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DOE EERE AMO Electrochemistry for Manufacturing Workshop Report

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Disclaimer

Foreword

The Advanced Manufacturing Office (AMO) in the U.S. Department of Energy's Office of Energy Efficiency and Renewable Energy held a workshop series titled "Electrochemistry for Manufacturing" in June 2021. The goal of the workshop series was to gain insight into potential applications within the manufacturing sector in which electrochemistry and electrochemical technologies could significantly improve energy efficiency and/or industrial emissions. In addition, AMO sought to identify research, development, demonstration, and deployment needs that could accelerate promising electrochemical technologies and/or enhance the efficacy of existing commercial technologies.

This report summarizes key findings from that workshop series.

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List of Acronyms

AMO	Advanced Manufacturing Office
CEO	chief executive officer
DOE	U.S. Department of Energy
ECS	The Electrochemical Society
GHG	greenhouse gas(es)
pH	a scale used to measure the acidity an aqueous solution
QA	quality assurance
QC	quality control
R&D	research and development
RD&D	research, development, and demonstration

Executive Summary

The Advanced Manufacturing Office (AMO) aims to improve the efficiency, productivity, environmental impact, and competitiveness of the manufacturing sector. The use of electrochemistry in manufacturing could help AMO achieve these goals with its potential to have significant impact on sustainability, energy and carbon efficiency, and U.S. manufacturing competitiveness. The "Electrochemistry for Manufacturing" workshop series was designed to help AMO understand (1) how electrochemistry can be used within the manufacturing sector to achieve AMO's goals and (2) the support for technology and workforce development that is needed from AMO to leverage crosscutting efforts that can enable successful outcomes.

The potential applications for electrochemistry are vast. Prior to the workshop, three key application areas were identified to have the highest potential for impact within AMO's core mission: metals manufacturing, chemicals manufacturing, and water purification. This report is organized to capture the key finding for each of those application areas as well as interdisciplinary areas that would facilitate a thriving innovation ecosystem across all applications.

The workshop brought together experts and practitioners of electrochemistry across academia, industry, national laboratories, and nongovernmental organizations. Based on talks and feedback in the workshop series, it is clear that electrochemistry is one of the critical pathways that the industrial sector is considering to reach emissions reductions targets. Emissions reduction is the primary driver for many within the industrial sector who are considering implementing electrochemistry-based technology. However, there are also potential energy and cost savings for many applications, and those additional benefits will likely incentivize early adopters.

Industry-specific breakout sessions were used to identify both the applications for electrochemistry in manufacturing and the associated research, development, demonstration, and deployment needs. Main takeaways from those sessions are detailed in this report. Although most of the applications are industry-specific, one issue discussed in multiple breakout sessions was the tension between targeting applications and products with high-volume (and, hence, high-emissions) impacts and targeting smaller applications that may have a smaller overall impact but produce higher-value products, which can accommodate the cost that comes with early innovation. The argument for addressing the higher-value/lower-volume products first is to use these applications to continue to de-risk the technology and lower the cost of implementation for commodity-like applications and products.

There were also several themes that spanned applications from the research, development, demonstration, and deployment needs identification. The need to invest in scaling technology to at least the pilot scale was reiterated in lightning talks and in multiple breakout sessions. Difficulties in receiving funding for demonstration-scale work was also highlighted as a potential area for government support. One challenge to scaling is the lack of fit-for-purpose equipment available. In this vein, there is significant opportunity to optimize electrochemical equipment since most applications currently use technology developed for fuel cells because of availability. Protocols and standards for accelerated performance testing are needed to accelerate deployment and provide a method of quantifying improvements. Finally, the need for life cycle analysis and techno-economic analysis tools and protocols was stressed across all applications.

Stakeholder input obtained through the Electrochemistry for Manufacturing workshop series confirmed that electrochemistry can support AMO in achieving its goals of reducing the energy and emissions impacts of the manufacturing sector. AMO will use the insight from this workshop to inform how future investment in electrochemical technologies fits into the broader portfolio of investment in the decarbonization of the industrial sector.

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1 Introduction

The Advanced Manufacturing Office (AMO) collaborates with manufacturers, small businesses, national laboratories, universities, and other stakeholders to catalyze research, development, and adoption of energy-related advanced manufacturing technologies and practices to drive U.S. energy productivity and economic competitiveness as part of the departmental priorities to combat the climate crisis, create clean-energy jobs, and promote energy justice. AMO's vision is for the United States to demonstrate global leadership in **sustainable** and **efficient** manufacturing for a growing and competitive economy. To achieve this vision, AMO has identified the following goals:

- Improve the productivity, competitiveness, energy efficiency, and security of U.S. manufacturing
- Reduce life cycle energy and resource impacts of manufactured goods
- Leverage diverse domestic energy resources and materials in U.S. manufacturing while strengthening environmental stewardship
- Transition DOE-supported technologies and practices into U.S. manufacturing capabilities
- Strengthen and advance the U.S. manufacturing workforce.

With the proliferation of solar and wind sources generating low-carbon electricity; an increased focus on efficient resource usage; and unprecedented climate crisis demanding decarbonization of all sectors, there is a greater-than-ever desire to electrify the large-scale processes of the manufacturing industry. Adoption of electrochemical technologies and strategies could substantially improve the performance of the industrial sector, including energy productivity, thermal efficiency, reduced greenhouse gas (GHG) emissions, and process intensification. The U.S. Department of Energy's (DOE) Advanced Manufacturing Office (AMO) held a virtual workshop series, titled "Electrochemistry for Manufacturing," to get feedback from stakeholders across industry, academia, and the national labs on:

- The most promising opportunities to use electrochemistry in manufacturing processes
- The benefits of employing electrochemical processes in the industrial sector
- The research, development, and demonstration (RD&D) needs to accelerate deployment of these technologies.

The workshop series included four sessions: "Introduction to the Workshop," which oriented attendees to the topic and objectives of the workshop series; "Application Identification," which focused on identifying promising applications for electrochemistry in manufacturing; "RD&D Needs," which aimed to identify key challenges and technology development opportunities in the application areas of interest; and "Crosscutting Enablers," during which the factors that contribute to a thriving innovation ecosystem were discussed. Each day included a series of talks and/or panel discussions followed by a breakout session. In some cases, additional talks were given after the breakout session. Breakout sessions for the Application Identification and RD&D Needs sessions were oriented about three application areas: chemicals manufacturing, metals manufacturing, and water purification. The detailed agenda for each day is included in the Appendix.

On Day 2, a series of talks, followed by a brief panel discussion, provided additional context for the workshop and insight into the role electrochemistry can play in the industrial sector as well as what is needed to facilitate commercialization of electrochemical technologies. Professor Nirala Singh (Michigan State University) highlighted several converging factors that make electrochemical technologies more attractive now than ever before, including a lower cost of renewable electricity, improved device efficiency through component development, and reduced component costs through manufacturing developments. Kathy Ayers (Nel Hydrogen) spoke to the state of the art of commercialized electrochemical technology, using electrolyzer manufacturing as an example. Finally, Shaffiq Jaffer (TotalEnergies SE) provided context for how electrochemistry may be deployed commercially, particularly in the petrochemical sector. Their talks, summarized below, provided introductory information for industry-specific breakout discussions intended to identify opportunities for electrochemistry to impact the industrial sector and what RD&D is needed to reach commercialization.

Industrial decarbonization is one of the main benefits of deploying electrochemistry in manufacturing. Electrification is expected to account for ~20% of emissions reduction from the industrial sector by 2050 and 30% by 2070 (International Energy Agency 2020), and electrochemistry will play a role. Production and cost reduction of renewable energy continues to outpace projections, resulting in increased adoption ahead of expectation. This may prematurely remove one of the key constraints of "electrifying" the industry. The following applications were discussed as potential avenues for electrochemistry to play a role in reducing emissions:

- Energy storage: There is a need for long-term energy storage, on the order of months to years, for which few options exist beyond chemical energy.
- Transportation fuels: The efficiency of charging a lithium-ion battery is higher than electroconversion of carbon dioxide (CO_2) to methanol. However, for modes of transportation where batteries are impractical, "e-fuels" should continue to be investigated.
- CO_2 conversion: CO_2 reduction is incredibly energy intensive and inefficient. Formic acid and CO are the only products of CO_2 reduction that currently reaches a relatively high efficiency. Electrophotoreduction of CO_2 has high efficiency potential but requires significant improvements and investment. Ethylene is another platform chemical that could be of interest, but the cost of ethylene from petroleum sources is sufficiently low that the economics for production via electroreduction methods are challenging.

- Other promising applications: These include but are not limited to chemicals synthesis, separations, and electrodeposition for corrosion avoidance.

As companies assess these opportunities, the cost of electrochemical technologies is a major consideration.

Electrolyzers can provide an example of how electrochemical technologies can progress toward commercial deployment. Electrolyzers have been scaled to megawatts (1–2 megawatts), and there is interest in even larger installations.

As the reactor scales, cost savings are realized through economies of scale in manufacturing and from a reduction of certain components in the stacks. Surrounding operations, such as downstream separations, will also scale traditionally with volume, providing additional value at larger scales. For example, there are several opportunities to reduce the cost of proton-exchange membrane technology based on fuel cell development, including thinner membranes and catalyst films. Process development is needed to improve the precision and efficiency of the operation. Costs will also come down with more experience in manufacturing electrolyzers and by manufacturing higher volumes of the same system, which typically drives up to 5% cost reduction. Power electronics also impact the price of electrolyzers, so cost reductions in power electronics would also drive down costs. Considering all factors, workshop participants estimated that $400 per kilowatt should be achievable in 5 years.

In addition to the cost of electrolyzer parts and manufacturing, the electrolyzer market will also set the price. Typically, the highest-value industry will drive the prices for these devices and components, because the technology providers will get the largest margin for their product. As the market diversifies into other products through the broadening of uses for electrolyzers, the cost will likely come down.

Several critical needs to advance the use of electrochemical technologies in manufacturing were highlighted and are summarized by the following:

- Reducing the cost of electrolyzers by:
  - Using process design expertise to optimize the full system, including auxiliary and downstream operations, rather than a single unit process
  - Looking at how power electronics interfaces with renewable energy, including co-optimization with and quality improvements to the input power
  - Moving from batch and/or manual processes to automated and continuous processes such as roll-to-roll to see improvements in consistency, production rate, and material efficiency
  - Improving the life cycle stability and durability of materials and systems
  - Better understanding how process variables impact produced parts and other fundamentals of manufacturing

- Improving efficiency by:
  - Optimizing smart systems through the process
  - Improving the efficiency of electrolytic hydrogen production and adjacent processes
  - Improving single-pass conversion rates
  - Improving downstream separation, which is a critical piece of total process efficiency
  - Using materials designed for electrochemistry rather than using readily available fuel cell materials
- Coupling electrochemical processes with renewable energy by:
  - Enabling industry to have at least 80% of their processes electrified
  - Leveling out fluctuations in renewable power, which is currently nowhere near where capacity utilization will need to be (50%–60%), with hydropower/solar power likely being the first cases
  - Enabling the deployment of these assets at scale.

To delve more deeply into relevant applications, barriers, and RD&D needs in the metal manufacturing, petrochemical, and water purification industries, breakout sessions were held to solicit stakeholder input. Input received both through lightning talks and in the breakout sessions are summarized in the following sections. Across all of these areas, communication and collaboration between labs, industry, and academia will be advantageous in accelerating development of these technologies.

2 Metals Manufacturing

2.1 Background

Electrolysis is advantageous in metal processing because it lowers the otherwise high heat requirements needed to reach a molten state and reduce metal. It is used in the production of several critically important metals, including aluminum, magnesium, sodium, potassium, zinc, gallium, and copper. Although many of these processes have been commercialized, there may be potential improvements that result in energy and emissions savings. Advancements are needed to improve the efficiency of the electrolytic processes that produce metals. Since the energy intensity of this sector of manufacturing is relatively high and the energy consumption is a substantial cost for many of these processes (U.S. Energy Information Administration 2019), any advancement in metals processing efficiency could make a large impact. Possible improvements in the energy efficiency of metals manufacturing may be made with advanced technologies, such as new electrode and membrane materials that result in longer life cycles and higher efficiencies, optimization of cell design and configurations, and novel processes that use different chemical pathways. Conventional iron production uses coke (made by heating coal or oil in absence of air) to reduce iron oxide to iron, generating CO_2 in the process. Direct iron reduction of iron oxide using electrolysis is a pathway that is currently being explored by Boston Metal and would eliminate the CO_2 generated by the reduction process (Advanced Manufacturing Office 2018). While still under development, this process may provide energy efficiency, emissions, and cost benefits over other iron manufacturing processes that attempt to reduce emissions.

As part of the workshop, speakers representing the state of the art in metals manufacturing provided insight in detailed technical presentations and lightning talks, including several that spoke to the importance of electrochemistry in metals manufacturing. In addition to these talks, breakout sessions on Days 2 and 3 were organized by industry or application area and sought stakeholder input on promising applications for electrochemistry in metals manufacturing as well as the challenges and RD&D needs to thrive commercially. A summary of the talks and feedback from the relevant breakout sessions are detailed in the following sections.

2.2 Presentations

Nirala Singh (University of Michigan) spoke broadly about the potential applications of electrochemistry and the benefits to industry. In his talk, he emphasized the external factors of reducing CO_2 emissions, reducing waste and pollution, safety, changing feedstocks, and lowering the cost of electricity to motivate shifts to electrochemical processes. Novel electrodeposition processes for microelectronics production were one of the key applications highlighted for potential development. In addition, electrochemical processes related to electrodeposition could be used to prevent corrosion, which is estimated to cost $276 billion per year in the United States (Fuller and Harb 2018). The open questions for electrodeposition of metals are understanding deposition kinetics and ensuring consistent deposition.

Rich Bradshaw (Vice President of Engineering at Boston Metal) described their innovative molten oxide electrolysis process for electrolytic metals production. It has the advantages of avoiding chlorine and fluorine use, it can produce high-temperature metals such as iron and titanium, and it is a modular process.

Another critical advantage of this process is that it does not directly emit CO_2 because of a lack of carbon introduced to the process. Theoretically a renewable energy fed iron-making process could be emissions-free.

The main technical challenge to commercialization of molten oxide electrolysis is the scaling of inert anode technology from lab to industrial scale while ensuring the durability of the anode. A major challenge of any technology in steel production is the low price of commodities that often do not support innovation.

E. Jennings Taylor (founder and senior advisor of Faraday Technology, Inc.) spoke about pulse current electrolysis, which can enable simpler electrolytes and lower chemical consumption. This method avoids operational instabilities, including thermal runaways, which result from the electrolyte and ultimately reduce associated operating expenses and capital expenditures. It has been used in applications such as electrochemical deburring of gears, electropolishing, pretreatment of metals prior to electrodeposition, and electrochemical machining.

2.3 Workshop Feedback

The following statements represent feedback from workshop participants in the breakout sessions and polls regarding metals manufacturing.

Applications that were identified could be grouped into a few categories:

- Extraction
    - Electrochemical extraction of metal from seawater can be critical for countries with limited resources. For others, direct, *in situ* electrochemical mining/metal extraction from buried natural ore deposits could be promising. This was investigated in the 1970s and should be revisited. Extraction of copper, iron, and sulfur via electrolysis is a class of applications that holds potential for energy efficiency and/or decarbonization in the next 5 years.
    - Combining wastewater treatment and efficient metal (particularly heavy metal and/or rare earth metal) recovery using electrochemical processes is a potential added-value area.
- Recycling
    - The use of electrochemistry for primary extraction and recycling of battery materials was broadly important for industry applications for batteries. It was highlighted that processes may exist for this application, such as Idaho National Laboratory's process for battery recycling.

  - Electrorefining could be used to replace high-temperature processes for scrap metal recovery. Tonnage metals (e.g., iron) show the largest opportunity, although other metals, such as titanium, can also offer some interesting opportunities to reduce energy intensity and promote greater adoption (such as lightweighting applications).
- Use of electrochemistry for feedstocks in metals manufacturing
  - Using electrochemistry to generate low-carbon feedstocks to reduce iron oxide represents a lower barrier to use in existing iron-making operations. Potential feedstocks made electrolytically include hydrogen and syngas, both of which can be made with biomass to further improve CO_2 impacts. The key challenges are operating expenses versus capital expenditures. The cost must come down to be economically competitive with other sources of energy.
  - Value-added materials, such as alloys, plastics, and graphite, may be produced via electrolytic processes by integrating nonfossil carbon (plastic, municipal solid waste, biomass) feedstocks.
- Direct electrochemical metals production and deposition
  - There is considerable interest among the aerospace industry community in electrodeposition of early transition metals, like niobium and tungsten, for high-temperature-stable coatings and thin, superconducting films. Electrochemical plating of zinc to replace hot-dip galvanizing was also mentioned as an application area of interest.
  - Electrodeposition and electrochemical machining can improve the components of metals additive manufacturing.
  - Electrochemical oxide reduction is being explored, with direct iron reduction being one of the applications that has the highest likelihood of impact within the next 5 years. Direct electrochemical manufacturing of titanium metal or alloys could also have a high value in the near term.
  - Replacing traditional carbon-based, high-temperature reduction of metals with electrowinning (also known as electro-extraction, which is the electrodeposition of metals from their ores) was something particularly of interest to national lab participants.

Several participants in the breakout sessions mentioned that the biggest impact on emissions reduction will be on metals extraction and recycling at the largest scales, such as with iron. Since it is significantly larger than that of all other metals, emissions reduction technologies specific to iron production are needed to notably impact industrial decarbonization. However, there is a danger in focusing only on iron, since it may be easier to absorb the costs of innovation in the production of higher-value metals and alloys made at smaller scales. Learnings from those applications may be applied to commodity metals.

Several barriers were identified in deploying electrochemical technologies in metals manufacturing. One major barrier was cost, particularly for commodity materials, like iron and steel. Another barrier was workforce development, which is addressed in later sections. There was an acknowledgment that long-term planning has not been a strength of the industry in the United States. There has also been limited sustained funding for work in this area, particularly on fundamental science.

The RD&D needs identified were:

- Establishing production methods that allow the incorporation of scrap and recycled feedstocks. All metals processing should attempt to consider incorporating recycled materials into virgin materials within the same process, which is an advantage of pyrometallurgical processes.
- Quantifying environmental benefits as well as other policy drivers that may lead to increased commercial viability, because analyses, including techno-economic analysis, are critical for commercial viability of electrochemistry of metals manufacturing or recycling.
- Improving, standardizing, and reducing the cost of the “balance of plant,” including power electronics and pumps.
- Performing applied research into scaling up processes, particularly at pilot scale or near-pilot scale. Pilot scale needs to be selective because costs go up dramatically with scale. A potential target for applied research is electrolytic oxide reduction or conversion of batch to continuous processes. For scale-up to be successful, industry needs to be involved.
- Running detailed capital expenditures modeling of industrial deployment, which can be used to drive decisions on which RD&D areas to emphasize. This information is powerful; cost reduction road maps can be made.
- Developing inert anodes that can reduce carbon emissions or increase efficiency to minimize the emissions for aluminum production.
- Solvating scrap metal for electrochemical processing, which is difficult in comparison to heating in a furnace in the presence of reductant. Development of better processes for metal separation from scrap is needed.

3 Chemicals Manufacturing

3.1 Background

Electrochemical pathways for chemicals production provide opportunities for more carbon- and energy-efficient synthetic routes of commodity and specialty chemicals that traditionally rely on large-scale, energy-intensive thermochemical processes. Electrochemical pathways can provide additional benefits, including less water usage, reduced solvent handling, and improved product quality. There are well-known commercial applications of electrochemistry, including the manufacturing of sodium hydroxide and adiponitrile. Additionally, emerging chemical pathways include reduction of CO_2 into fuels and chemicals; electrolysis-based synthesis of hydrogen, methanol, and ammonia; and synthesis of specialty chemicals and pharmaceuticals. Electrochemical synthesis provides only a small fraction of the many thousands of commodity and specialty chemicals in the marketplace. Electrochemical manufacturing for chemicals production is underutilized compared to conventional thermal-based routes because process heat from fossil fuel use is currently relatively cheap compared to electricity. Thus, reductions in the energy consumption of the electrochemical process and increased availability of clean electricity are needed for widespread adoption of electrochemical manufacturing in the chemicals sector. The energy efficiency of electrochemical processes can be improved through optimization of individual components including anode, cathode, catalysts, membranes, and integrated cell designs. Optimization via modeling and process intensification can increase the yield and selectivity of reactions at reduced energy input. Additionally, electrochemistry can be leveraged to reduce the energy-intensive separation steps by improving selectivity or through targeted applications, such as electrodialysis.

Due to the high maturity of processes for the manufacturing of the identified chemicals, the willingness of industry members to uptake new technology was debated. Potentially, the order in which chemicals classes are pursued can impact the broad uptake of electrochemical manufacturing of chemicals. Multiple pathways were suggested by participants.

A potential pathway included starting with high-margin specialty chemicals, like pharmaceuticals, to assist in early-stage implementation, followed by commodities and then fuels.

Other participants indicated commodity chemicals, like olefines, should be the starting targets due to the largest potential to reduce CO_2 emissions. Another option was to pursue pathways relying on less-energy-intensive steps by starting with exothermic reactions that can generate energy while producing chemicals, like ethylene from methane or ethane, epoxides from olefins, or propylene to acrylic acid via electrooxidation.

3.2 Presentations

Kendra Kuhl (Twelve) discussed her company's work in carbon transformation using proprietary catalyst technology that transforms CO_2 into critical chemicals, materials, and fuels that are conventionally made from fossil fuels. Through electrochemical CO_2-reduction technology, industry organizations and brands can meet emissions targets faster while creating essential products—from polymers in automobile dashboards to aviation fuel to laundry detergent—at the same or higher quality as conventional products made from petrochemicals. To realize the full potential of carbon transformation, there is a need to scale the technology and develop a greater fundamental understanding to drive continuous performance improvement.

Sumit Verma (Shell) commented that the combined result of an increased societal push toward decarbonizing the energy and chemicals sectors as well as the continuous decline in the levelized cost of renewable power is that electrochemical manufacturing technologies are currently realizing an increased level of interest in development and deployment at the industrial scale. The most prominent commercial application in the works today is hydrogen produced via water electrolysis (often termed "green hydrogen"), with industrial deployments in the 10- to 200-megawatt scale (e.g., Shell REFHYNE and the Rotterdam Green Hydrogen Hub in Europe).

Other emerging opportunities include electrolysis of CO_2 to create valuable products, such as carbon monoxide, ethylene, or ethanol; the electrochemical synthesis of hydrogen peroxide; and electrochemical separation, like electrodialysis or electrochemical swing adsorption. As the chemicals industry starts to scale and deploy these options, common barriers that cut across these technologies need to be addressed by:

- Improving the availability and scale of renewable power, which is a necessity for enabling industrial-scale deployment of electrochemical technologies
- De-risking technology options at scale (hundreds of megawatts)
- Increasing the availability of high-performance as well as standardized electrolyzer components, such as anion-exchange or bipolar membranes and oxide- or proton-conducting ceramics.

Some of these barriers can be addressed through government funding. For example, this funding could help with improving manufacturing capabilities of electrolyzers and their components by establishing "gigafactories"; promoting research and development (R&D) to boost component performance (e.g., membrane stability and conductivity); establishing and securing a robust supply chain for critical components, including for recycling them; and researching manufacturing options that could reduce the cost of linear-scaled electrolyzer modules. All these examples fit into AMO's mission space.

Bob Snyder (CEO of Chemetry) spoke about the challenges his company has faced progressing their electrochemistry-based technologies. A key focus was the need for government funding to support the development phase to de-risk the scaling-up of processes. Bob highlighted the relative ease of receiving funding for early-phase R&D due to the relatively low cost and short time horizon for results. The gap between a pilot plant and a commercial plant can be quite large, and bridging that gap can be costly, resulting in a preference toward incremental improvement over stepwise changes in technology and performance. To attain these stepwise changes in improvement, novel processes must be de-risked at sufficient scale, often requiring commercial-scale equipment and extended timelines. The economics of conducting trials at this scale may be justified for specialty products but are much more challenging for commodities. There is an opportunity for government support in this step of technology development.

3.3 Workshop Feedback

During breakout sessions focused on chemicals manufacturing via electrochemical processes, stakeholders highlighted the most promising target chemicals, including production of intermediates and end products, like olefines, alcohols, oils, lubricants, urethanes, and solvents.

- The production of commodity chemicals, like ethylene and propylene, from CO_2 was an agreed-on opportunity space due to its decarbonization impacts.
- The generation of hydrogen and hydrogen carrier molecules, like ammonia, methanol, and methane, was identified as an application that addresses a critical need: long-term renewable energy storage.
- Specialty chemicals that require high-purity end products, like pharmaceuticals, agrochemicals, and silicon, are ideal candidates for electrochemical processes due to higher selectivity and increased tunability than traditional pathways.
- Other inorganic processes, including nitration, fluorination, and salt formation, were also identified, through survey studies, as essential to expand the range of synthesizable chemical products.

3.4 Research, Development, and Demonstration Needs

The RD&D needs for chemicals manufacturing via electrochemical processes spanned from fundamental and applied RD&D for both component and electrolyzer platforms to pilot-scale testing facilities and plant-scale demonstrations. Key RD&D opportunities discussed in the breakout sessions included:

- Component research on advanced membranes, including oxidatively stable anion membranes, membranes compatible with organic solvents, and proton-exchange membranes
- Research on the development of electrolyzers and reactors, including flow reactors, hybrid reactors, and tandem reaction reactors, with particular attention given to mass transport and cell-catalyst architectures, including available catalyst areas, local catalyst environments, and water management, for selective reactions

- Research focused on separations, including process and environmental conditions that allow for chemicals separations following electrochemical reactions, which rely on pH changes and can be used for bipolar membranes, or direct electrolysis, which can produce the pH shift
- Scaling of electrodes from surface areas of a few square centimeters to many square meters prior to plant-scale demonstrations
- Development of frameworks and protocols that accelerate the testing of performance and stability of electrochemical conversion processes, which, at the pilot-scale takes months or longer, including defining short- and long-term performance standards for yields, durability, and roughness and understanding the impact of feedstock impurities on performance
- Ensuring protocols for short- and long-term performance, considering tradeoffs between single-pass conversion and industrial-scale currents
- Use of techno-economic analysis and life cycle assessments to identify the chemical conversions and/or process stages that yield the greatest improvements for end-product costs and energy-efficiency testing with analyses compared to current mature processes and intensified production techniques.

4 Water Purification

Water contamination is of growing concern due to traditional infrastructure decay, population increase, industrial development, and technological progress. Increased detrimental pollutants, such as inorganic minerals, radioactive minerals, organic contaminants, or biological toxins, find their way into water resources, impacting water treatment and purification strategies. In some instances, the use of electrochemical technologies as a coarse treatment process (i.e., pretreatment), can better the performance of fine treatment and disinfection technologies. Electrochemical disinfection methods can remove or convert nontoxic materials by combining one or more treatment processes, including electrochemical oxidation, electrochemical reduction, electrodialysis, and/or electrocoagulation methods. The advantage of electrochemical disinfection processes is that they can be used in both centralized and distributed treatments where the transport and storage of hazardous materials are not needed, they can be scaled, and they reduce energy consumption in current processes. In addition, there is potential for energy recovery through the production of fuels at the cathode, which allows further reduction in their energy footprint.

4.1 Potential Electrochemistry Applications

In Shankar Chellam's (Texas A&M University) presentation, electrocoagulation was highlighted as an electrochemistry application that delivers the aforementioned benefits over conventional chemical water treatment. This was reinforced and built upon in the breakout sessions, where the most promising applications of electrochemical water purifications were identified. These included but were not limited to sensors, chemical removal and destruction, nutrient extraction, capacitive deionization, micropollutant removal and remediation, and modular and automated distributed treatment. Some opportunities that exist in these applications that were identified are:

- Capacitive deionization for high-salinity wastewater streams
- Operation of advanced bipolar membranes at much higher current densities, such as through an on-site acid and base generation
- Chemical and microbial (e.g., volatile organic compounds, polyfluoroalkyl substances) removal and destruction.

Daniel Bar (Ameridia) spoke about Ameridia's separation and fractionation technology that, among other applications, can be applied to wines and juices, and water treatment. The technology combines electrodialysis and bipolar membrane electrodialysis, ion exchange resins, chromatography, and membrane filtration. He used electrodialysis for the tartaric stabilization of wine and grape juice as an example of how this technology is applied commercially and the potential benefits. Use of this electrochemical technology compared to cold stabilization leads to major energy savings and reduced product losses.

4.2 Research, Development, and Demonstration Needs

It was unanimously agreed that most areas of electrochemical water purification require a deeper understanding of the fundamentals needed due to the underlying electrochemical and bulk water reactions, which are not well understood, before being able to scale up procedures. The field of electrochemical use for water treatment is new and, as a result, has a lot of room for efficiency improvement. To become a more viable technology, the following challenges need to be addressed:

- Presence of trace contaminates, which are difficult to detect and can interfere with desired chemistry. Further, byproducts from electrochemical processes, like chloride ions, can lead to increased toxicity through the formation of toxic chemicals, like perchlorates, through side reactions.
- Process selectivity, which is dependent on many factors, including various oxidation states of metal contaminants, salinity, pH, and other micropollutants, and can vary significantly.
- A lack of understanding of surface interactions in sorption and conversion, as well as interfacial mass transfer at the electrode.
- Development of inexpensive sensors, detectors, and electrode materials, which will need to be scalable, modular, and fully automated.
- Electrode fouling, which increases ohmic resistance and reduces energy efficiencies and contaminant removal efficacy.
- Techno-economic analysis/life cycle assessments, which have not been developed and are needed to help guide process intensification paths.

Overall, the RD&D needs are multiscaled and include technical and economic aspects. Process intensification should be leveraged to achieve many of these objectives. Broad RD&D needs include:

- The bench-scale development of highly selective ion-exchange membranes for water softening or heavy metal recovery
- Pilot-scale and prototype testing of distributed/automated electrochemical processing units
- Full life cycle economic assessment of distributed electrochemical units (extended operation energy use, reliability, operation cycle duration, maintenance needs, etc.)
- Small-scale distributed treatment units that are modular and automated
- Process intensification powered by green energy for remediating contaminated waters

5 Crosscutting, Enabling Technology

In addition to sector-specific opportunities and technology development needs, AMO sought to better understand the crosscutting factors that enable faster technology advancement and contribute to a thriving innovation ecosystem. Those factors were classified into four segments:

- Reactor design and scale-up
- Quality assurance and quality control
- Modeling and simulation
- Education and workforce development.

Each of these areas were explored more deeply through expert talks and breakout sessions on Day 4. The discussions and talks are summarized in the following sections.

5.1 Reactor Design and Scale-Up

5.1.1 Background

Research in materials discovery and device optimization are universally performed with routes that are most expedient and available at the lab scale. These early-stage efforts rarely consider factors important for scaling up, such as waste volume, cost of equipment and material feedstock, or the safety and availability of hazardous chemicals used in the scaled processes. Simple translation of methods developed at the laboratory scale into large-volume manufacturing is rarely possible. To assist in the acceleration of scale-up activities, there is a need to leverage scientific approaches that consider systemwide data analytics in the advanced manufacturing of materials (U.S. Department of Energy Office of Science 2020).

Despite the breadth of applications, the manufacture of components and materials for electrochemical systems often encounter similar challenges. Electrode performance is highly dependent on composition and morphology from the catalysts and active materials to polymeric constituents that provide ion transport and/or binder properties. Often, wet-processing routes are preferred, requiring that inks and slurries be formulated to provide desired material interactions and compatibility, while also providing for acceptable processability. Low-cost manufacturing methods for the electrodes are needed, and often use roll-to-roll processes capable of high throughput and quality. The application processes used must enable thin and uniform layers with the right distribution of the assorted phases, and often include various pre-metered methods (Hanft et al. 2018; Mauger et al. 2018; Schmitt et al. 2013). While these methods are relatively well known, the development of proper slurry formulations and processing conditions to achieve desired morphology and performance is a challenge for each new electrochemical material set (Shen et al. 2019; Khandavalli et al. 2018; Khandavalli et al. 2019). In addition, for some material systems, reactivity during processing is a concern, and processes must be designed to minimize or eliminate exposure to water or oxygen. Methods to reduce capital expenditures or processing steps, reduce energy consumption, and utilize less-hazardous processing aides are ongoing development needs (Wood, Li, and Daniel 2015; Hawley and Li 2019).

5.1.2 Presentations

Michael Ulsh (National Renewable Energy Laboratory) presented challenges in scaling and testing on Day 4 of the workshop, with some of the content summarized in the preceding two paragraphs. While his description used the example of manufacturing of electrochemical devices, the lessons learned from those endeavors are applicable in designing and scaling electrochemical reactors in other manufacturing processes not targeting electrochemical device production.

5.1.3 Workshop Feedback

Because greater than half of the workshop participants expressed interest in discussing reactor design and scale-up, two breakout groups were devoted to this topic on Day 4. Several common themes emerged from these two separate groups in response to the question "What advances are needed in reactor design and scale up to enable and support electrochemistry adoption in manufacturing?"

- Product separation and purification from the electrolyte and the electroactive catalysts is a requirement for manufacturing. Funding opportunities for purifying and recycling realistic electrolytes from state-of-the-art studies would accelerate this necessary development. Product specifications should incorporate industry regulations for purity in transportation and storage. Creating paired electrochemical reactions and separations also would be advantageous.
- There is a need for off-the-shelf reactors from lab scale to pilot scale that can be readily sourced. Though some small-scale reactors are commercially available, it is tougher to find mid- to pilot-scale sizes. We need to move away from lab-scale H-type cells where mass and heat transport are poorly defined into standardized electrochemical cells where the relation between hydrodynamics and mass and heat transfer are well defined (reactors where the Reynolds, Sherwood, Schmidt, and Prandtl Numbers and their relations are fully characterized). These should allow the study of kinetics in electrocatalytic systems under an understanding of the transport-reaction relations, and this should, in turn, facilitate modeling, design and scale-up. We also need to define pilot scale, because, in academic research, "pilot" is considered ~100–1,000 square centimeters, while for industry, it usually includes stacks upwards of 5,000 square centimeters (application-specific).
- Development of more selective and active catalysts, keeping catalyst manufacturability in mind, will enable high-efficiency processes.

Modular designs and units provide advantages, such as the ability to bridge from pilot to production scale and to quickly replace components with minimum loss of onstream factors.

- Better understanding of design principles and requirements regarding durability would accelerate implementation of electrochemical processes by industry. For example, how much will it cost to open up cells every year versus every 10 years to replace membranes?
- It is important to develop process-specific reactor engineering (liquid versus gas) from electrode/diffusion layer/catalyst/membrane. This depends on the process, so scale-up cannot be generalized; it has to be system-specific. Liquid-based versus gas-based processes are especially different.
- High raw-material costs have highlighted a need for lower-cost electrode catalyst materials, especially alternatives to precious-metal-based water oxidation catalysts.
- Electrolyzer scaling design rules (i.e., how to use pilot or bench data to design multimegawatt systems) should be developed, similar to those available for commercial-scale thermochemical reactors. Identifying what parameters scale up in what form is a critical need to avoid unnecessary repeated trial-and-error experimentation.
- We need greater knowledge of scale-up parameters. Models are well tested in industry except for multiphase systems, so standard approaches to scale up would be valued.

5.2 Quality Assurance and Quality Control

5.2.1 Background

Quality assurance (QA) typically refers to material property measurements of incoming raw materials that verify that critical properties are with specification ranges. QA measurements are similar to benchtop characterizations used in R&D, though are often modified to provide fast and easy operations for use by production-line operators. Measurements of dimensions, as well as chemical and mechanical properties, are frequently made for QA.

In addition to QA of raw materials, there is also a need for real-time, in-line inspection during production for quality control (QC) (Ulsh et al. 2013; Yuan et al. 2021). Valuable material can be consumed quickly during high-throughput manufacturing and, if improperly processed, can incur significant cost while yielding a product that does not meet specifications (Debe 2012). Physical and morphological properties (e.g., thickness variation, void fraction, surface roughness) of produced materials can be just as important as quality (performance) and should also be monitored. In-line monitoring is particularly useful to track consumption of precious metal catalysts in fuel cell or electrolyzer electrodes to ensure adequate loading and prevent over consumption of rare, costly materials. Feedback from continuous measurement of the weight of electrode layers emerging from roll-to-roll extrusion can be used to control the feed rates of raw materials to achieve optimal loading.

A detailed description of metrology for inspection and control of roll-to-roll manufacturing processes can be found in the Factual Document for the Basic Energy Sciences Workshop on Basic Research Needs for Transformative Manufacturing (Jenks et al. 2020).

5.2.2 Presentations

The presentation from Mike Ulsh on Day 4 on reactor design and scale-up also covered QA/QC. The background content above is primarily from the read-ahead document and from his presentation.

5.2.3 Workshop Feedback

There was no breakout session devoted to this topic, as participants preferred to discuss reactor design and scale-up.

5.3 Modeling and Simulation

5.3.1 Background

Electrochemistry involves many different phenomena that interact across various time and length scales from atomistic to macroscopic and from picoseconds to hours or longer for rare events related to durability. To understand these interactions, multiscale modeling approaches have been used. Due to the advent of efficient and less-costly computation, multiscale, multiphysics modeling is increasingly utilized for the evaluation of designs and concepts before and during experimental fabrication and testing. In this fashion, the design-build-test paradigm can be greatly sped up, thereby realizing drastically shorter concept-to-market time.

Multiscale modeling encompasses many different concepts, each with their own strengths and weaknesses. At the atomistic scale, *ab initio* models, such as molecular dynamics, quantum mechanics, and density functional theory, provide detailed descriptions of atomic and subatomic motions and interactions that can be used to understand intrinsic material interactions and properties. Such models are limited, though, in predicting larger-scale phenomena either in space or time, which is more often the case in manufacturing process and evaluation. At longer time and length scales in terms of seconds and micrometers—the so-called mesoscale—there are stochastic models that enable reaction pathway and mechanism exploration and event-based phenomena such as phase coexistence inside materials. Continuum models at the longest length and time scales provide less granular information due to the averaging of atomistic interactions but enable a much more detailed understanding of multiple, coupled physics in realistic domains on the order of micrometers or larger. These physics-based models at the continuum level can explore the intricacies of new designs and processes, including reactions, transport phenomena, aggregation behavior, fluid flow (i.e., computational fluid dynamics), and others. This has been key in the development of complex environments and optimization of designs that can then be fed into additive manufacturing or provide insight into design targets and new synthesis trains, especially where transport and separation phenomena become critical. Examples of technologies where such modeling has provided great impact and insight include batteries, fuel cells, CO_2 reduction, and other electrochemical technologies.

5.3.2 Presentations

The use of modeling and simulation to enable and support electrochemistry adoption in manufacturing was the subject of a presentation by Adam Weber (Lawrence Berkeley National

Laboratory) on Day 4 of the workshop. Adam made the case that modeling can be used to explore the underlying physics of electrochemical processes as well as help interpret experimental data. Modeling is also a tool that can elucidate controlling phenomena and bottlenecks. Another goal of modeling is to conduct virtual experiments that enable sensitivity studies for process optimization, including examining different cell architectures. These virtual experiments can save time and money by avoiding a trial-and-error approach and accelerate the transition from concept to market.

On Day 3, Daniela Blanco (Sunthetics) spoke about the application of machine-learning techniques to speed the discovery and development of electrochemical systems for chemical systems. Sunthetics develops machine-learning platforms that accelerate the optimization of electrochemical transformations in academia and industry. The technology addresses the need for new approaches to model reaction behavior quickly and efficiently, significantly shortening process development timelines. The main remaining challenge is the integration of hardware and software for automated process optimization solutions for varying process scales. There is a need to better understand the possibility to leverage data sets across industry sectors, how to develop integrated hardware and software solutions, and how to best integrate physical models and artificial intelligence. Several challenges currently limit the use of artificial intelligence in the development of electrochemical systems. Those include a lack of knowledge in artificial intelligence and statistical learning, the need to build large data sets to learn from, and data privacy and quality.

5.3.3 Workshop Feedback

A breakout session on modeling asked participants to respond to the question "What advances are needed in modeling and simulation to enable and support electrochemistry adoption in manufacturing?" Responses included:

- "There should be a dedicated crosscutting modeling center that can engage and help various projects. It could be useful for industry to have a central point of contact to figure out the best modeling strategy and subteam for their need."
- "More user-friendly reactor models at the process simulation level, such as integration into Aspen Plus, ChemCad."
- "Public, open-source models for others to build on, whether techno-economic, transport, electrochemical reactions, or others."
- "Predictive modeling of (electro)chemical degradation under operation would be a very valuable tool."

5.4 Workforce Development

Education to build the next-generation workforce that will be equipped to innovate and apply electrochemistry to manufacturing plants of the future and education to retool the existing workforce are key priorities for AMO. To discuss the topic of education and workforce development, Vimal Chaitanya (New Mexico State University and member of the Education Committee at The Electrochemical Society [ECS]) spoke. In the talk, Vimal identified one of the main challenges in education is that very few colleges and universities offer programs in electrochemistry, highlighting three that have graduate programs: Penn State, Oregon State University, and Columbia University. Professional societies, such as ECS, offer professional development opportunities through awards, educational offerings, professional development, and community engagement. However, these societies could benefit from increased engagement from industry and government. This could help bridge the gap between academia—which makes up the majority of ECS membership—and industry (or the workforce they employ).

In the breakout session focused on education and workforce development, participants discussed what advances are needed to support the advancement of electrochemistry in manufacturing. One of the key barriers that was raised by several participants is the barrier to develop and offer new content within universities. Some indicated a general "inertia" of universities to changing programs; however, others commented on the need for content to follow demand in the form of funded research projects and jobs. The following suggestions and comments were made to address this barrier:

- Short courses or "modules" on electrochemistry and electrochemical manufacturing concepts should be offered. This content should be offered online to overcome the inertia of developing new content and/or changing programs at universities. They could be easily adapted and could be inserted into standard curriculum as appropriate. *DOE could provide seed funding to establish these or similar courses related to focus areas of interest.*
- The curricula developed should emphasize industrial connection and seek industrial internships and industry-funded projects in academia. Growing energy conversion and storage industries are going to provide ample opportunities for research and employment in the next decade.
- University engineering departments should create and maintain robust advisory committees with industry representation. *DOE could sponsor or co-sponsor industry-academia symposia to facilitate this dialogue.* The National Science Foundation has had success with this in the past.
- Coupling electrochemistry with other, related content, such as electrochemical engineering and chemistry, could provide options for future careers and facilitate the connection between electrochemistry fundamentals and applied disciplines. This includes making components, cells, stacks, and production units.

Another barrier identified is the lack of degrees and official certification covering major fundamental aspects of electrochemistry. When the workforce does not get this training in school, their employers want them to receive training in basic electrochemistry and fundamentals related to the processes they interact with. This was confirmed by industry stakeholders present. To address this challenge, the following recommendations were posed:

- From a solid undergraduate basis, the details of electrochemistry can be learned through continuing education and sponsored research at universities. This would ensure students have exposure to a wide range of process technologies but may require universities to support one or a few experts in their chemical or metallurgical engineering departments.
- Textbooks or lab manuals for electrochemistry lab courses are needed to provide hands-on learning.
- Practical engineering and plant management training for the operation and maintenance of electrochemical systems that is different from training electrochemical engineers to develop technology is needed. These may be offered by equipment suppliers or through trade associations and professional societies.

5.5 National Laboratory Capabilities

During the workshop, DOE's national laboratories summarized their capabilities and expertise in electrochemistry through a series of lightning talks.

DOE's national laboratories have extensive experience in electrochemical R&D, including water electrolysis, chemical conversion, and energy conversion and storage, which can be leveraged for electrochemistry in manufacturing. The national laboratories' expertise can be leveraged to meet the current RD&D needs associated with electrochemistry in manufacturing. Specific work includes manufacturing of chemicals, fuels, metals, and electricity conversion, such as:

- CO_2 conversion
- Activation of natural gas
- Nitrogen reduction
- Water electrolysis
- Sulfide and halide production
- Solid oxide fuel cell and flow battery design and manufacturing.

The national laboratories have developed R&D capabilities from individual component development to reactor designs to manufacturing capabilities. These include capabilities in:

- Component research includes materials, membranes, electrolyte development, characterization and degradation, phase interface management, separations, and purifications
- Both *ex situ* and *in situ* testing of components
- Physics-based modeling capabilities at multiple scales

- Reactor development, including research using button cells, short/large stacks, and system integration
- Manufacturing in quality control diagnostics including *in situ* and *ex situ* monitoring
- Manufacturing scale-up of components and reactors, including research in additive manufacturing, roll-to-roll demonstrations, advanced synthesis, and bulk supply of powders.

For further information on laboratory-specific information, Table 1 provides contact information for each presenter, and their presentation titles are available in the Appendix.

Table 1. Laboratory Contacts

National Laboratory	Presenter	Email
Lawrence Berkeley National Laboratory	Nem Danilovic	ndanilovic@lbl.gov
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SLAC National Accelerator Laboratory	Apurva Mehta	mehta@slac.stanford.edu
Savannah River National Laboratory	Scott McWhorter	scott.mcwhorter@srs.gov
National Renewable Energy Laboratory	Bryan Pivovar	bryan.pivovar@nrel.gov

6 Next Steps

The Electrochemistry for Manufacturing workshop successfully collected input from industry, academic, and national lab stakeholders. Input spanned a broad spectrum of industries, including small, medium, and large companies. From this input, it is clear that electrochemistry will play a role in industrial decarbonization, one of the central missions of DOE's AMO. The input obtained in this workshop will inform future programming within AMO in the area of electrochemistry for manufacturing and industrial decarbonization.

Appendix: Detailed Agenda

Day 1: June 15, 2021 – Introduction to the Workshop Series

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1:10–1:25	Connecting Electrochemistry with DOE Priorities	Mike McKittrick, Acting Director, AMO
1:25–2:10	Electrochemistry at DOE Panel Discussion	Kate Peretti, AMO Sonia Hammache, DOE Bioenergy Technologies Office Amishi Kumar, DOE Office of Fossil Energy and Carbon Management Eric Miller, DOE Hydrogen and Fuel Cell Technology Office Peter Faguy, DOE Vehicle Technology Office
2:10–2:15	Break	
2:15–2:35	Introductory Breakout Sessions	Everyone
2:35–2:55	Read-Ahead Overview	Todd Deutsch, National Renewable Energy Laboratory
2:55–3:00	Wrap-Up and Close Session 1	Kate Peretti, AMO

Day 2: June 17, 2021 – Opportunity Identification

1–1:05 p.m. ET	Welcome, Day 1 Recap	Kate Peretti, AMO
1:05–2:10	Electrochemistry in Manufacturing Expert Panel Discussion	Moderator: Ross Brindle, Nexight
	• Translating State-of-the-Art Electrochemistry to Industry	Nirala Singh, University of Michigan
	• Commercial Reactor Overview	Kathy Ayers, Nel Hydrogen
	• Potential Applications Ready for Industry	Shaffiq Jaffer, Total
2:10–2:20	Break	
2:20–2:50	Industry Lightning Talks	Rich Bradshaw, Boston Metal Gareth Williams. Johnson Matthey Sumit Verma, Shell Shankar Chellam, Texas A&M Daniel Bar, Ameridia
2:50–3:30	Application Identification Breakouts	Everyone
3:30–3:35	Wrap-Up and Close Session 2	Kate Peretti, AMO

Day 3: June 22, 2021 – Research, Demonstration, and Development (RD&D) Needs

1–1:05 p.m. ET	Welcome	Kate Peretti, AMO
1:05–1:15	Summary From Day 2	Ross Brindle, Nexight
1:15–1:45	Industry Lightning Talks	Bob Snyder, Chemetry Kendra Kuhl, Opus 12 Daniela Blanco, Sunthetics Todd Brix, OCO EJ Taylor, Faraday Technology
1:45–2:25	RD&D Needs Breakout Sessions	Everyone
2:25–2:35	Break	
2:35–3:30	National Lab Lightning Talks	Representatives From the National Labs
3:30–3:35	Wrap-Up and Close Session 3	Kate Peretti, AMO

Day 4: June 29, 2021 – Crosscutting Enablers

1–1:05 p.m. ET	Welcome	Kate Peretti, AMO
1:05–1:15	Summary from Day 3	Ross Brindle, Nexight
1:15–1:35	Lessons Learned and Considerations for Commercialization of Reactors for H2	Chris Capuano, Nel Hydrogen Hui Xu, Giner
1:35–2:15	State-of-the-art and Challenges in:	
	• Reactor Design and Scale-Up	Miguel Modestino, New York University
	• Modeling and Simulation	Adam Weber, Lawrence Berkeley National Laboratory
	• Standardization and Quality Assurance/Quality Control	Michael Ulsh, National Renewable Energy Laboratory
	• Education and Workforce Development	Vimal Chaitanya, New Mexico State University
2:15–2:25	Break	
2:25–2:55	Crosscutting Enablers Breakouts	Everyone
2:55–3	Next steps and Closeout	Kate Peretti, AMO

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