and Day One Wrap Up		
3:45 pm	Sessions I & II Report Outs & Panel Discussion of Cross-Cutting Synergies	Clubhouse Ballroom
5:30 pm	Adjourn	

Friday, April 15, 2016		Room
8:00 am	Check-in	Clubhouse Ballroom
Renewable H_2 Production and the Advanced Water Splitting EMN		
8:30 am	EMN Framework Examples, Neha Rustagi, *DOE*	Clubhouse Ballroom
8:50 am	Innovative Demonstration Platforms: Electrolysis: Bryan Pivovar, *NREL* PEC: Frances Houle, *JCAP/LBNL* STCH: Tony McDaniel, *SNL*	
9:20 am	Breakout Session Instructions	
Breakout Session on Demonstration and Benchmarking Platforms		
9:30 am	Breakout Session III: Innovative Benchmarking/Demonstration Platforms • *For each of the three technology areas, suggest a realistic near-term demonstration platforms to: serve as a materials benchmarking tool under technology-specific operating conditions; and provide a pathway for advancing TRL and MRL for attracting potential industry investors*	Electrolysis: Clubhouse Ballroom PEC: Cardinal Room STCH: Oak East
11:00 am	Lunch Pickup and Return to Full Assembly	
11:30 am	Session III Report Outs and Panel Discussion	
Breakout Session on EMN Resource and Gap Mapping		
12:45 pm	Breakout Session IV: EMN Gap & Resource Mapping • *Populate a resource map of state-of-the-art tools in materials theory, computation, synthesis, characterization, analysis and benchmarking relevant to establishing an advanced water splitting EMN consortium, and developing related FOA topics* • *Perform gap analysis of important resources for the EMN consortium*	Electrolysis: Clubhouse Ballroom PEC: Cardinal Room STCH: Oak East
2:30 pm	Coffee Break	
Group Re-assembly and Workshop Wrap Up		
2:45 pm	Session IV Report Outs and Panel Discussion of Synergistic Opportunities	Clubhouse Ballroom
4:00 pm	Wrap-up and Path Forward	
4:30 pm	Adjourn	

Appendix C: Workshop Attendees

Last Name	First Name	Organization
Ager	Joel	LBNL
Ahlborg	Nadia	Stanford University
Alia	Shaun	NREL
Allendorf	Mark	SNL
Ardo	Shane	UC, Irvine
Atwater	Harry	Caltech
Ayers	Katherine	Proton OnSite
Aykol	Muratahan	LBNL
Bhavaraju	Sai	Ceramatec, Inc.
Blum	Monika	University of Nevada
Boardman	Richard	INL
Brennan	Tom	AVP
Britto	Reuben	Stanford
Brosha	Eric	LANL
Cargnello	Matteo	Stanford University
Chakthranont	Pong	Stanford University
Chueh	William	Stanford University
Coda	Matthew	Clark Street Associates
Deutsch	Todd	NREL
Dinh	Huyen	NREL
Dismukes	Charles	Rutgers
Eichman	Josh	NREL
Elangovan	S (Elango)	Ceramatec, Inc.
Elgowainy	Amgad	ANL
Emery	Antoine	Northwestern University
Ermanoski	Ivan	SNL
Gaillard	Nicolas	University of Hawaii
Gao	Yong	SIU
Ginley	David	NREL
Gomez*	Carlos	DOE
Gorensek	Maximilian (Max)	SRNL
Gregoire	John	Caltech
Hamdan	Monjid	Giner, Inc.
Harrison	Kevin	NREL
Hartney	Mark	SLAC
He	Ting	INL
Hellstern	Thomas	Stanford University

Last Name	First Name	Organization
Holladay	Jamie	PNNL
Houle	Frances	LBNL
Hu	Shu	Yale
Hu	Shu	Yale
James	Brian	Strategic Analysis Inc.
Jaramillo	Thomas	Stanford University
King	Laurie	Stanford University
Klahr+	Benjamin	DOE
Kopasz	John	ANL
Lewinski	Krzysztof	3M
Lim	Kipil	Stanford
Lordi	Vincenzo	LLNL
Lyubovsky+	Max	DOE
Ma	Zhiwen	NREL
Majumdar	Arun	Stanford University
McDaniel	Anthony	SNL
McEnaney	Joshua	Stanford University
Mehta	Apurva	SLAC
Miller	James	SNL
Miller+	Eric	DOE
Mills	Michael	DOE
Mittelsteadt	Corky	Giner Inc.
Molter	Trent	Sustainable Innovations, LLC
Mukerjee	Sanjeev	Northeastern University
Mulholland	Gregory	Citrine Informatics
Musgrave	Charles	CU, Boulder
Narkeviciute	Ieva	Stanford University
Nelson	Jeffrey	SNL
O'Brien	James	INL
Ogitsu	Tadashi	LLNL
Osterloh	Frank	UC Davis
Palm	David	Stanford
Partridge	Harry	NASA Ames
Pellow	Matthew	Stanford
Perret	Robert	NTSLLC
Peters	Mike	NREL
Peterson+	David	DOE, FCTO
Petri	Randy	FuelCell Energy Inc
Pivovar	Bryan	NREL

Last Name	First Name	Organization
Prasher	Ravi	LBNL
Randolph+	Katie	DOE
Roemer	Andrew	Proton OnSite
Rustagi+	Neha	DOE
Saleh	Amr	Stanford
Sanders	Michael	Colorado School of Mines
Sarkar	Reuben	DOE
Satyapal	Sunita	DOE
Saur	Genevieve	NREL
Scheffe	Jonathan	University of Florida
Schwartz	David	PARC
Selman	Nancy	Sustainable Innovations, LLC
Shinde	Subhash	SNL
Snedaker	Matthew	LBNL
Sokaras	Dimosthenis	SLAC
Spurgeon	Joshua	U of L
Stechel	Ellen	ASU
Summers	Bill	SRNL
Sunkara	Mahendra	U of L
Tan	Chor Seng	Stanford University
Tang-Kong	Robert	Stanford University
Toma	Francesca	LBNL
Turner	John	NREL
Van Duren	Jeroen	Intermolecular
Van Overmeere	Quentin	PARC
Weber	Adam	LBNL
Weimer	Alan	CU, Boulder
Westlake	Brittany	EPRI
Wipke	Keith	NREL
Wood	Brandon	LLNL
Xiang	Chengxiang(CX)	Caltech
Xu	Hui	Giner Inc.
Yang	Hong	University Of Illinois
Zakutayev	Andriy	NREL
Zheng	Xiaolin	Stanford University
Zhu	Kai	NREL
Zimmerman	Jonathan	SNL

+ Workshop Organizers * Note takers

Appendix D: Breakout Session Tables

Low - T Electrolysis

Break Out Session I:
What are the major issues in framing analysis and system and component metrics?

Reported high level takeaways from breakout group discussion on Technoeconomic Analysis (TEA) and Life Cycle Analysis (LCA) (w/ sensitivity)

TEA
• Design for manufacture and assembly (DFMA) analysis • Valuation of technology readiness level (TRL) or maturity level – How to quantify costs to increase readiness? • Do not understand scaling factors well (currently made on small scale); these costs will be used in LCA calculations. Need for both size kW → MW → GW • How to handle dynamic pricing? How can it be worked into these models? • Ancillary services – How to quantify benefits like stability to grid over large frequencies? • Quantify value of pressure and purity – What is the end use? – Storage related
LCA
• IBID • If natural gas is the electricity source, process doesn't make sense • Energy return on energy invested (EROEI)/energy return on investment (EROI)? • Recyclability of parts? • CO_2 footprint? • Water implications/availability? • DOE targets, \$/kg H_2, stack efficiency, electricity costs, stack costs • Short-term performance – Slew rate – Start-up and shut down – Turn-down ratio

System Definitions and Goals
• Water flow rates needed, dive cycle (intermittency) equivalent for durability • Operating conditions • Durability • H_2O utilization • System response time • Water footprint (water in) • Electrical efficiency, integration with intermittent energy sources • Power conversion costs and efficiency • Durability, reliability (especially constant versus variable load) AST, start-up and shut down time • Turn-down ratio. When giving costs at what volume scale? • Recyclability (scrap value), inlet water needs • Dryer efficiency • Maintenance requirements, outlet pressure. Value waste heat.
Component Definitions and Goals
• Separator durability, hydrogen evolution reaction (HER) under alkaline conditions. • EIS standards, open circuit, operation, slight load? • Creep, voltage stability • Conductivity/permeation ratio, membrane mechanical definitions AST for catalyst, F- tolerance of materials, diffusion media cost (surface area?) hydrogen embrittlement • Cycling durability targets • Percent of H_2 production, rectifying efficiency as function of duty cycle • Active surface area method, RDE testing/definition, MEA durability and ASTs supply and pricing of BP plates, g PGM per kg H_2 • Pressure drop • Dryer metrics • Percent H_2O uptake of membranes, temperature range, gas diffusion layers span wise strength, plate cost, durability and resistivity • \$/kg H_2 how to amortize over time, GM loading/kg H_2, strategic value of non PGM, membrane interfacial resistance • Regeneration protocols, cell voltage drop broken down by component • Crossover targets, standards (how to measure)

Break Out Session II:
What are key issues and needs in improving functional and structural materials performance metrics?

STACK Level

Membrane

- X over <1% product loss
- 100 mV at 2 A/cm^2
- Durability as function of FER 1% per 10,000 hours
- Standard tests for conductivity and permeability
  - Standard conditions?
  - In-situ versus ex-situ

Catalyst

- Loading anode + cathode < 0.5
- 2 A/cm^2 <1.6 V iR Corrected
- <2mV/1000 h
- Cycling protocol needed 1.4-2.0 V, < 1mV/5000 cycles
- Method for active surface area and metric for loss as function of time
- ASTs
- Cost metric in terms of H_2 produced over lifetime
- Mechanical durability/delamination
- Need for standard for catalyst activity
- OER supports
- Tests
  - RDE standard
  - (Glassy carbon) bad
  - Gold?

MEA

- 2A/cm^2 < 1.75 total
- Full cell benchmarking
- Stability on reversal; carbon stability on cathode side
- Freeze tolerance

Support Materials

- Pressure drops
- Porosity
- Pore size
- Hydrophilicity
- Conductivity
- Interfacial resistances

Separators/Frames

- Durability in terms of H_2 uptake; function of conditions
- Resistance targets
- Strength
- Cost
- Embrittlement, Oxidation resistance. Resistance to F-
- Traceability

End Plates

- Bolts and coatings

Standard Conditions

System Level

Pump

- Efficiency, lifetime, ion shedding

Rectifier

- Wide band gap power convertor

Deionizer

- Pump and clean up, needs separate loop, would like in line

Dryer

- Regeneration efficiency
- High pressure cyclibility

Phase Separator

- H_2 separators at high pressure hard to find, including level sensors
- Liquid water (mist) removal is important
- Instrument drift
- H_2 in O_2 sensors
  - Water dependence
- Plastic O_2 resistance
- Replace 316 SS with lower costs
  - Valves, containers, pumps, DI H_2O compatibility, lower cost
- Filters, scrubbers for non-ionic contaminants
- Freeze aspects
- Corrosion measurements
  - ICP, standard
- Inorganic and non-ionic contaminants, way to measure online, and know their impact.

Break Out Session III:
What are the major issues in framing analysis and system and component metrics?

Progression
Bench top cell platform

• 25-100 cm^2
• Example test conditions: ambient pressure, 80C, 2A/cm^2
  - Need to define porous anode materials
• What can be evaluated at this level
  – Catalyst, membrane, bi-plates-, porous materials,
  – Durability: 100's of hour range
  – Membrane- in situ testing: Crossover, F- release
• BOP: Sensors

Subscale stacks/system s (1- 10kW)

• Durability: single vs multi-cell, 100-5000 hour
• Delta P: 300 psi
• BOP/Materials:
  – Hydrogen dryers
  – Gas-phase separators
  – Pumps
  – Power electronics; size, input requirements (3-phase 480 VAC), 250 kW modules

MW/Sub-MW or Large Format (0.1-1MW)
• Power Electronics • Large format cell –stack area
AST needs to defined:
• Catalyst test example: 1.4-2.2V, 30s at each 10,000 cycle • Cell degradation   – Uncontrolled shutdown impact • Need understanding of failure mechanism (example: membrane under various operating conditions – P, T)

Break Out Session IV:
What are the essential resources for an advanced water splitting materials EMN consortium?

Resource Needs

- Better information around different plastics for BoP, techniques to better characterize compatibility with DI water and pure O_2
- Direct Mechanical Testing (DMT) at operating conditions (specific to plastics)
- Capability to manufacturer/fabricate electrodes at scale (at least sheet size, method translatable)
- Detailed characterization/analysis of components post test
- Large scale polymer synthesis (fabrication) (polymer and membrane)
- Membrane material mechanical properties at operating conditions (fully hydrated, relevant pressures and temperatures)
- Hydrogen embrittlement testing
- Electrolysis hardware: standardized hardware available (flow field, gas diffusion media)
- AST protocol, fast paced way to identify material
- How to measure crossover, what condition?
- Standard test methods for components (corrosion rate in bi-polar plates)
- In-situ characterization capabilities (e.g. neutron imaging, X-ray…)
- In-line defects in manufacturing, quality control
- Leveraging FC industry and academia with materials work
- Database for material compatibility, effective contamination, reversible contaminates
- Flow modeling on the anode (fits in CFD modeling)
- Modeling transport & defining descriptors & linkage to test data (inform CFD)
- At higher TRL level so manufacturing. How to get size of manufacturing, is there a tooling database for manufacturing?
- Rapid prototyping – additive manufacturing to make repeatable; Advanced manufacturing for mass production
- Better understanding of degradation mechanisms (e.g. AEM)
- More opportunities to scientific exchange/meetings focusing on H_2O splitting

Capability

- Proton has CFD modeling of porous materials but could be improved at labs
- Giner: membrane crossover at different levels (H_2 sensor, GC…)
- SNL: Hydrogen embrittlement testing

Gaps/Needs

- Reduced cost
- Connection between research and industry
- Insufficient industry participation
- (supply chain engagement)
- Understanding of H_2 interactions (ex. H_2/H_2O mixing/drying, H_2 embrittlement)
- Commercial sensors
- Experienced knowledge in scale-up science-related to electrolyzer materials
- Knowledge of AEM interfacial interactions
- Codes/standards

High - T Electrolysis

Break Out Session I:
What are the major issues in framing analysis and system and component metrics?

System level TEA
• H2A, Nuclear coupled /distributed / industrial • CAPEX – SECA ? • Current density vs. degradation in TEA • Hybrid / intermittent operation • SOEC + SOFC operation / thermal storage / Co-electrolysis
System Metrics
• Electricity usage, electricity price, CAPEX • Intermittent duty cycles, efficiency, ramp rate, degradation, turn down • Degradation, corrosion, migration, contaminants • Operation at 1.5A/cm^2 @ 1.3V, pressure, • Cost as a function of performance • Scale, minimum operating pressure
Components Metrics
• Thermal gradient, thermal management, interfaces, mechanical properties, thermal cycling, stack design, seals • Standard testing protocol, configuration, accelerated testing • ASR 0.2; 1.5A/cm^2 at 1.3V, 3mbar, 0.005 sccm/cm^2-psi, water purity • Maintenance schedule

Break Out Session II:
What are key issues and needs in improving functional and structural materials performance metrics?

Functional Materials
• Electrolyte: superionic conductors, intermediate-temperature ionic conductors, durability under pressure operation • Electrode: microstructure, catalytic, thermochemical stability, steam stability, microstructure stability, interface, 3D characterization • Interconnect: coating, corrosion • Seals: leakage, steam stability • Operation: pressurized, life time (3-5-10) • Manufacturing: capability, QA/QC • Benchmark: protocol, ASR, degradation (11mv/1000h @ 1.5A/cm2)
Structural Materials & BOS
• HEX, recuperater, steam generator, water treatment, high temperature (HT) tubing, corrosion, sensors, controllers, seals, insulation • Water purity, AC/DC, power electronics • HT thermal storage • System controller / integration

Break Out Session III:
What are the major issues in framing analysis and system and component metrics?

Parameter	Tech Qualifications	Benchmark	Demo
1. Purpose/Test Platform	Materials verification & Single Stack Repeat Unit Cell	Stack Module	TRL: 6. Stack plus BOP
2. Instrumentation	heavy	Module intensive	Mass balance
3. Thermal Input	Agnostic (lab power); high precision/control	Agnostic (expensive steam generator, E of NG fired)	Actual waste heat stream
4. Electric input	Expensive programmable power supply	Simulated Hardware in the loop	Actual Solar of wind source
5. H_2 output delivered to			Sent to a buffer tank; prove amenable to subsequent compression step
6. Production: kg H_2 per day (% of Forecourt, 1.5mt/day)			~42 kg/day; (3% of Forecourt), minimum
7. Capacity, kW		~1-2kW SOEC minimum.	~ 60 kW SOEC ; [20kW SOFC], minimum; to 200kW SOEC (70kW SOFC)
8. Key Minimum Conditions	Pressurized	Pressurized	

8. Metrics	ASR, Degradation, V-eff at j; minimum 2000h degradation characterized. Platform proves materials, and early manufacture methods. Real IC materials, cell, and contacts as in stack. Parametric polarization; and constant current and constant voltage ops. EIS. Seal Protocol; real duty cycles	Effective ASR; 4000 Durability minimum (e.g. <1.0%/1000h); lifetime; scope manufacturability; proves cells and stack integration/design; Seal protocol; voltage distribution; min/max temps; correlation versus Tech Qualifications; real duty cycles	H_2 Production Rate; Durability; Efficiency; All subsystems needed at large scale; Stack Cost Metric; Cost of H_2; H_2 recycled; Operation & Maintenance real; real duty cycles.

Break Out Session IV:
What are the essential resources for an advanced water splitting materials EMN consortium?

MATERIALS THEORY, COMPUTATION, MODELING, AND DESIGN			
Capability	**Institution**	**Description**	**Limitations**
Atomistic modeling	INL	to look at solid state interdiffusion of electrode/ electrolyte materials	Computational intensive
Fluent CFD	INL	Expertise using it in electrolysis mode. Validated it against real world data	
System modeling	INL	ASPEN/HYSYS for system development	
CFD, transient, mechanical stress, system	Ceramatech		
Stack design	Ceramatech	Extensive experience in cell and stack design	
Microstructure modeling	INL	How structures change at temperature	
Design	PNNL	Designed cells, headers, cassettes, flow fields, stacks, systems + BOP (HYSYS/ASPEN)	
SO - MP	PNNL	Models fundamental microstructural phenomena, half cells, single cells, stack and full systems. Mech. Stress, heat transfer, fluid flow, electrochemical performance, microstructural electrochemistry, structural reliability, Weibull statistics, devitrifying, compliant, and reinforced glass seals, porous ceramics and sintering, creep, fatigue, micromechanics, damage, fracture and failure modeling. Works with FEA (ANSYS, Abaqus, CFD (Star CD, Fluent), CARES, Matlab, Excel, Solidworks	Doesn't work on Mac.
MATERIALS/CELL/STACK FABRICATION AND DEVELOPMENT			
Capability	**Institution**	**Description**	**Limitations**
Combinatorial / high throughput	INL	Ionic conductivity, protonic conductivity, composite conductor	
Fabrication	INL	Tape casting, screen printing, plan on ultrasonic spray, electro infiltration.	
Powder synthesis	PNNL	Liquid & solid precursors, combustion synthesis, calcining, attrition, ball milling, powder comminution (processing)	

Cell Fabrication	PNNL	Tape casting (5', 8' casters), screen printing, compression molding, injection molding, tape calendering, isostatic and uniaxial pressing, slip casting, laser cutting, roll lamination, sintering (air and controlled atm)	5' and 8' casters for tape casting. No extrusion
Thin Film	PNNL	Spin coating, PVD, slurry and solution coating, ultrasonic spray coating. High volume capable, but not combinatorial	No extrusion, 200 cm2 size
Seals and protective coating	PNNL	Seals: Compliant Glass-ceramic (fix in place) Metal to ceramic, Air brazed Typical braze, Hybrid seals Coatings: oxidation/ corrosion, conductive & insulating. High volume capable, but not combinatorial	
Manufacturing	PNNL	Capable of small scale production (~75 cells/week, 200 cm^2), developed QA specs for high volume production of powders, tapes, cells, stacks, leak testing	200 cm2 size
CAPABILITIES: BUTTON CELL / SINGLE CELL / SHORT STACK			
Capability	**Institution**	**Description**	**Limitations**
Button cell/single cell	INL	8 channels	
Button Cell	PNNL	50 cells. Single test, multiple test (allows testing under same conditions), Contaminant testing,	Competition with other projects
Single Cell/Short Stack	PNNL	6 test stands, 1 kW	1 kW, competition with other projects
Systems testing	PNNL	3 test stands, 5kW, 1 at 10kW	Competition with other projects
Reliability testing	PNNL	10 test stands, >1000hrs, button cells to short stacks, contaminant test capability	Competition with other projects
Protocols	PNNL	Developed acceptance testing, and reliability protocols for cells and stacks	
STACK TESTING / DEMONSTRATION / BOP			
Capability	**Institution**	**Description**	**Limitations**
Full stack testing	INL	15 kW, 12 stacks can be tested in the hot zone. Each group of 4 stacks has its own steam, H_2, exhaust, and electronics. All 12 stacks was 15 kW. Included heat recuperation, steam generation, and H_2 recycle, monitoring system.	Can do multiple stacks that add up to 15 kW. Can't do single stack at 15 kW
Systems testing	PNNL	3 test stands, 5 kW, 1 at 10 kW	Competition with other projects
Full scale stack and system	Ceramatech	5 kW routinely	

CHARACTERIZATION			
Capability	**Institution**	**Description**	**Limitations**
Physical Characterization	INL	Microscopy techniques (SEM, TEM, acoustic SEM, optical), LEAP, Raman, XRD, CT scanner, Gas chromatography, Mass spectrometry	
Physical Characterization	Ceramatech	Scanning acoustic microscopy, CT scanner, Gas chromatography, Mass spectrometry,	
Electrochemical	INL	Seebeck, EIS (8 channel), ionic & ohmic conductivity	
Physical characterization	PNNL	2D and 3D optical microscopy SEM with EDS and EBSD, TEM, particle size analysis, surface area determination, Thermal gravimetric analysis (TGA), differential scanning calorimetry, Dynamic mechanical analysis, Dilatometry (including controlled atmospheres), X-ray diffraction (including high temperature), Gas chromatography, Mass spectrometry, Mechanical testing load frames, SIMS, XPS TGA/DSC, Raman, FTIR, leak testing, surface profilometry, oxygen permeability, ionic & ohmic conductivity, EMSL capabilities	
Electrochemical Characterization	PNNL	Electrical conductivity and seebeck measurements, current-voltage and impedance spectroscopy analysis, EIS, TEM at HT operating	E TEM- 20 Pa

GAPS

- Database of SOA materials and how they perform
- Models
  - Computational predictive modeling for SOEC type materials particularly to go to lower temperatures
  - Phenomenological models to search materials databases to help identify potential candidates
  - Models to predict interface
  - Models to predict corrosion at high temperature
  - High throughput testing for screening (current capabilities are limited, or we have them, but haven't applied them to solid oxide)
- Preventive coating- effectiveness, long term, other contaminants
- Contaminants impact
- Microstructure evolution with time
- How to do high temperature operation and in-situ analysis
- R&D opportunity
  - Medium T systems – 600C
    - TEA / LCC to determine if it's worth it.
    - Materials development, catalyst, electrolyte, seals?

Photoelectrochemical

Break Out Session I:
What are the major issues in framing analysis and system and component metrics?

- Tools are available to everyone for analysis (e.g. H2A)
- Publications on TEA and EROI
- Defining efficiency is key. At a given pressure in terms of KWh/kg
- What is hydrogen? Different definitions (purity, composition) for different applications
- Research metrics vs commercial metrics (e.g. The community should recognize the unique diurnal energy source in assessment)
- Discussed durability and accelerated stress testing
- GHG assessment for PEC is necessary

Break Out Session II:
What are key issues and needs in improving functional and structural materials performance metrics?

- Materials compatibility between different components
- Special considerations for separators (e.g. crossover versus conductivity)
- Bipolar membranes
- How do we benchmark catalysts. Need definition standards and protocols.

Break Out Session III:
What are the major issues in framing analysis and system and component metrics?

Tech Qualification and Benchmarking

- Reproducibility
- Developed for realistic lighting conditions (spectra, intensity, orientation, diurnal)
- Collects and measures H_2 (quality and quantity) and O_2
- Open to any/most integrated systems
- Measures durability and evaluates degradation
- Capable of accelerated wear testing, different water feeds

Demonstration

- 1 m^2 demonstration
- 10% gives 24 grams / day
- Evaluate kg H_2/kWh sun, days to years
- Simplicity
- Weber Grill

Particle Systems
• TRL for particle systems much lower than for panel systems (type 3 and 4) • Emerging particle systems summarized in Fabian, D. M. et.al., Energ. & Envi. Sci. 2015, 8, 2825-2850. • New systems must continuously evolve stoichiometric H_2/O_2 against 0 bar or against 1 bar of products, under 1 or 10 sun illumination • Need to exclude air contamination during testing: requires closed loop H_2/O_2 detection • Need for lifecycle analysis and TEA for particle systems that and effects of stirring • and mass transport • Need for analysis of mass transport for type 2 system (separate compartments for O_2 and H_2 evolution) • Need for functioning type 1 and 2 reactor demonstration generate industry interest • Need for successful gas separation for type 1 reaction (co-evolves H_2/O_2) • Need to eliminate back reactions for both type 1 and type 2

Break out session IV:
What are the essential resources for an advanced water splitting materials EMN consortium?

CAPABILITIES				
Theory and Computation	**Synthesis and Scale-up Fabrication**	**Screening and Characterization**	**Data and Informatics**	**Manufacturing and Commercial**
• Band mapping • Computational spectroscopy • Structure and mechanism (JCAP) • Multi-physics modeling (LLNL, JCAP) • TEA and LCA (NREL, LBL) • Supercomputing infrastructure	• Combinatorial synthesis (inkjet - JCAP) • Combinatorial thin films (NREL) • Plasma spray oxidation • Micro plasma jets • Spray pyrolysis • Sputtering • PDIL (NREL) • Methodologies for materials scale up and integration	• X-ray (SLAC, LBL, ANL) • High throughput characterization • In-situ and operando characterization (SLAC, LBL) • Thin film characterization (e.g. TEM, SEM, AFM, etc.) (national labs)	• Data and informatics infrastructure • Demonstrated machine learning capabilities for materials optimization	• Roll to roll • High pressure H_2 experience (SNL) • Risk assessment from H_2 refueling could be used in PEC systems.
NEEDS				
Theory and Computation	**Synthesis and Scale-up Fabrication**	**Screening and Characterization**	**Data and Informatics**	**Manufacturing and Commercial**
• Predict kinetic and thermodynamic stability (chemical, mechanical) of materials • Computational spectroscopy • Interface modeling	• Spatial ALD (large format) • High throughput process development • High throughput device development	• Quantitative degradation testing (QCM, ICP-MS, X-ray) • Photoelectrode imaging	• Network Database (materials, metrics) • Automated data collection (barcodes?) • Connecting theory to real work experiments • Incorporating historical data	• Leaking/safety testing • Sensor systems • Commercial advisory board

Solar Thermochemical (STCH) - Two-step metal oxide redox systems

Break Out Session I:
What are the major issues in framing analysis and system and component metrics?

- Detailed process and component flowsheets necessary
- System designs will need to be better defined
  - Moving particle, fixed bed, all the components, operating conditions, etc.
- Due to low TRL, difficult to predict components that will ultimately be in system being modeled for a materials bill of materials
- Need to capture components that are peripheral to reactor and CSP (e.g. vacuum pumps, inert gas, heat exchangers, separations, condensers)
- STH efficiency may not be best metric; may not adequately capture overall cost, many tradeoffs; GHG may not be related to efficiency
- Metrics should be filtered into a handful of overarching parameters- cost and GHG
- Cost and source of water used should be captured
- Land footprint
- Need to consider embedded energy (e.g. kg CO_2 required to build plant)
- Sunshot targets and assumptions (DHI or GHI) should be consistently used

Break Out Session II:
What are key issues and needs in improving functional and structural materials performance metrics?

- <10 mol H_2O and metal per mole of H_2
- Maximum temperature (e.g. 1400C)?
- $P_{O2} < 10$ Pa not practical
- Metric for oxidation temperature (e.g. max temperature or delta) would guide system design
- Durability should be quantified in a configuration that is structurally relevant to the ultimate application (e.g. particle, monolith, RPC, etc.)
- Morphological changes with cycling
- Reliable measurements of thermodynamics and kinetics under high flux conditions necessary
- Measurement techniques should be developed
- Relevant range of measurements should be defined?
- Should set up center for computational resources; e.g. materials database that's accessible from multiple sides.
- Technology roadmap is necessary to define material needs for BOP
- Configuration must be characterized to determine material constraints; e.g. thermal stresses are not important if electricity is used to aid heating
- Materials that can resist oxidation at high temperatures (1500C) are needed
- Working group to determine what and how critical materials perform
  - Computational center should be established that captures data from experimentation, and makes available to theoretical community

Breakout Session III:
What are the promising platforms for technology qualification, benchmarking and demo?

Education of industry and developing protocols to consider and test new concepts
• We are more able to speak the same language with a single voice to a global/universal audience– which is more compelling • How do you make a flexible platform to demonstrate? • Develop a user facility to engage the community– the facility is the thermal source or reactors that people plug into • Develop common engineering models • Cannot look too far forward; but we need to accelerate the timeline to build the interest • Combine material characterizations with engineering models to educate industry—create near-term numerical platforms for materials and engineering (Fluent? Aspen?) • Validate numerical models and develop virtual platforms for large scale • Should we look into integration with the PV and CSP communities?

Break out session IV:
What are the essential resources for an advanced water splitting materials EMN consortium?

	Resource Location	Capabilities	Strength or Limitation
Theory/ Computation	Computational: DOE (LBNL, Oak Ridge, ANL, NREL, Brookhaven, LANL), Northwestern, U.Colorado, Mines, Stanford, Georgia Tech, Ames, Rutgers Eng: DOE (Sandia, NREL), MIT, CalTech, DLR, ETH, EMPA, Stanford	Computers, expertise (Schoell, Schlossen, Carter, Julia Galley, Maricceli, Sater, Vincent Gabriel) Jenna, Al's Post-doc, Boiczek, Peter (GT), Fletcher Murray, Icarino (particulate flow in combustion)	
Synthesis/Scale-Up Fabrication	Coorstek, Zircar, Ceramics, Advanced Ceramics, Ceramatech	People with business interest	
Screening/ Characterization	Screening: N/A Characterization: National Nanotechnology Infrastructure Network, UT Austin, Purdue	Expertise, equipment, diagnostics	Need to survey outside the network
Data/ Informatics	OQMD, Citrine, Materials Project (model)	External company with expertise, handle atomistic information	Teaming with computational scientists and computational chemists
Manufacturing/ Commercial	Chemical Engineering Departments, DOE (NREL), LightSpeed	TEA, LCA	

Solar Thermochemical (STCH) - Hybrid and other multi-step cycles

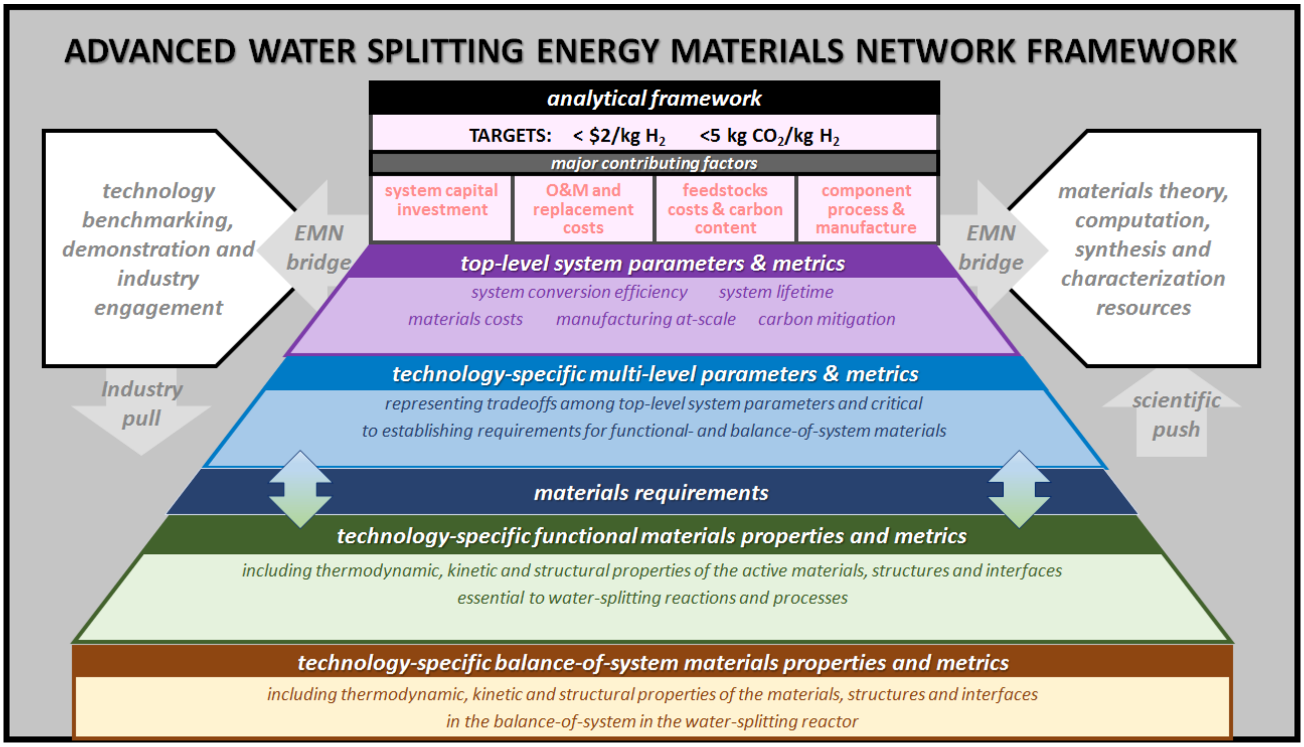
Break Out Session I:
What are the major issues in framing analysis and system and component metrics?

- Plant designs, and corresponding flowsheets of material and energy balance are incomplete
- Detailed component-level understanding has not been developed
- High-level assumptions (e.g. solar energy efficiency) should be more consistent
- Current literature does not capture peripheral equipment (e.g. pumps)
- Analyses should allow for optimization of system design; parameters within the design can be varied and affect one another
- More data sharing in common location is necessary to inform models
- Should explore potential for ancillary equipment (e.g. heat pumps)
- Should characterize production rate over time
- Consider ancillary value (e.g. grid stability)
- Consider thermal energy storage
- Theoretical thermodynamic efficiency, reaction kinetics, and durability of materials should be captured. A defined method to measure thermodynamics and kinetics necessary.

Breakout Session III:
What are the promising platforms for technology qualification, benchmarking and demo?

PLATFORMS FOR QUALIFICATION		
Concepts	**Benefits**	**Challenges**
Pressurized button cell test facility to evaluate catalysts and membranes	Versatile- used for other electrolysis studies as well Can leverage membranes from PEMFC Would be of great value to industry partners to demonstrate technology potential	Corrosion of electrodes SO_2 depolarization
Bayonet acid reactor	low-temperaute metal-ceramic connections heat recuperation	heat transfer from helium
High temperature solar receiver and high-temperature storage demonstration	could be funded through SunShot	efficiency of receiver high-temperature operation
Electrolyzers to demonstrate technology	Air Products CRADA used this	
FUNDAMENTAL R&D TO GUIDE PLATFORM		
Concepts	**Benefits**	**Challenges**
Heat transfer from bed to helium through computational modeling and experimentation	Being assessed at universities (e.g. Georgia Tech, U. South Carolina)	Working with other labs that have capabilities
Catalyst benchmarking in sulfuric acid (INL) + morphological analysis • need to conduct fundamental computational + experimental work • lab round robin approach like in PEC	May be opportunities for collaboration with EU	Data unavailable for sulfuric acid behavior at extremely high temperatures and pressures
BOP materials qualification in high temperature and high pressure	Collaboration with SNL/other offices	

Appendix E: AWSM Workshop Framing Pyramid



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