Hydrogen Production Technologies – 2024

Hydrogen Production Technologies Subprogram Overview

Introduction

The Hydrogen Production Technologies subprogram supports research, development, and demonstration (RD&D) to reduce the cost and improve the efficiency and durability of technologies used to produce hydrogen from diverse clean energy sources (such as wind, solar, hydropower, geothermal, or nuclear power) with natural resources (including water and organic material such as biomass or waste streams). Activities of this subprogram support the Hydrogen Energy Earthshot (Hydrogen Shot) goal of $1 for one kilogram of clean hydrogen in one decade. Subprogram activities also align with the U.S. National Clean Hydrogen Strategy and Roadmap in its direct support of reducing the cost of clean hydrogen, a strategic priority that is foundational to all the priorities identified in the roadmap. The subprogram also incentivizes the development of innovative off-roadmap technologies with potential to meet the Hydrogen Shot goal through the American-Made H-Prize: Hydrogen Shot Incubator, also known as the Hydrogen Shot Incubator Prize.

One RD&D focus of the Hydrogen Production Technologies subprogram is electrolytic water splitting through low- and high-temperature electrolysis using clean, low-carbon energy sources. The Infrastructure Investment and Jobs Act (also known as the Bipartisan Infrastructure Law [BIL]) includes a provision for clean hydrogen production from water electrolysis. Since the enactment of the BIL, all electrolysis activities have been supported through BIL funding, including both the Sect. 816 Clean Hydrogen Electrolysis Program and Sect. 815 Clean Hydrogen Manufacturing and Recycling Program. Electrolysis RD&D has been coordinated through activities with four consortia: Hydrogen from Next-generation Electrolyzers of Water (H2NEW), HydroGEN Advanced Water Splitting Materials (HydroGEN), Electrocatalysis (ElectroCat), and Roll-to-Roll (R2R). Additionally, the Hydrogen and Fuel Cell Technologies Office announced project selections for a national lab call and a $750 million BIL Sect. 815/816 funding opportunity announcement, which included projects supporting RD&D for electrolyzer manufacturing and for new components and materials.

The Hydrogen Production Technologies subprogram also continues to fund non-electrolysis, clean hydrogen production technologies at lower technology readiness levels (TRLs) through the subprogram's annual appropriations. These advanced hydrogen production pathways include direct solar water-splitting processes, such as photoelectrochemical (PEC) and thermochemical (TCH), as well as biological processes that can convert biomass or waste streams into hydrogen.

Goals

The Hydrogen Production Technologies subprogram aims to develop clean, low-carbon hydrogen production technologies. Specific subprogram objectives include the following:

- Develop and validate low-cost, sustainable, and low-carbon-intensity hydrogen production technologies with the potential to meet an intermediate hydrogen production cost target of \$2/kg H_2 by 2026 and the Hydrogen Shot target of \$1/kg H_2 by 2031.
- Develop new, low-cost materials and components to improve performance and durability of hydrogen production technologies, including high- and low-temperature electrolysis and lower-TRL approaches such as PEC and TCH hydrogen production.

Key Milestones

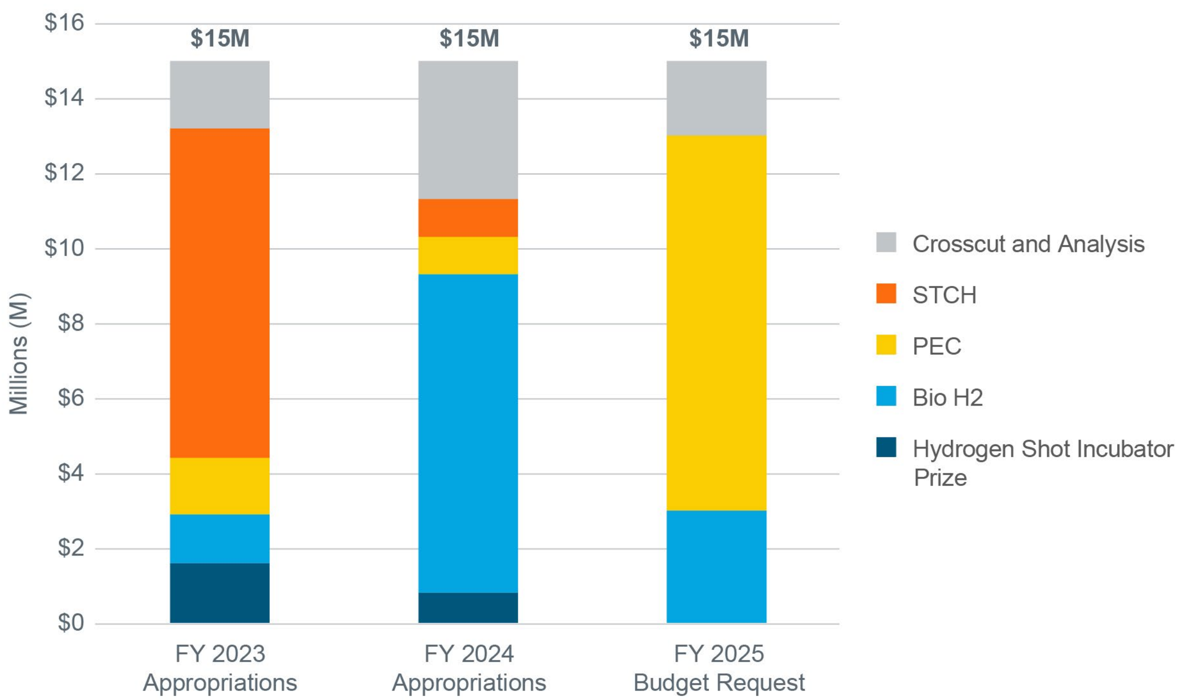
The Hydrogen Production Technologies subprogram has established the following key milestones:

- Develop clean hydrogen production technologies able to meet cost targets of \$2/kg H_2 by 2026 and \$1/kg H_2 by 2031.

- Develop proton exchange membrane electrolyzer technologies able to meet stack targets of $100/kW at 3 A/cm^2 and 1.8 V with an 80,000-hour lifetime by 2026.
- Develop high-temperature electrolyzer technologies able to meet stack targets of $125/kW at 1.2 A/cm^2 and 1.28 V with a 40,000-hour lifetime by 2026.
- Develop technology enabling direct solar-to-hydrogen conversion efficiency of >10% for >500 hours by 2025.

Budget

The Fiscal Year (FY) 2024 appropriation for the Hydrogen Production Technologies subprogram was $15 million, which covers all non-electrolysis work, with an emphasis on advanced pathways. All electrolysis work is supported under the BIL Sect. 816 Clean Hydrogen Electrolysis Program and Sect. 815 Clean Hydrogen Manufacturing and Recycling Program, which, in total, provide more than $200 million/year.



The funding received for FY 2023 and FY 2024 ($15 million each) supported direct solar water-splitting research, including work toward advancing PEC and TCH durability and efficiency; hydrogen production cost analysis; and biological hydrogen production using microbial processes and carbon-negative pathways, including a partnership with the Office of Fossil Energy and Carbon Management on small biomass carbon removal and storage pilots with hydrogen production. Funding also supported the Hydrogen Shot Incubator Prize to incentivize development of innovative off-roadmap technologies with the potential to produce clean hydrogen at $1/kg in one decade. The FY 2025 request is $15 million to continue research and development (R&D) in advanced pathways for hydrogen production.

In FY 2024, the BIL (Sect. 816, in particular, and provisions in Sect. 815) funded a range of electrolysis activities to improve efficiency, increase durability, and reduce the cost of producing clean hydrogen using electrolyzers to less than $2/kg by 2026. Emphasis is on efforts to improve and develop new materials and components for multiple types of electrolyzers, as well as to advance manufacturing technologies to get to economies of scale for electrolyzer manufacturing. A total of 36 projects with $1.1 billion in total project costs (~$470 million federal cost share) were competitively selected. One outcome will be to enable 10 GW/yr of electrolyzer manufacturing capacity. Another 11 projects on five electrolyzer technologies across 10 national labs were competitively selected under the Clean Hydrogen Electrolysis Program Lab Call.

BIL Sect. 816 funding continued to support national-lab-led consortia (H2NEW, HydroGEN, and ElectroCat) focused on electrolysis R&D, as well as efforts to develop megawatt-scale electrolyzer test and validation facilities. BIL Sect. 815 funding supported a recovery and recycling consortium for both electrolyzers and fuel cells. In addition, a national-lab-led consortium (R2R) focused on roll-to-roll manufacturing for both electrolyzers and fuel cells was launched and co-funded by BIL Sect. 815 and Sect. 816.

Annual Merit Review Results

During the 2024 Annual Merit Review, 52 projects funded by the Hydrogen Production Technologies subprogram were presented, and 21 were reviewed, including 10 HydroGEN Seedling projects (a breakdown of number of projects reviewed by budget category is shown in the table on the right). The 10 HydroGEN Seedling projects received scores ranging from 3.1 to 3.6, with an average score of 3.3. The other 11 reviewed projects received scores ranging from 2.7 to 3.7, with an average score of 3.3. The complete list of reviewed projects and the average score for each can be found in the Prologue Table.

Number of Projects Reviewed by Budget Category	
BioH2	3
PEC	7
TCH	3
Electrolysis[a]	5
Crosscut and Analysis	3

[a] Not including FC-160 or MNF-BIL-001, which are reviewed and scored in the Fuel Cell Technologies section.

Two additional projects include electrolysis work that is funded in part by the Hydrogen Production Technologies subprogram. Please refer to the Fuel Cell Technologies subprogram section to find results for these projects:

- FC-160: ElectroCat 2.0 (Electrocatalysis Consortium)
- MNF-BIL-001: Roll-to-Roll Consortium.

Following are reports for the 21 reviewed projects. Each report contains a project summary, the project's overall score and average scores for each question, and the project-level reviewer comments.

Project #ELY-BIL-001: Megawatt-Scale Low-Temperature Electrolyzer Research Capability

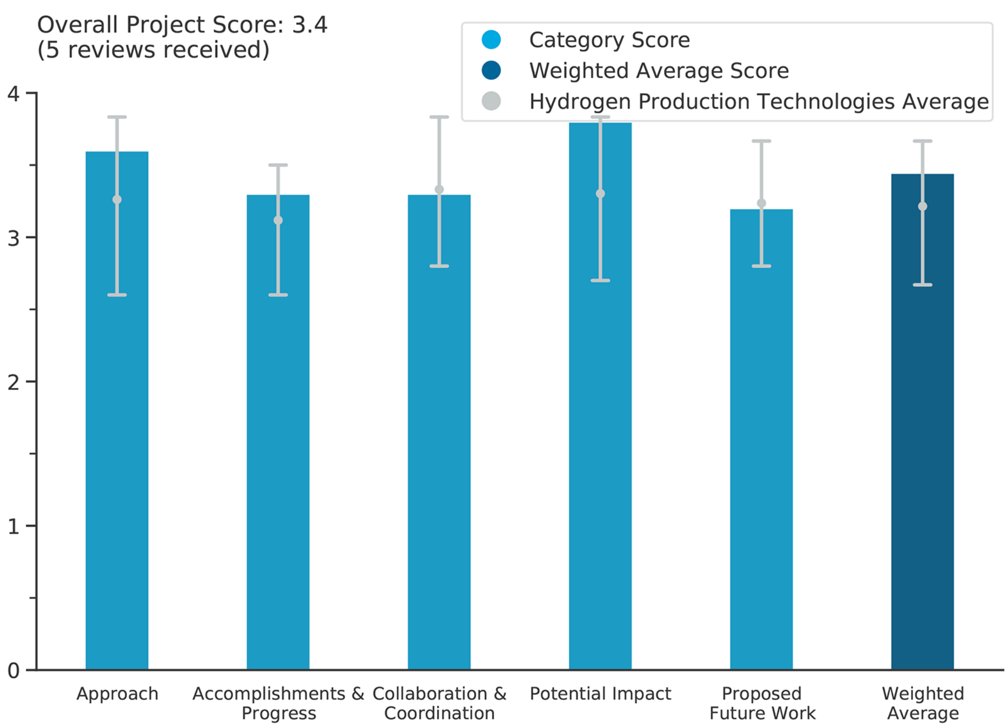
Daniel Leighton, National Renewable Energy Laboratory

DOE Contract #	WBS 12.5.0.501
Start and End Dates	4/18/2023
Partners/Collaborators	
Barriers Addressed	• Demonstration and performance evaluation of low-temperature electrolysis stacks and systems up to 10 MW • Production of hydrogen using directly coupled zero-carbon energy sources

Project Goal and Brief Summary

The project goal is to support industry partners participating in the DOE Clean Hydrogen Electrolysis Program by developing a flexible, multi-megawatt low-temperature electrolyzer research capability at the National Renewable Energy Laboratory (NREL) Flatirons Campus. The project aims to facilitate the flexible operation and evaluation of proton exchange membrane (PEM) and liquid alkaline electrolyzers, ultimately contributing to the commercialization of these technologies and supporting the Hydrogen Shot goal of $1/kg H_2 within a decade.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Hydrogen Production Technologies projects.

Question 1: Approach to performing the work

This project was rated **3.6** for identifying and addressing objectives and barriers and for project design, feasibility, and integration with other relevant efforts.

- NREL has a clear approach to completing the work proposed, as highlighted in the presentation. The critical barriers have been identified and are being addressed. The proposed test facility will benefit and potentially allow for standardization across the industry. NREL is using the safety process required by NREL's prime contract with DOE. It might be of benefit to industry to publish the hydrogen safety processes NREL follows such that others might follow them as a template. The timeline discussed in the proposed future work seems well-planned and should be achievable.
- The team is asked to elaborate on how NREL will ensure the absence of any bias/unfair allocation of time for customers/vendors/technologies signing up for evaluation and testing. The team should describe how this process will work in practice and determine whether it will be on a first-come, first-served basis. If so, the team should also determine whether there will be any entry criteria to determine eligibility for testing. If the vendor/customer/technology is not funded via public grants (and is thus proprietary), the team should ask themselves what benefit it will add to the common knowledge of the community. The team should also ask whether there will be a requirement that testing/durability data must be disclosed to the community to be eligible for such tests. If this criterion is not considered by the team, they should be able to justify their decision against it.
    - The team should list/discuss electrolyzer vendors under consideration and testing, or interconnection studies, both for PEM and alkaline. The team should name them. If the research is proprietary, the team should determine what value such future tests provide to the wider community. Proprietary tests can be conducted on the customer's/vendor's time and resources. The NREL platform should serve the wider research and engineering community and be open to the public to further advance common knowledge to accelerate knowledge-sharing.
    - During the next update, the team should consider spending 30 seconds to a minute explaining coupling with renewables and perhaps introduce the big picture, which can be later addressed in detail in another presentation.
    - The team should elaborate on how a flexible balance of plant (BOP) can exist to accommodate various technologies. Usually, stacks are designed around a specific BOP configuration to increase system efficiency. The team should determine the priorities in terms of measured variables if maximum system efficiency cannot be achieved. The team should also determine how tests will be compared/normalized against each other.

  Overall, the project has resulted in great work. The reviewer looks forward to following progress at NREL. The team should consider these questions and recommendations as the reviewer's best attempt to help accelerate successful development of PEM and alkaline testing platforms at NREL.
- It is great to see NREL providing a stack/system testing platform for various vendors and companies eager to further develop/characterize/investigate their technologies. The presentation addresses the major objectives well. The reviewer looks forward to seeing data from all tests and comparisons across the data. Also, the reviewer challenges NREL to consider incorporating internal research and development technology to be tested in stacks and systems and working with vendors to incorporate such technology in commercial stacks. There is limited time to share the updates, and possibly some of the questions are already being addressed but were not presented for the obvious reason of the allocated presentation time. However, it would be valuable, during the next update, for the team to elaborate on status/progress regarding the following: (1) water rights and whether they are fully secured, (2) wastewater discharge permitting and where discharged water will go, (3) an air permit for possible venting/flaring, and (4) how lye will be recycled from the site for the alkaline systems.
- Expansion to 10 MW testing will tremendously expand the testing capabilities. This will be very helpful for the electrolyzer industries. The project needs to explain how the test capabilities will be distributed between alkaline and PEM electroyzers. The project needs to address how to explain the current and voltage, as the users have different stack designs. The project needs to develop a comprehensive testing protocol. It seems that the principal investigator discussed only integration with the wind turbine and did not address solar

energy. It is recommended that the project use an external consultant to develop a comprehensive and independent hazard and operability (HAZOP) study.

- The project demonstrated having identified methods to have parallel work completed to ensure the timeline and goal are achieved.

Question 2: Accomplishments and progress

This project was rated **3.3** for its accomplishments and progress toward overall project and DOE goals.

- NREL has shown clear progress toward expanding the Advanced Research on Integrated Energy Systems (ARIES) capability at the Flatirons Campus to operate multi-megawatt low-temperature electrolyzers. The full system layout, BOP, and detailed piping and instrumentation diagrams presented show great progress.
- The project has just started. It is unclear whether the design has been completed, but the project has already spent $18,630,000. Internal hydrogen HAZOP needs are insufficiently addressed. The project needs an external consultant.
- The project team has identified clearly that water supply is a challenge. A clear plan with updated progress was demonstrated to address the supply of water to ensure project success.

Question 3: Collaboration and coordination

This project was rated **3.3** for its engagement with and coordination of project partners and interaction with other entities.

- The project team mentioned collaboration and requested that original equipment manufacturers (OEMs) provide their input to ensure the system developed can accommodate the variety of requirements from different OEMs.
- NREL is collaborating and coordinating with both PEM and liquid alkaline commercial vendors. It is unclear whether stack purchases are being funded through this effort. If NREL is purchasing stacks, it might be beneficial to list the manufacturers of the stacks being purchased. It might also be beneficial to publish data benchmarking efficiencies.
- The project team needs to listen to the test demands of the industries. The project also needs to have an external consultant to do hydrogen safety.

Question 4: Potential impact

This project was rated **3.8** for supporting and advancing progress toward Hydrogen Program goals and objectives.

- This project is strongly aligned with the Hydrogen Program's goals. Testing is a pain point for every large-scale (>1 MW) water electrolysis stack manufacturer. Being able to benchmark stacks from various manufacturers could help guide the research required to meet hydrogen production targets of $1/kg.
- The development of this project is essential to reducing the risks and accelerating the success of electrolyzer manufacturing and development at scale.
- If successful, the project will address high demands for large stack testing from the new electrolyzer developers.

Question 5: Proposed future work

This project was rated **3.2** for effective and logical planning.

- NREL has presented a project that could benefit all in the water electrolysis industry. The plans build on the vision previously set forth in ARIES. The proposed future work can be summarized as Design, Procure, and Build, all logically laid out.
- The project demonstrates a clear path and plan for the development of testing capabilities for PEM.
- The future plan is too simple. It needs to have more explanations for each box.

Project strengths:

- The project's strength is in addressing testing/benchmarking of large-format (>1 MW) water electrolysis stacks, a capability that can benefit the water electrolysis community. The capability for testing ~4 MW stacks will be prized.
- Expansion to 10 MW testing will tremendously expand the testing capabilities, which will be very helpful for the electrolyzer industries.
- Capabilities to test full-scale electrolyzers are coupled with intermittent renewable energy.
- There is a clearly defined plan and progress demonstrated.

Project weaknesses:

- There are no project weaknesses in this reporting period.
- The project has a very large amount of funding. It has received $18,630,000. It is unclear how that amount was spent. Internal hydrogen HAZOP needs are insufficiently addressed. The project needs an external consultant.
- A description of the plan for alkaline electrolyzers was not presented.

Recommendations for additions/deletions to project scope:

- NREL has demonstrated the capability and knowledge of testing PEM stacks and developing testing systems. The project team mentioned the plan to develop alkaline testing capabilities; however, a plan focused on alkaline testing capabilities was not presented.
- The team needs to better explain how the spending was commensurate with the project progress and milestone delivery.
- A task to benchmark commercially available large-format (100 MW) stacks could be beneficial.

Project #P-148: HydroGEN Overview: A Consortium on Advanced Water-Splitting Materials

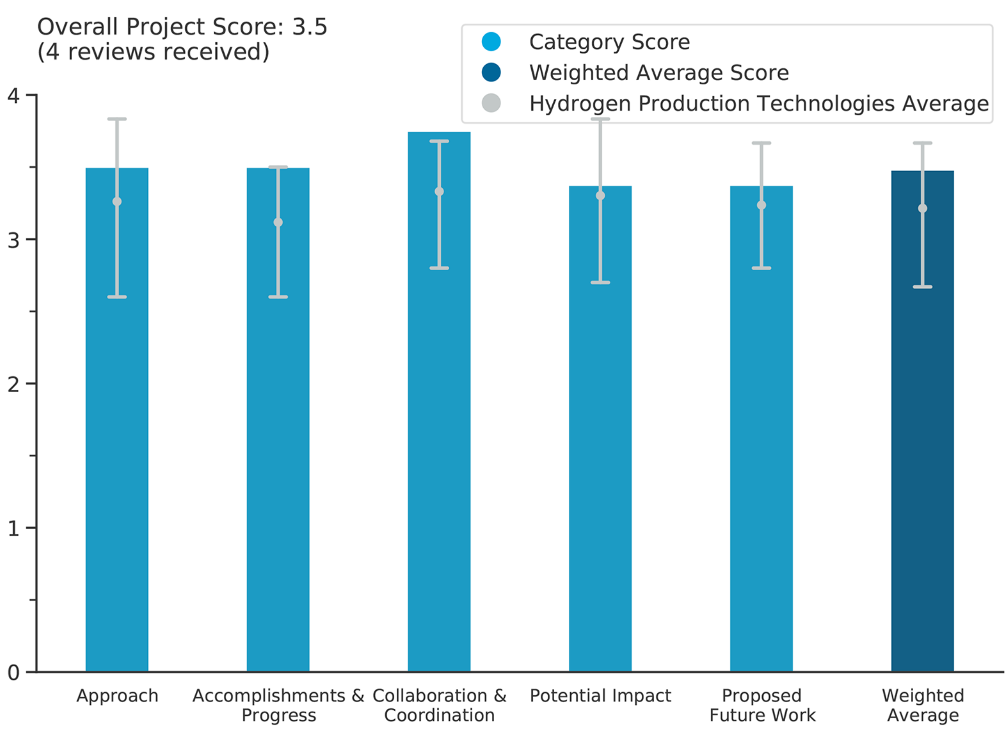
Huyen Dinh, National Renewable Energy Laboratory

DOE Contract #	WBS 2.7.0.518 (HydroGEN 2.0) and 2.7.0.513 (Node Support)
Start and End Dates	6/1/2016
Partners/Collaborators	Lawrence Berkeley National Laboratory, Sandia National Laboratories, Idaho National Laboratory, Lawrence Livermore National Laboratory
Barriers Addressed	• Cost • Efficiency • Durability

Project Goal and Brief Summary

The HydroGEN Advanced Water Splitting Materials Consortium's (HydroGEN's) objective is to facilitate collaborations between federal laboratories, academia, and industry to evaluate and accelerate the research and development (R&D) of innovative, advanced materials that are critical and necessary to advanced water-splitting (AWS) technologies for clean, sustainable, and low-cost hydrogen production. Water-splitting technology pathways supported by HydroGEN include photoelectrochemical (PEC), solar thermochemical (STCH), low-temperature electrolysis (LTE), and high-temperature electrolysis (HTE). In addition to collaborating with industry and academia, HydroGEN uses a synergetic, multi-laboratory approach, utilizing and integrating the labs' world-class capabilities to address the critical research gaps identified by the lab teams and HydroGEN Benchmarking and Protocol workshops in each of the AWS technologies.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Hydrogen Production Technologies projects.

Question 1: Approach to performing the work

This project was rated **3.5** for identifying and addressing objectives and barriers and for project design, feasibility, and integration with other relevant efforts.

- Below is a discussion of the project objectives and critical barriers.
  - The project has clearly identified the objectives. The primary objective of this project is to accelerate foundational R&D of innovative materials for AWS technologies to enable low-cost clean hydrogen production ($1/kg H_2). This objective is clearly defined and aligns well with national goals.
  - The project focuses on key barriers such as cost, efficiency, and durability across all AWS technologies. Each technology area (LTE, HTE, PEC, STCH) has specific targets and milestones, demonstrating a clear understanding of the challenges involved.
  - Regarding the safety plan, although this project is not required to submit a safety plan for review by the Hydrogen Safety Panel, each participating national lab adheres to rigorous DOE-approved safety procedures. These include integrated safety management processes that are regularly reviewed and monitored.
  - The project emphasizes a strong safety culture with principles ensuring safe operations, hazard evaluation, and continuous improvement. The project includes engineered control strategies specific to hydrogen operations.
  - Regarding the diversity, equity, inclusion, and accessibility (DEIA) plan and initiatives, the project has recruited diverse talent through programs such as the Graduate Education for Minorities (GEM) program, Student Training in Applied Research (STAR) program, and Science Undergraduate Laboratory Internship (SULI) program. The project has also initiated collaborations with institutions such as the University of Puerto Rico, and there are efforts to actively mentor diverse researchers.
  - Regarding the community benefits plan (CBP) and community engagement, the project plans to develop DEIA and CBPs further, including activities such as participating in the Faculty Applied Clean Energy Science (FACES) program, visiting minority-serving institutions (MSIs) for talks and recruitment, and engaging students at levels from kindergarten through grade 12 in AWS technologies. In terms of current implementation, 11 new seedlings, awarded through funding opportunity announcements (FOAs), have incorporated DEIA/CBPs, highlighting efforts to recruit and engage underrepresented groups and educate students on AWS technologies.
  - The project is well-designed and feasible, with a clear structure, defined goals, and a collaborative framework leveraging the strengths of multiple national labs and partners. The approach includes theory-guided R&D, advanced characterization, and cross-disciplinary collaboration, ensuring comprehensive and feasible research.
  - Regarding integration with relevant efforts, the project effectively integrates with other DOE initiatives, in particular H2@Scale, and collaborates with industry, universities, and other research institutions. This integration maximizes resource utilization and fosters innovation.
  - The project takes a comprehensive approach, addressing most major AWS pathways and ensuring a holistic approach to clean hydrogen production. The development of standardized protocols and benchmarking practices enhances the reliability and comparability of research outcomes across different technologies.

  Considering all the aspects—project objectives, safety plan, DEIA plan, and overall project design and feasibility—the project received a high rating that reflects a high level of excellence in its approach, execution, and potential impact. The project demonstrates strong alignment with national clean energy goals, effective collaboration, and a robust framework for advancing advanced clean hydrogen production technologies.
- HydroGEN has a difficult task in coordinating activities across multiple technologies, and the principal investigators do an excellent job of managing this complex task. It is very good to see the breakdown of budget between lab calls and FOA support, which has not been as transparent in the past. A good balance of these activities is important for both HydroGEN and H2NEW (Hydrogen from Next-generation Electrolyzers of Water) to ensure relevance while giving the labs freedom to grow new capabilities and innovative approaches.

- The HydroGEN consortium has a massive portfolio of technologies and projects. There are sufficient cross-cutting efforts, particularly in materials, to warrant this approach. The consortium is doing an outstanding job in its organization and pulling together quite disparate technologies. The efforts on outreach and education are very impressive and set examples that other consortiums may follow to engage a broader community. Good advancements are being made in anion exchange membrane (AEM) water electrolysis (AEMWE) electrode development and the role of ionomer. More details on catalyst morphology and its impact should be captured and presented. A unified assessment of the various technology thrusts should be created and presented—perhaps a spider chart with plots for all the technologies, including performance, durability, and cost metrics, as well as the largest scale of demonstration to date and technology readiness level (TRL) assessment. Some of the technology-specific spider charts need up bounds that are related to ultimate goals or some other targets. The proton-conducting solid oxide electrolyzer cell (p-SOEC) spider chart particularly needs to be updated with upper-level values consistent with commercially viable value.
- It is good to develop advanced electrolysis technologies. Some projects under HydroGEN have generated promising results. However, the project needs an overall roadmap (e.g., TRL) for STCH, PEC, and AEM. The project has a large budget: $10 million for 2023 and $9.6 million for 2024. The project team needs to explain how the funding was spent commensurate with milestone delivery. It would be helpful if the project could show how many of the technologies it has developed have been higher TRLs and are getting closer to commercialization.

Question 2: Accomplishments and progress

This project was rated **3.5** for its accomplishments and progress toward overall project and DOE goals.

- Below is a discussion of the progress toward project objectives.
    - Significant milestones have been achieved. The project has demonstrated substantial progress in advancing material innovations for AWS technologies. Examples include performance improvements in LTE through ionomer studies, enhanced durability and efficiency in HTE, stable PEC devices with high solar-to-hydrogen efficiency, and the development of new STCH materials.
    - The project has well-defined performance indicators, such as cost targets ($1/kg H_2), efficiency metrics, and durability benchmarks. Regular updates and milestones show steady progress toward these goals, with achievements in both laboratory-scale research and initial steps toward scalability.
    - The project is addressing critical barriers to DOE goals and has made notable advancements in reducing costs and improving the efficiency and durability of AWS technologies. For instance, HTE projects have achieved significant current density and durability improvements, while PEC projects have demonstrated high efficiency with long-term stability. In addition, the project leverages some cross-technology insights to address barriers. For example, the understanding of ionomer stability in LTE informs similar challenges in HTE and PEC, enhancing the overall research impact.
    - The project is incorporating safety considerations. Regarding safety culture, each participating national lab follows rigorous DOE-approved safety procedures, ensuring that all research activities comply with high safety standards. These efforts include regular reviews and hazard assessments as part of the integrated safety management process. In addition, the project employs engineered control strategies for hydrogen operations, such as robust ventilation systems and high-quality materials to prevent hydrogen embrittlement, enhancing the overall safety of the research environment.
    - Regarding the DEIA plan or CBP, the project has actively recruited diverse talent and engaged in various DEIA initiatives, such as the GEM, STAR, and SULI programs. Additionally, the project has established collaborations with MSIs and is planning further DEIA activities. Further, the implementation of DEIA/CBPs in new FOA-awarded projects demonstrates a commitment to diversity and community engagement. However, there is room for further development and expansion of these plans to maximize their impact.
    - Considering all the aspects—progress toward objectives, addressing critical barriers, safety incorporation, and DEIA implementation—the project has shown excellent progress in advancing

AWS technologies, addressing key barriers, and incorporating safety and DEIA considerations into its research framework.

- For much less funding than some major consortia (Energy Frontier Research Centers, H2NEW, etc.) across a high number of projects, the output is impressive. There have been significant papers, project output, support of FOA projects, etc. It was also good to see new emphasis on safety and CBP, even if not "required." Metrics were proposed for all four technologies, which has been a challenge but represents an important starting point.
  - LTE: Good progress was demonstrated on AEM understanding, in collaboration with industry/ academic partners.
  - HTE: Work focused on progress on SOEC durability, modeling, and new testing protocols for dynamic operation.
  - PEC: Mechanistic work focused on density functional theory and fundamentals, while device testing was more focused on practical environments.
  - STCH: Significant modeling was performed, particularly degradation modeling for materials and devices. High-throughput screening is also being developed.
- The teams have made excellent progress. Year-over-year advancements are indicated for many of the sub-programs. The AEMWE analysis of ionomer stability and catalyst integration are very valuable to the AEMWE R&D community.
- For the reviewer's convenience, roadmaps for PEC and STCH technologies, along with progress made in past 10 decades, are needed. For the AEM electrolysis, regarding ionomer–catalyst interactions, the mechanisms are unclear. Regarding Inconel, it seems that stainless steel ability may be an issue, and it is unclear whether there is any durability data. For stainless steel porous transport layers, after 1,400 hours, there are concerns of surface changes and membrane contamination.

Question 3: Collaboration and coordination

This project was rated **3.8** for its engagement with and coordination of project partners and interaction with other entities.

- Below is the discussion on engagement and coordination with project partners.
  - The project employs a consortium model that effectively engages multiple national labs (National Renewable Energy Laboratory, Lawrence Berkeley National Laboratory, Idaho National Laboratory, Sandia National Laboratories, and Lawrence Livermore National Laboratory), universities, and industrial partners. This structure facilitates comprehensive collaboration and resource-sharing. The project demonstrates strong coordination among national labs, leveraging their unique capabilities and expertise to address complex challenges in AWS technologies. This inter-lab collaboration accelerates progress and enhances the quality of research outputs.
  - The project is well-integrated with other DOE initiatives, in particular H2@Scale. This alignment ensures that the project contributes to and benefits from broader national energy goals and efforts.
  - The project actively shares knowledge and data through the HydroGEN and H2NEW Data Hub, community benchmarking workshops, and numerous publications. These efforts promote wider dissemination of findings and foster cross-pollination of ideas across different projects.
  - The project has made commendable efforts to engage with MSIs and minority business enterprises. Initiatives such as the collaboration with the University of Puerto Rico and recruitment through programs such as GEM and STAR highlight these efforts.
  - The project has outlined plans to further enhance DEIA engagement, including visiting MSIs, developing DEIA minutes in meetings, and incorporating DEIA elements in new projects. However, the current level of engagement can be expanded further to maximize impact.
  - Considering all the aspects—engagement and coordination with partners, interaction with other entities, and collaboration with MSIs and minority business enterprises—the project demonstrates outstanding collaboration and coordination, effectively leveraging partnerships to accelerate progress and enhance its impact, with ongoing efforts to strengthen diversity and inclusion.

- HydroGEN interacts with many institutions both within and outside the consortium. For a community that has not always had to work together and is more used to individual contributor projects, the collaboration within the labs is impressive. Employee exchange for PEC seems like a very effective exercise to transfer knowledge. The mechanism for HydroGEN to work with outside partners also has major advantages over the old model, in which project partners not only had to fund the lab work but also provide additional cost share.
- The consortium is large and features fairly disparate approaches to generating hydrogen. However, an impressive degree of coordination is demonstrated. The coordination of the AEMWE work with that in the Electrocatalysis Consortium (ElectroCat) should be further elaborated or increased. There is a concern about duplicative efforts or under-utilized synergies.
- There is collaboration with national laboratories, but more collaboration with industry is needed.

Question 4: Potential impact

This project was rated **3.4** for supporting and advancing progress toward Hydrogen Program goals and objectives.

- Below is the discussion on the project's potential impact.
    - The project has made significant progress toward its specific performance targets, including achieving cost-reduction pathways, efficiency improvements, and enhanced durability across different water-splitting technologies. For example, the LTE projects have made strides in ionomer research, leading to better performance and stability. The project's comprehensive approach addresses most major pathways (LTE, HTE, PEC, STCH) for AWS, ensuring that advancements are made across the board. This holistic strategy increases the likelihood of meeting the specific performance targets.
    - Regarding advancement toward Hydrogen Program goals and objectives, the project is closely aligned with the Hydrogen Program goals, particularly the H2@Scale initiative, which aims to integrate hydrogen production into the national energy framework. By focusing on producing clean hydrogen at $1/kg, the project directly supports the goal of making clean hydrogen a competitive energy carrier and feedstock. The project's focus on developing sustainable and low-cost hydrogen production technologies is highly relevant to national and global clean energy transitions. Successful outcomes from the project can significantly reduce greenhouse gas emissions and enhance energy security.
    - The project's research has the potential to revolutionize clean hydrogen production by making it more efficient, cost-effective, and durable. The impact of achieving the project's targets extends beyond energy production, influencing sectors such as transportation, industry, and long-duration storage. The long-term benefits of the project include creating a more sustainable, resilient, and secure energy future; reducing reliance on fossil fuels; and promoting technology innovation. The project's advancements contribute to a cleaner environment and economic growth through the creation of new markets and job opportunities.
    - Considering all aspects—support for specific performance targets, advancement toward Hydrogen Program goals, and overall relevance and impact—the project demonstrates excellent potential to advance clean hydrogen production technologies and contribute significantly to achieving DOE goals, positioning the project as a key player in the transition to a sustainable energy future.
- This project has potential for high-level impact, providing support to several lower-TRL approaches to generating hydrogen that could address challenges with incumbent hydrogen production technologies. The AEMWE sub-program could help enable electrolyzers without per- and polyfluoroalkyl substances (PFAS).
- All technologies seem to have worked diligently to develop more concrete metrics, which is not simple because of the interacting variables. While the consortium and DOE should be open to modifying the targets if fundamental research shows they no longer represent the best pathways, having metrics at least focuses the work and allows for better measurement of progress.
- The project is meaningful for next-generation clean hydrogen technology. The project started in 2016. The presentation should tell where the project started and where it would go. It is unclear whether there are any funded projects that could improve the TRL from <2 to >5.

Question 5: Proposed future work

This project was rated **3.4** for effective and logical planning.

- Below is the discussion on proposed future work.
    - Regarding logical and effective planning, the project has laid out comprehensive plans for its next steps, focusing on critical areas such as improving material durability, enhancing efficiency, and reducing costs. The project outlines specific research goals and milestones for each AWS technology, ensuring a clear and logical progression. The future work includes well-defined decision points that allow for regular assessment of progress and adjustments as needed. This iterative approach helps in maintaining the project's focus and direction.
    - The project has effectively identified key barriers to achieving its goals, such as cost, efficiency, and durability challenges in various AWS technologies. By addressing these barriers head-on, the project ensures that its research remains relevant and impactful. The proposed future work targets these barriers through focused research efforts. For example, in LTE, there are plans to optimize catalyst layer composition and processing techniques, while in PEC, the focus is on understanding and mitigating device degradation mechanisms.
    - The project has incorporated risk mitigation strategies into its future plans, such as developing accelerated stress tests (ASTs) to understand durability in LTE and exploring alternative cell architectures in HTE. These strategies help to anticipate potential challenges and proactively address them. The project outlines alternate pathways to achieve its goals, ensuring flexibility in its approach. For instance, if certain materials or processes do not yield the desired results, the project has identified alternative methods and technologies to explore.
    - Considering all aspects—logical planning, consideration of barriers, and risk mitigation—the project demonstrates a solid and strategic approach to planning its next steps, effectively addressing potential challenges and ensuring continued progress toward its objectives.
- The proposed consortium work is important and should be prioritized for funding. For example, reactor development for PEC and STCH is vital to the community's ability to test new materials against existing benchmarks and beyond bench testing indoors. Outreach and communication are also necessary to get the most value from HydroGEN.
- The AEMWE proposed future work on catalyst layer composition and processing is merited. Alternative electrode structures and electrode-optimized catalyst morphologies should be given consideration. Component-specific ASTs for AEMWE are needed; this is listed as future work. Separate ASTs for the AEM and the electrode ionomer are needed (in addition to catalyst ASTs).
- The future plan is generally good, but it should have an overall roadmap.

Project strengths:

- The project is conducting comprehensive research that covers major AWS technologies, providing a holistic approach to clean hydrogen production. In addition, there is a strong collaborative network. The consortium leverages the strengths of multiple national labs and partners, facilitating cross-disciplinary research and accelerating technology development. Finally, the project focuses on durability and efficiency. Addressing these critical aspects ensures that developed technologies will be viable in real-world applications.
- The strength of this project is its comprehensive approach to advancing lower-TRL hydrogen production technologies leveraging cross-cutting techniques for materials. Another strength is the outreach and broad impact component of the consortium.
- The project has a cross-functional team and develops diversified technologies. It builds the foundation for the next-generation hydrogen technologies.
- It was very good to see the team jointly present, which gave a better flavor for how the team works together as a consortium. Also, more transparency on spending and definitions of draft metrics were good additions.

Project weaknesses:

- Regarding early-stage focus, while early-stage R&D is critical, the transition from lab-scale innovations to commercial-scale applications remains a significant challenge. There is a risk that promising technologies might not be fully developed or might face hurdles in scaling up to commercial production levels. Regarding current DEIA implementation, there may be limited reach and impact. Although the project has taken commendable steps toward DEIA, the current level of engagement can be expanded. The existing initiatives, while valuable, might not fully capture the potential diversity and inclusivity benefits that could be achieved with a more comprehensive strategy. Regarding coordination and integration, there is potential for enhanced coordination. Despite strong collaboration, there is always room for improved coordination and integration across different technology areas. More structured mechanisms could further ensure regular, systematic cross-fertilization and maximize the use of shared insights and technologies.
- The project's main weakness is the diversity of approaches and establishment of metrics that apply to all systems to perform technology-to-technology comparisons.
- The project has not had a clear roadmap since this program was launched in 2016.
- The main past/existing weaknesses (lack of significant durability testing, target setting, etc.) are being addressed.

Recommendations for additions/deletions to project scope:

- The recommendations are below.
    - Regarding the focus on commercialization pathways, the project should develop clear plans for transitioning from lab-scale to commercial-scale applications. This could involve engaging with industry partners early, focusing on scalable processes and ones that can benefit from learning curves similar to photovoltaics, and conducting demonstration projects to gain insights into commercial viability. In terms of market readiness, the project should identify potential market barriers and work on solutions to ensure that developed technologies can if successful be adopted widely.
    - DEIA efforts could be enhanced. Engagement could be expanded by broadening the scope of DEIA activities to include more MSIs, diverse research groups, and underrepresented communities. For example, the project might consider increasing its outreach efforts, offering more internships and mentorship programs, and creating partnerships with organizations focused on diversity. In addition, the project could regularly monitor and evaluate DEIA efforts to measure their impact and effectiveness. Strategies should be adjusted as needed to ensure that diversity and inclusivity goals are being met comprehensively.
    - Coordination and integration could be improved with structured collaboration mechanisms. Dedicated cross-technology working groups could be established that focus on integrating insights and innovations from different AWS approaches. These groups can meet regularly to share progress, discuss challenges, brainstorm solutions, and focus on developing common apples-to-apples metrics beyond just the levelized cost of hydrogen. In addition, the project could implement biannual or annual reviews specifically aimed at cross-technology integration. These reviews could help identify areas where one technology's advancements can benefit others, fostering a more cohesive and synergistic research environment.
    - Regular and updated techno-economic analysis (TEA) should be conducted to inform research directions and ensure focus on the most impactful innovations. TEA can help in aligning the R&D efforts with market realities. In addition, TEA findings can be used to refine performance metrics, ensuring that research targets are realistic and aligned with economic viability. It might help in setting clearer goals and evaluating progress more effectively.
- It is highly recommended that a clear overall roadmap be added to this project.
- There are no suggestions regarding any changes to the scope.

Project #P-170: Benchmarking Advanced Water-Splitting Technologies: Best Practices in Materials Characterization

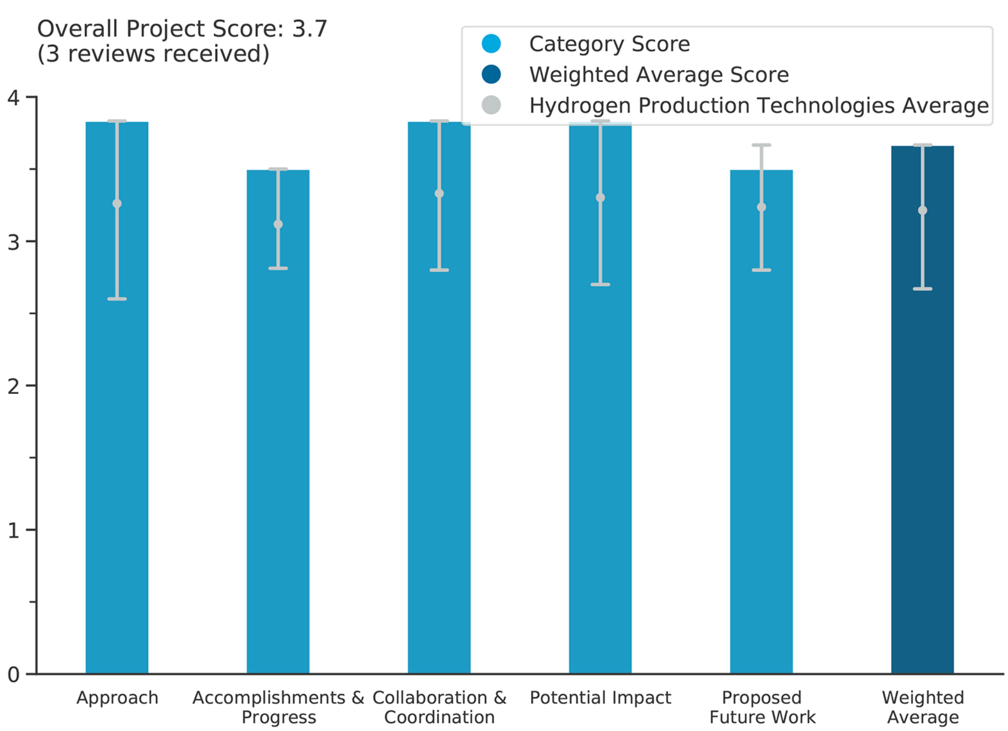
Olga Marina, Pacific Northwest National Laboratory

DOE Contract #	WBS 2.3.0.708
Start and End Dates	10/20/2021
Partners/Collaborators	Nel Hydrogen, Arizona State University, California Institute of Technology, H2 Technology Consulting LLC
Barriers Addressed	• Generate hydrogen using different technologies • Improve energy resilience and sustainability • Establish a universal system for benchmarking • Provide access to benchmarking results to community

Project Goal and Brief Summary

Making significant advances in advanced water-splitting technologies (AWST) requires the effective use of AWST research, development, and demonstration resources. To that end, this project will help establish a universal system for benchmarking. Researchers will develop and verify protocols for AWST validation testing and improvement within the categories of low-temperature electrolysis (LTE), high-temperature electrolysis, photoelectrochemical, and solar thermochemical hydrogen. This project will contribute to the strategic coordination of benchmarking in the water-splitting community and the advancement of test protocols.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Hydrogen Production Technologies projects.

Question 1: Approach to performing the work

This project was rated **3.8** for identifying and addressing objectives and barriers and for project design, feasibility, and integration with other relevant efforts.

- The strategic coordination of benchmarking and protocols is more critical than ever for the advanced water-splitting community, as dozens of new hydrogen production funding opportunity announcement (FOA) projects are beginning in 2024. The approach is sound: benchmarking and protocol development through community engagement, workshops, round-robin validation, and strategic publications across the four topic areas.
- There is a good focus on benchmarking and measurement protocols, as opposed to going straight to analysis. The idea of a round-robin testing verification program with the community is great.
- This approach contributes to overcoming some barriers in the scientific community.

Question 2: Accomplishments and progress

This project was rated **3.5** for its accomplishments and progress toward overall project and DOE goals.

- It is nice to see the project working on Volume 2 of the protocols technical publication and the sixth workshop. There is good current, consistent progress within the mature project.
- The protocol upload to the Data Hub and in-progress publication of Volume 2 of protocols in Frontiers lead the list of significant accomplishments and progress of the benchmarking effort. The Quarter 2 (Q2) and Q3 milestones are rather vague. The milestone descriptions could have indicated the number of articles to identify, as well as a specific metric associated with the development of a detailed protocol validation plan.
- The greatest strength is the educational aspect of the effort across the scientific community, which, according to the publication and use of the protocols, is significant. The key question is whether electrolyzer performance can reach an optimum if operated at some best protocol. It is unclear whether there is a best protocol. Perhaps the benefit of developing protocols is just not operating in the many incorrect, unverifiable, unreproducible, and inconsistent ways that are unshareable and useless in the scientific community.

Question 3: Collaboration and coordination

This project was rated **3.8** for its engagement with and coordination of project partners and interaction with other entities.

- The project has strong collaboration and coordination, both between the specific topic areas and with the community, as evidenced by the interest and attendance at the annual Advanced Water Splitting Technologies Workshop. In addition to the ongoing coordination with H2NEW (Hydrogen from Next-generation Electrolyzers of Water) and HydroGEN (the HydroGEN Advanced Water Splitting Materials Consortium), the LTE portion of the project should consider adding coordination efforts with the new liquid alkaline effort in H2NEW, the alkaline oxygen evolution reaction effort in ElectroCat (the Electrocatalysis Consortium), and recycling efforts in H2CIRC (the Hydrogen Electrolyzer and Fuel Cell Recycling Consortium).
- There are great partnerships and collaboration with clear roles. The focus on strategic coordination is good. Involvement of the user community is great.
- Collaboration by the principal investigator is world-class.

Question 4: Potential impact

This project was rated **3.8** for supporting and advancing progress toward Hydrogen Program goals and objectives.

- The project is very relevant given the importance of hydrogen production, especially getting ready for H2Hubs (the Regional Clean Hydrogen Hubs Program). The project addresses a critical need for consistent ways of characterizing and measuring production methods using water-splitting technology.
- The development and dissemination of best practices, benchmarks, and protocols are particularly impactful, as dozens of new projects in hydrogen production begin this year. It will be critical to ensure the

new FOA projects are aware of and following the latest protocols and best practices arising from this project to accelerate their impact and ensure accurate evaluation of their progress.

- The greatest strength is the educational aspect of the effort across the scientific community.

Question 5: Proposed future work

This project was rated **3.5** for effective and logical planning.

- There is a clear plan for future work and understanding the importance of completing the work given the visibility of and investment into electrolysis technologies.
- The team should continue the effort as needed.
- The round-robin and validation efforts are a critical part of future work of this project. The project should also have a plan for identifying and engaging with the relevant FOA projects announced this year, which will likely need to be closely coordinated with the applicable consortia (H2NEW, HydroGEN, etc.).

Project strengths:

- The project is doing a great job of collaboration and industry involvement. Benchmarking and establishing protocols are underappreciated in our industry, so thanks to the team for addressing them.
- The project continues its strong engagement with the advanced water-splitting water community and should be commended for being able to do so across a broad range of topic areas.
- The greatest strength is the educational aspect of the effort across the scientific community.

Project weaknesses:

- There are no apparent project weaknesses.
- A significant challenge in the ongoing development of best practices, benchmarking, and protocols is how to disseminate and ensure timely adoption of updates to established or published protocols. Using the Data Hub as a repository helps to address this challenge, but it is not clear how the project will attract attention to the Data Hub repository or advertise updates or new uploads to the Data Hub.

Recommendations for additions/deletions to project scope:

- A recommendation for additions to scope is the addition of system-level measurement protocols and metrics. The protocols for materials and components are critical, particularly for researchers and labs, but system-level definitions are also important for system integrators and purchasers. The team may or may not adopt the methods outlined by the project, but providing a protocol establishes a baseline.
- Per slide 14, the LTE topic currently does not have any protocols in development for liquid alkaline. The Hydrogen and Fuel Cell Technologies Office has recently funded several new projects on liquid alkaline electrolysis, including in the H2NEW consortium, and this topic should be considered as an addition to the scope of this project.
- The key question is whether electrolyzer performance can reach an optimum if operated at some best protocol. It is unclear whether there is a best protocol or if the benefit of developing protocols is just not operating in the many incorrect, unverifiable, unreproducible, and inconsistent ways that are unshareable and useless in the scientific community.

Project #P-179: BioHydrogen (BioH2) Consortium to Advance Fermentative Hydrogen Production

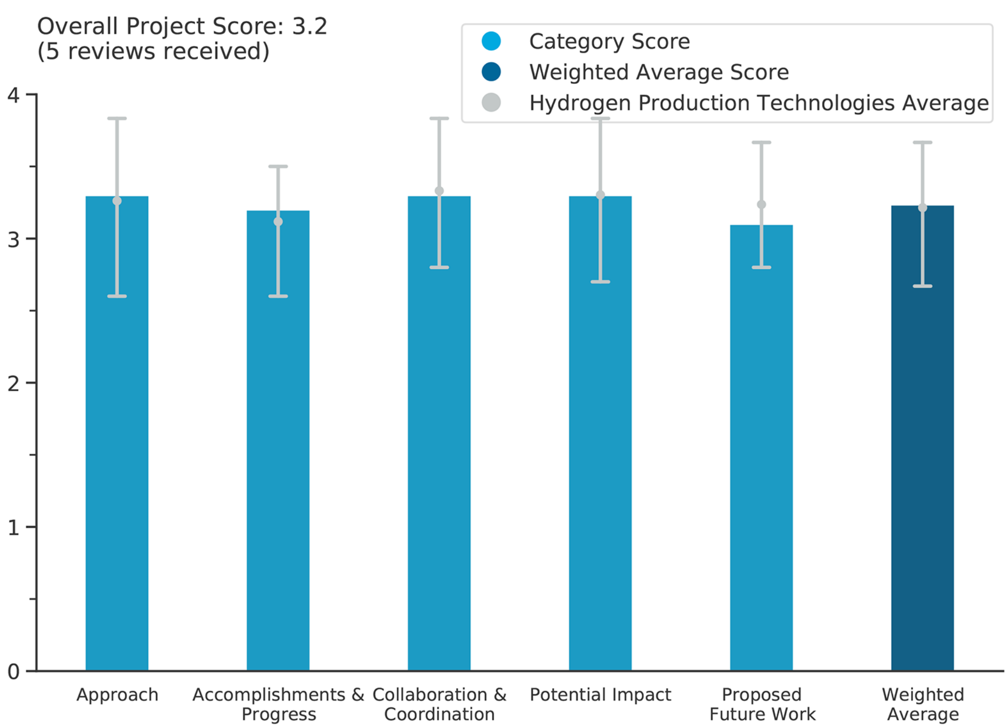
Katherine Chou, National Renewable Energy Laboratory

DOE Contract #	WBS 2.4.0.516
Start and End Dates	10/1/2018
Partners/Collaborators	Lawrence Berkeley National Laboratory, Argonne National Laboratory, Pacific Northwest National Laboratory
Barriers Addressed	• Capital cost

Project Goal and Brief Summary

The goal of the BioHydrogen (BioH2) Consortium is to develop a carbon-neutral microbial dark fermentation technology integrated with a microbial electrolysis cell (MEC) to convert waste lignocellulosic biomass into low-cost hydrogen. This collaborative team of national laboratory scientists aims to (1) improve the rates and molar yields of hydrogen production (moles of hydrogen/moles of sugar) via metabolic engineering of the cellulose degrader, *Clostridium thermocellum*, (2) optimize the bioreactor for high solids loading to reduce reactor cost, (3) develop an integrated MEC system to improve hydrogen molar yield and reduce fermentation waste product, and (4) conduct a techno-economic analysis (TEA) and life cycle analysis (LCA) with data generated by team partners to identify major cost drivers and guide integration efforts.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Hydrogen Production Technologies projects.

Question 1: Approach to performing the work

This project was rated **3.3** for identifying and addressing objectives and barriers and for project design, feasibility, and integration with other relevant efforts.

- The National Renewable Energy Laboratory's (NREL's) approach consists of four related tasks to simultaneously improve hydrogen yield, increase the solids content, increase MEC current density, and conduct TEA and LCA to identify the best feedstock. It is a comprehensive and thoughtful approach. NREL's approach assigns tasks to four national laboratories, each very well-suited to the tasking. The approach fundamentally rests on improving the conversion of sugars to hydrogen. This task can be accomplished only with genetic engineering, and that is one of the four core tasks.
- NREL has presented a clear approach to addressing the critical barriers in developing an MEC. The presentation reviewed the progress toward addressing feedstock cost. The status of continuous reactor development was also addressed. The consortium is well-defined and well-led. The work has shown good progress toward meeting DOE goals for hydrogen production cost.
- The project clearly identifies the critical barriers to reducing the price of hydrogen production through the MEC approach, and the work is focusing on reducing these barriers. The potential for significant cost reduction has already been demonstrated.
- NREL's systematic strain improvement approach to achieve nearly all sugar (C5 & C6) fermentation is excellent, and this step is critical to improving overall hydrogen yields.
- Slide 2 identifies the theoretical hydrogen production yields, which include 4 mol via fermentation and 8 mol via MEC. Based on this information, it seems that the approach should be based on two-thirds of the effort directed toward improving the MEC technology. Even if one considers the state of the technologies, MEC technology is probably not as advanced as the fermentation technology. Therefore, more effort may need to be focused on the MEC approach. This may require an assessment of the approach taken in this project, considering the expertise available at national laboratories and how the Hydrogen and Fuel Cell Technologies Office (HFTO) can advance its BioH2 program to reach the Hydrogen Shot target in the shortest timeframe. Research and development (R&D) definitely needs to be conducted to reach the target performance in the next two to three years so the United States can deploy technologies to produce green hydrogen by 2030. The project has spent $6.5 million on R&D to date. One of the priorities is capital expenditure (CAPEX)/bioreactor cost reduction. It is unclear whether the fermenter cost has been reduced. It seems the pre-treatment has been eliminated, and use of solids in the fermenter is implemented, which is good, but the impact of that on the TEA is not clear. Unfortunately, the TEA and LCA work showed totally different feedstocks from what was used in experiments, so there does not seem to be a real assessment of hydrogen cost of production for the work that is ongoing using biomass feedstock. It is unclear whether one can claim the results from slides 13 and 14 to be relevant, considering the experimental work conducted in this project, since there is no experimental work on food waste or cheese whey. Actually, cheese whey is one of the most difficult wastes to treat biologically, even in anaerobic digestion systems, so claiming that one can get to -$2.2/kg H_2 using the fermentation–MEC technology without experimental data seems like an apples-to-oranges comparison. Furthermore, on slide 4, it is unclear whether the cost reduction to $12.4/kg H_2 is proposed to be achieved via the bulleted points shown in red (use of solids, reduced electricity use, decarbonization) and whether this reduction was achieved in the last six years since the project started. If not, the information seems misleading. It is also unclear whether the claim of reducing electricity by more than half is exhibited in the TEA results. If the team has identified the electricity use for the integrated fermentation–MEC process, it would be good to show those data to illustrate the reduction in energy use. Regarding the technical approach to converting different sugars, it is unclear how feasible it is to engineer multiple pathways to use all sugars into Clostridium thermocellum, how robust this organism is to real feedstock conditions, and how this approach has been evaluated. It is also unclear how long (length of experiment) the engineered strain has been used for converting the biomass and whether the experiments are continuous or batch. If these are batch experiments, it is unclear whether subsequent batches can be run using inoculum from a previous batch versus inoculating with a freezer stock. This information will illustrate strain robustness. It is unclear whether the current strain has pathways to convert all engineered sugar pathways, i.e., combined glucose, xylose, arabinose conversion pathways in one strain, and what the return on investment of research dollars is on hydrogen yield improvement. If a particular sugar is present at less than 10% of total chemical oxygen demand, it is unclear whether it is worth pursuing strain

engineering to convert that sugar and whether the strain will have similar growth and conversion rates if it is fed with a different biomass, such as forest biomass or energy crops. Industrial biotechnology R&D over the last three decades has shown that introducing the engineered organisms into the field with real feedstocks results in strain failure due to hosts' inability to handle contaminants present in real feedstocks. It is critical to understand long-term goals for this research considering the existing knowledge base.

Question 2: Accomplishments and progress

This project was rated **3.2** for its accomplishments and progress toward overall project and DOE goals.

- The NREL consortium is making great progress toward achieving DOE goals on hydrogen cost. Cost has been reduced from approximately \$58/kg H_2 to \$12.4/kg H_2 with a pathway to \$5.6/kg H_2 (prior to tax incentives). Future work is focused on addressing the barriers to reduction in hydrogen cost.
- The team has made solid progress in each of its four main tasks. Progress in all four is required to achieve the overall project and DOE goals. The engineered microbe increased hydrogen production by 105%. Testing on high solids content feed resulted in a 15% higher yield. MEC current density increased to greater than 30 A/m^2. A reported peak current density of 66 A/m^2 is cited but without further specification of conditions. While MEC current density improvements were achieved, a much higher current density is needed to achieve the overall project goals.
- Achievements against the targeted tasks is significant; however, a wider selection of feedstocks needs to be included. Some grass varieties as feedstocks need to be studied to make the pathway universally attractive for green hydrogen production. Sugar utilization needs to be improved.
- The technology is at a very low technology readiness level (TRL), and the current cost projection of \$12.4/kg H_2 is still significantly higher than the project target of \$2/kg H_2 and the DOE ultimate goal of \$1/kg H_2 production. It is not clear from the results and pathways analysis if the potential for further significant cost reduction exists.
- The hydrogen production was reported to be doubled to 1.2 L-H_2/L-reactor. Typically, the productivity is given by L-H_2/L-reactor-day. It is unclear whether the operating period for this is 96 hours (same as the growth period). If this assumption is correct, the rate is estimated to be approximately 0.3 L-H_2/L-reactor-day. The following slide from the Pacific Northwest National Laboratory (slide 10) suggests the rate to be approximately 0.4 L-H_2/L-reactor-day for milled corn stover (MCS). The TEA work done to date does not seem to report on what hydrogen productivity is needed for economic feasibility (say, at a given CAPEX). It is not clear what the parameter is for assessing techno-economic progress or whether the TEA can identify a rate of hydrogen production that needs to be reached using current CAPEX. The MEC work identifies a current density of 30 A/m^2; however, the most important parameter is, once again, L-H_2/L-reactor-day. This parameter was reported to be 1 L-H_2/L-reactor-day. So the current density does not translate into hydrogen productivity. This is a function of the reactor configuration. Literature reports suggest the target hydrogen productivity for achieving economic feasibility should be greater than 20 L-H_2/L-reactor-day, which indicates the need to increase the rate by an order of magnitude. It is unclear whether there is a path to achieve this rate. Slide 11 indicates use of a single-chamber MEC. It is unclear how the hydrogen produced is going to be prevented from being used by methanogens or whether the cage design is capable of addressing this issue.

Question 3: Collaboration and coordination

This project was rated **3.3** for its engagement with and coordination of project partners and interaction with other entities.

- The NREL consortium has excellent alignment with the Hydrogen Program and DOE research, development, and demonstration (RD&D) objectives and has the potential to advance progress toward DOE RD&D goals and objectives.
- The combination of four national laboratories on this project is excellent and appears to be fostering excellent collaboration.
- All relevant organizations in the DOE setup are involved.

- The project is an effective collaboration between several national laboratories, each developing a component of the overall technology process. However, better collaboration and joint effort should be shown on the integration of the system components developed by different project partners, which may produce significant improvements in the overall system performance.
- The four national laboratories seem to be doing relatively individualistic projects. They are all working on BioH2; however, it seems each has gotten a separate piece of the project. The laboratories have exchanged some materials, but the relative impact of how one laboratory's activities alter another laboratory's work is not clear. The relationship of at least the TEA and LCA work to each experimental task should be direct; however, at least in the results from this year, the use of cheese whey and food waste as feedstocks shows no relation to any other laboratory's experimental work. Based on the TEA and LCA results, it is unclear whether there is a path for using MCS or other agricultural waste/energy crops' biomass as a feedstock to get to less than \$2/kg H_2. Alternatively, based on the Argonne National Laboratory (ANL) results, it is unclear whether the national laboratories are all going to focus on food waste and cheese whey as feedstocks starting this year. It is also unclear how the TEA/LCA is helping to direct the experimental work. There are many organizations outside the national laboratories that have expertise in the areas in which the national laboratories are working. It is unclear whether there is any way to collaborate/coordinate with outside entities in this project to address the common goal of achieving a hydrogen production cost less than \$2/kg.

Question 4: Potential impact

This project was rated **3.3** for supporting and advancing progress toward Hydrogen Program goals and objectives.

- The project has excellent potential impact, as confirmed by the TEA, which shows a potential for less than \$1/kg H_2 (when factoring in some scenarios for tipping fee credits).
- Biologically derived hydrogen can be a game changer when carbon sequestration potential is considered. The project is strongly aligned with DOE goals. The focus on developing continuous reactors and improving hydrogen production densities (A/cm^2) will address the barrier to meet DOE hydrogen production cost targets.
- Bio-pathways for cost reduction of green hydrogen production will have a significant impact.
- The project provides good new data and fundamental understanding of the MEC hydrogen production. However, because of high cost and many remaining challenges to system integration, it is unlikely that this technology will be able to be successfully commercialized in the 10-year timescale at which the Hydrogen Program goals need to be achieved.
- The timeline published by HFTO to achieve clean hydrogen production cost reductions is steep. It is not clear whether the BioH2 Consortium has a path to achieve the near-term goal (\$2/kg H_2) or the long-term Hydrogen Shot goal (\$1/kg H_2 by 2030). The amount of funding in the HFTO biological hydrogen production program is not huge. Given this limitation, it is unclear what the best chance is for this pathway to be a successful pathway in achieving the Hydrogen Shot goal. While the BioH2 Consortium is conducting good scientific research, it is oriented toward achieving HFTO research, development, demonstration, and deployment goals. The national laboratory project does not seem to address the question of directing research in this field. It is a microcosm in itself, and the potential impact on the advancement of this field in general does not seem to be addressed.

Question 5: Proposed future work

This project was rated **3.1** for effective and logical planning.

- The project has identified remaining challenges and barriers for each component of the hydrogen production system and proposed a reasonable work plan to continue addressing these challenges.
- The focus of the proposed future work addresses the critical barriers to meeting the DOE hydrogen production targets. Risk mitigation may not have been completely reviewed.
- The listed future activities are adequate and in the right direction. Feedstocks of some grass varieties need to be included in the study.

- Future work plans are good but could include more numerical targets. The plans also could be more expansive, as they represent a significant annual investment.
- It is unclear whether the BioH2 consortium is required to set Specific, Measurable, Achievable, Relevant, and Time-Bound (SMART) goals. There were no quantified goals in the Future Work slide, only qualitative objectives. The future goal for Task 1 (directed at engineering additional enzymes to increase conversion) should be based on whether the resulting strain is stable and usable in a continuous operation in the field, with real feedstocks with potential contamination and other real-life issues. Considering the second goal (demonstrate process robustness via long-term continuous operation with MCS biomass), it is unclear what long-term means (one week, one month, or one year). It is also unclear how robustness is defined. Regarding Task 3 (optimization of milled biomass wastewater conversion to achieve higher hydrogen production rates), for example, it is unclear what "higher production rates" means and what is guiding the rate target. Regarding Task 4 (identify/explore additional cost reduction pathways, e.g., lignin upgrading, MEC design, low-cost feedstock), for example, it is unclear why lignin is upgrading a cost reduction pathway, whether there is a possible path to produce hydrogen from lignin, and whether there is any path to breakdown lignin economically, based on the past two decades of R&D at NREL. It is very difficult to gauge whether proposed future work is based on quantitative or even qualitative analysis of risks and rewards.

Project strengths:

- The team has excellent capabilities and division of labor among the four national laboratories. The team has made significant incremental progress toward increasing hydrogen yield and solids content. The team's achievement in gene engineering to allow an additional pathway to convert a sugar is a strong project strength. The team's use of TEA to explore specific scenarios of feedstock selection, feedstock cost, tipping fees, and subsidies is a significant project strength. The team's identification of scenarios that result in negative cost of hydrogen (using tipping fees and tax credits) is a project strength. The use of NREL nuclear magnetic resonance (NMR) to identify bonds to target to enhance hydrogen production is a project strength.
- The project continues successful development of all the components of the MEC-based, biomass-based hydrogen production technology, and the project achieved significant reduction in the projected cost of hydrogen. The technology can be used with various organic waste streams. The project has good collaboration between several laboratories.
- The project's strength is in national laboratory leadership, which provides the appropriate environment for developing technologies, such as biologically derived hydrogen.
- The project is a well-structured collaborative model and has focused, dedicated work by partners.
- The genetic engineering work related to utilization of sugars is good; however, it needs to be based on an approach that evaluates necessary and sufficient conditions for achieving production of hydrogen (a gas), which could potentially be produced, say, using a consortia approach as well, and can be easily separated from the broth, as it is a gaseous product. The Advanced Biofuels and Biproducts Process Development Unit has a state-of-the-art fermenter and bioreactor capability. It is certainly a strength; however, it is unclear whether such expensive equipment can be economical for the production of a fuel gas. In comparison with anaerobic digestion, it is unclear whether a huge cement/metal (non-stainless steel) tank can work for this fermentation. ANL has clear strengths in the Greenhouse Gases, Regulated Emissions, and Energy Use in Transportation (GREET) modeling, so its work in evaluating the environmental impact of BioH2 is critical. It is certainly a huge strength for the project and needs to be used as such for defining the milestones for the technical work.

Project weaknesses:

- There are no immediate weaknesses observed in this reporting period.
- Maybe some academic biotechnology laboratories will bring in additional value and fast-pace the strain development.
- The presenter shared few details on the MEC progress. MEC current density needs to be substantially higher to produce cost-competitive hydrogen without production tax credits. MEC current density is listed

as greater than 30 A/m^2 but is also cited as 66 A/m^2. While both may be true, the voltage for peak current density is not listed, suggesting perhaps that peak value occurs at an undesirably high cell voltage. No target MEC current density is stated.

- The project continues to be at a low TRL, and the cost of hydrogen production remains very high. It is unlikely that the technology could mature and that cost would decrease within the timeframe of the DOE hydrogen cost targets.

Recommendations for additions/deletions to project scope:

- A realignment of the tasks based on potential return on R&D dollars could be helpful. A clear example is the potential for a specific pathway to generate hydrogen (based on stoichiometric yield) using a complex biomass stream. Investing in tasks that may yield max return in the time available may be advisable. Also, use of relevant expertise in a given field should be recruited if it is not available at national laboratories. Alternately, tasks/funding allocations should be focused on expertise available at national laboratories.
- It is suggested that the project chart a list of conditions (MEC current density, solid content, hydrogen yield) that can be combined to yield a low cost of hydrogen without subsidies. It is suggested that the project add more numerical goals for each task of future work.
- It is suggested that the project include solid grass feedstocks for the study.
- One addition could be technology transition to an industrial partner.

Project #P-196: H2NEW Consortium: Hydrogen from Next-Generation Electrolyzers of Water

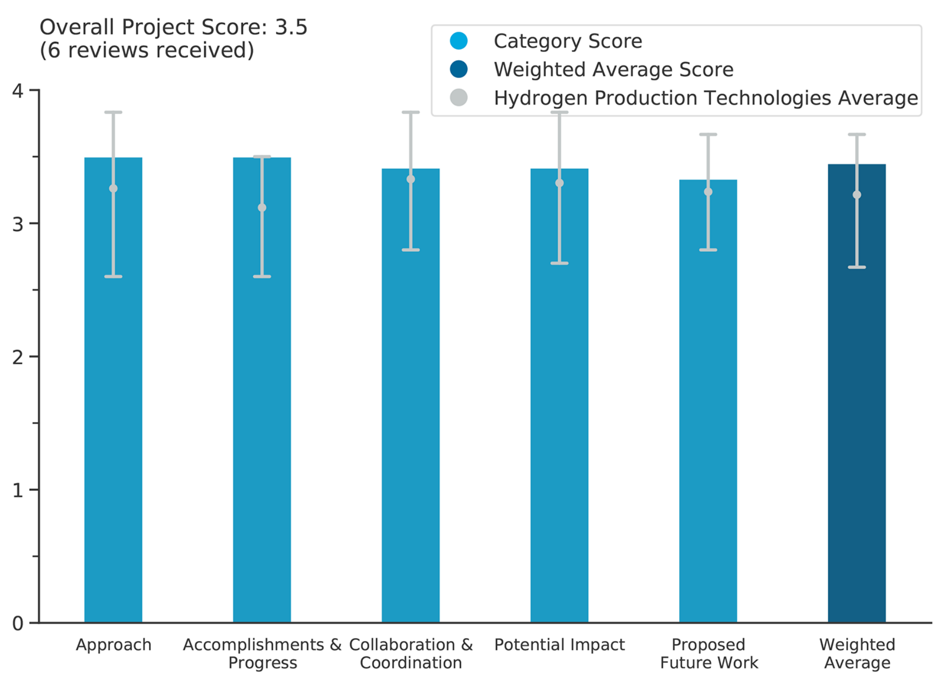
Bryan Pivovar, National Renewable Energy Laboratory, and Richard Boardman, Idaho National Laboratory

DOE Contract #	Multiple
Start and End Dates	1/1/2020
Partners/Collaborators	Argonne National Laboratory, Lawrence Berkeley National Laboratory, Lawrence Livermore National Laboratory, Los Alamos National Laboratory, National Energy Technology Laboratory, Oak Ridge National Laboratory, Pacific Northwest National Laboratory, National Institute of Standards and Technology, SLAC National Accelerator Laboratory, University of California, Irvine, Carnegie Mellon University, Colorado School of Mines
Barriers Addressed	• Durability • Cost • Efficiency

Project Goal and Brief Summary

The H2NEW (Hydrogen from Next-generation Electrolyzers of Water) consortium is a comprehensive, concerted effort focused on overcoming technical barriers to enable affordable, reliable, and efficient electrolyzers that can achieve <$2/kg H_2 by 2026. H2NEW is studying both low-temperature electrolysis (LTE), based on proton exchange membrane (PEM) and liquid alkaline technologies, and high-temperature electrolysis (HTE), based on oxide-ion-conducting solid electrolyte. The core H2NEW national laboratory team is addressing components, materials integration, and manufacturing research and development (R&D). The team is working to improve scientific understanding of the performance, cost, and durability tradeoffs in electrolysis systems, including under predicted future dynamic operating modes, by using a combination of experimental, analytical, and modeling tools.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Hydrogen Production Technologies projects.

Question 1: Approach to performing the work

This project was rated **3.5** for identifying and addressing objectives and barriers and for project design, feasibility, and integration with other relevant efforts.

- It is great to see dynamic collaboration among a strong and far-reaching team. Dr. Boardman's vision is impressive, and Dr. Pivovar's leadership in the low-temperature arena is motivational. It is very clear that the team is very excited, high-energy, and agile to navigate various challenges from materials to stacks to future systems. The reviewer challenges H2NEW to consider incorporating internal R&D technology to be tested in stacks and systems and working with vendors to incorporate such technology in commercial stacks. Testing rainbow R&D stacks is one step, but incorporating one stack into a bundle of other industrial stacks (skids) would be even more valuable. These tests would allow excellent research and engineering teams to prioritize variables of interest for improvement of the overall system. Below are some topics it would be valuable to address, perhaps in one or two slides during the next update. (It is understood that the presentation is allocated limited presentation time to share updates, and possibly some of the questions below are already being addressed but were not presented for that reason.)
    - Accelerated test protocols (current pulsing) are certainly valuable on small cells or short stacks. It is unclear how such protocols (if possible) can be incorporated on larger stacks and systems where the balance of plant (BOP) would have to experience such changes as well.
    - The financial levelized cost of hydrogen (LCOH) work is interesting. With the understanding that it is early stages, the team is urged to consider calling major vendors, EPC (engineering, procurement, and construction) firms, and developers to understand true costs—and that the goals to achieve $2/kg by 2026 and $1/kg by 2030 set by DOE are far-fetched. It is imperative to set realistic expectations for the community to accelerate project deployment.
        - For example (and there are many), in slide 46, variable electricity cost with a 50% capacity factor (CF) leads to a reduction in LCOH of $0.52. If CF is 50%, that means the electrolyzer is producing 50% less product. To run such an electrolyzer when energy is low-cost, renewables would have to be oversized by 2x and the electrolyzer would have to be oversized by 2x to make up for lost hydrogen production, as the customer will want fixed tons/day of H_2. Therefore, as CF drops, the price of hydrogen will increase, not decrease. One can argue lower energy cost, but if capital expenditures (CAPEX) double for the whole plant, it is not clear how this still leads to reduction in LCOH. It is understood that this is a representative/preliminary graph, but these assumptions should be carefully discussed with the wider community.
    - A similar challenge is presented for consideration when LCOH for HTE is evaluated, as in the second sub-bullet above. Furthermore, if nuclear carveout is not approved by the Treasury and a hydrogen production tax credit cannot be collected, then perhaps creative solutions could be incorporated to allow for HTE and hydrogen to be at a competitive LCOH, but it is not clear what these solutions might be.
    - In slide 52, it was not clear where the CAPEX and BOP numbers are coming from, whether these prices are offered by industry original equipment manufacturers (OEMs) that have manufactured tens to hundreds of megawatts of solid oxide electrolyzer cells (SOECs), or whether these prices are simply projections. Perhaps it would be possible to tabulate each vendor and the vendor's projected prices. In step 2, it is not clear whether the $30/MWh of energy is indicative of energy delivered, including transmission, distribution, and delivery costs—and if not, why this was not the case.
    - It is very encouraging to see a massive focus on HTE testing reproducibility among collaborators and long-term operation.
- Overall, this is great work, and this reviewer is looking forward to following the team's progress. The team is asked to consider these questions and recommendations, as they are intended to help accelerate successful development of LTE and HTE testing/demonstration platforms.
- The main objective of the H2NEW consortium is to establish and utilize experimental, analytical, and modeling tools to gain a scientific understanding of the performance, cost, and durability tradeoffs of electrolysis systems under projected future operating conditions. To achieve this goal, a number of leading experts with diverse expertise have been brought together. Appropriate milestones, decision points, and

critical barriers that must be overcome have been clearly defined and are being effectively addressed. The integrated safety management process is well-designed and of high quality. Additionally, the diversity, equity, inclusion, and accessibility plan and the community benefits plan are well-designed, feasible, and integrated with other relevant efforts.

- Only recently (less than 10 years ago), national labs and R&D organizations, including universities, have focused resources to address the needed challenges within PEM water electrolysis and liquid alkaline water electrolysis (LAWE). This basically means that almost every single component in these stacks had to be tackled and understood, with fundamental aspects and in situ properties of materials unveiled. On one hand, H2NEW has the massive task to go through understanding many fundamental aspects of these devices, which might appear to lead to progress that is much slower. Moreover, not many of the researchers involved have been exposed to the hydrogen electrolysis industry, which make the task even more challenging, and much of the information needs to be obtained from collaboration with other groups and the existing electrolysis industry and OEMs. With all of that considered, the approach could not be any different. Yes, H2NEW is doing basic work such as benchmarking and screening of commercial materials, but these tasks are ultimately important and will make progress much less incremental in the later part of the project.
- The lead for the HTE SOEC part of H2NEW has been able to piece together an excellent team and appears supportive to team members. The SOEC effort has excellent organization and structure. Key issues have been methodically isolated and effective strategies developed there. The approach focus in HTE must be on quickly lowering cost, lowering area-specific resistance (ASR), increasing current (hydrogen production rate) of the SOEC, and disseminating the results to real energy system integrators.
- This is a very large, comprehensive project with many insightful results. It would be helpful to understand the roadmap for this large project, including SMART (Specific, Measurable, Achievable, Relevant, and Time-Bound) milestones and timeline. The project did not discuss shunt current characterization, which is a very important part of LAWE. The combination of low- and high-temperature electrolysis technologies is always logically sound.
- In slide 5, Tasks 4, 6, and 9 are not mentioned. Task 9 is mentioned on slide 9. Missing tasks should be described, even if succinctly, to avoid confusion.

Question 2: Accomplishments and progress

This project was rated **3.5** for its accomplishments and progress toward overall project and DOE goals.

- This project has made outstanding progress. It has come a long way to reach project milestones and important fundamentals for degradation mechanisms. Moreover, the project seems to be on track to reach the $2/kg goal, although a more empirical validation of the current status was not shown or not very clear. There was not a strong link to key suppliers (OEMs) of materials and components at scale, which could greatly assist in validating the numbers for the cost analysis used here. On another topic, the project should spend more time/resources on unveiling key properties of both porous transfer layer (PTL) and gas diffusion layer materials. Not much was reported, or not much progress was shown, in this area. The project is encouraged to demonstrate more durability data for liquid alkaline cells and short stacks in the next reporting period.
- The durability of high-temperature water electrolyzers (HTWEs) has significantly advanced compared to the results from the last year. The durability of PEM water electrolysis is poor (30 mV/1,000 hours). The project needs to pinpoint the causes as soon as possible. The microporous layer on the PTL is good. High-pressure hardware design is completed. This is quite meaningful for research institutions. The results of modeling hydrogen crossover are great. Some techno-economic analysis results (slides 12 and 46) are very valuable for the hydrogen and electrolysis communities. Slide 81 has operando high-temperature x-ray diffraction (XRD), and through XRD, there are powerful tools for HTWE diagnostics. In the LAWE part, the project needs to study the longer durability of stainless steel PTLs.
- Clear and measurable performance indicators/milestones have been outlined for the consortium. To date, sufficient results have been presented, which suggests that excellent progress is being demonstrated toward overcoming critical barriers and achieving project objectives.
- Excellent progress was made in both LTE and HTE.

Question 3: Collaboration and coordination

This project was rated **3.4** for its engagement with and coordination of project partners and interaction with other entities.

- As this is a consortium, the engagement and coordination of project partners are critical to promoting beneficial interactions among participants/members. In this regard, the consortium has done a good job in coordinating appropriate collaboration with other national labs. However, more collaboration with universities and industries could be more beneficial and impactful.
- This project has outstanding coordination at both the national and international levels.
- There is excellent collaboration among national laboratories and universities.
- There have been strong collaborations among national laboratories, but it was unclear how the industrial advisory board works, such as how often they meet and what their main contributions are.

Question 4: Potential impact

This project was rated **3.4** for supporting and advancing progress toward Hydrogen Program goals and objectives.

- This consortium is well-aligned with the Hydrogen Program’s goals and objectives and is likely to advance progress toward its performance targets. The unique capabilities developed by this consortium may also provide important support to other relevant R&D projects supported by the Office of Energy Efficiency and Renewable Energy.
- The project is quite impactful for the entire water electrolysis community in terms of depth and breadth. The project has provided many insights for electrolysis technology advances. The project needs to focus on durability studies. The current cell degradation rate of 30 mV/1,000 hours is too high.
- The $2/kg target is very much dependent on progress in other areas that are currently not being addressed in the project. Other relevant points of R&D in stacks and, to some extent, system components play an important role in reaching such an ambitious target. These are aspects that can be covered in the next phase by establishing a stronger collaboration with the electrolyzer industry and OEMs. This is an even more important aspect for both LAWE and high-temperature electrolyzers, as these have not obtained much attention in the development of stack components and balance of stack and system in the national labs.
- The impact on the industry should be to accelerate development.

Question 5: Proposed future work

This project was rated **3.3** for effective and logical planning.

- In addition to the progress made so far, the consortium has carefully planned its next steps. This includes incorporating appropriate performance targets and decision points and considering barriers to its goals. More collaborations with universities and industries could be included in future activities.
- All the research in the Hydrogen and Fuel Cell Technologies Office should be to drive to the 2026 goals of low ASR and high current and rapid acceleration to deployment to meet 2030 and 2050 goals.
- The project may need some SMART milestones and an overall project roadmap.
- The project has a very clear scope for the proposed work in the next H2NEW period, although a clearer roadmap is suggested for the progress expected in the LAWE space versus PEMs. The project does not seem to completely understand what can be done in this area from an innovation, research, and development perspective. However, as the labs have just started to work in this area, the limited scope is also somewhat expected.

Project strengths:

- The main objective of the H2NEW consortium is to develop experimental, analytical, and modeling tools to understand the performance, cost, and durability tradeoffs of electrolysis systems under future operating conditions. Leading experts with diverse expertise have been assembled to achieve this goal. The consortium has clearly defined milestones, decision points, and critical barriers, which are being effectively addressed.

- The project is quite impactful for the entire water electrolysis community in terms of depth and breadth. The project has provided many insights for electrolysis technology advances.
- Strengths include coordination, strong background on PEM fuel cell devices, national and international collaboration with other labs and universities, awareness of the need of technical economic analysis that can guide the scope and next steps, and multi-disciplinarity.
- Excellent leadership is a project strength.
- All project elements are strengths.

Project weaknesses:

- To maximize its impact, the consortium may consider broadening the engagement and coordination of institutions and participants. This would better utilize its unique capabilities, support additional related R&D projects, and significantly advance progress toward the Hydrogen Program's goals.
- There is a lack of work on crucial stack and system components, limited capability for electrolyzer single-cell and stack testing (suggestion to increase at least 100x), and inertia with accelerated stress test development, lack of background information from industry and intellectual property conflicts. Also, the project is sometimes too incremental.
- The project needs to focus on durability studies. The current cell degradation rate of 30 mV/1,000 hours is too high. The project may need some SMART milestones and an overall project roadmap.

Recommendations for additions/deletions to project scope:

- The project needs to focus on durability studies and pinpoint the causes of fast performance decay. The project also needs to develop a clear overall project roadmap to show a large picture of the project.
- It would be beneficial to provide more support to universities and industry.
- The reviewer has no recommendations or additions.

Project #P-200: Low-Cost Manufacturing of High-Temperature Electrolysis Stacks

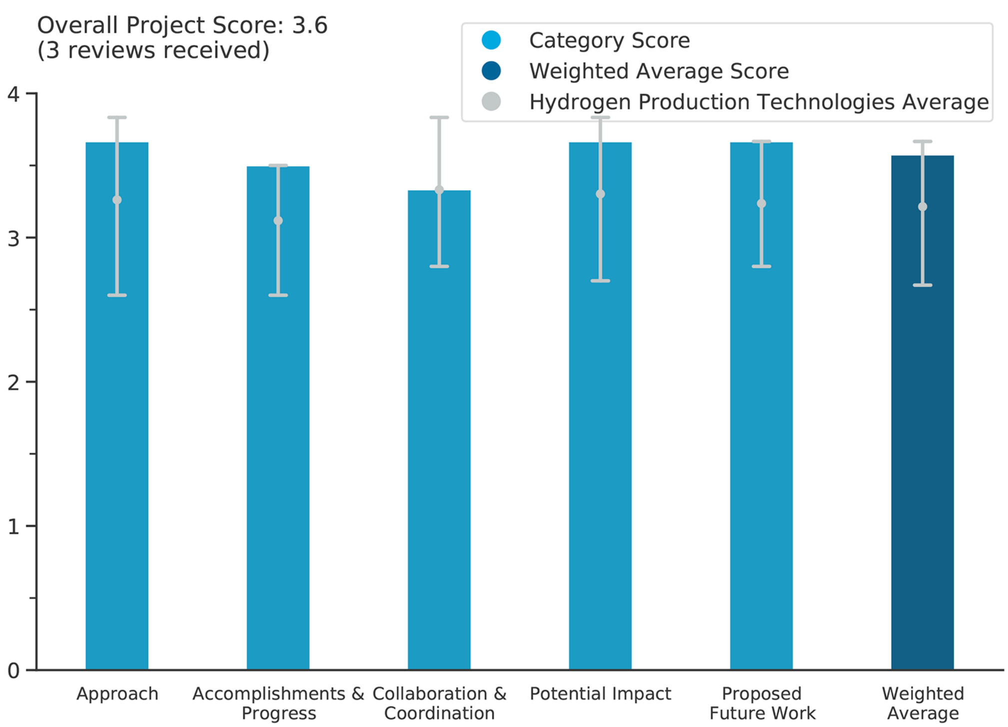
Scott Swartz, Nexceris, LLC

DOE Contract #	DE-EE0009621
Start and End Dates	4/1/2022–9/30/2025
Partners/Collaborators	Idaho National Laboratory, Strategic Analysis, Inc.
Barriers Addressed	• High-temperature electrolyzer stack cost • High-temperature electrolyzer electrical efficiency • High-temperature stack electrolyzer durability • Hydrogen production cost

Project Goal and Brief Summary

The project's goal is to develop cell and stack manufacturing technologies for high-temperature electrolysis stacks. The primary objective is to achieve stack manufacturing costs below $100/kW, with a 15% reduction in cell costs through design optimization. The project will address key barriers, including high-temperature electrolyzer stack cost, electrical efficiency, and durability, by enhancing cell performance, stack durability, and manufacturability. The approach involves developing innovative cell and stack designs, reducing manufacturing costs, and conducting rigorous testing and analysis.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Hydrogen Production Technologies projects.

Question 1: Approach to performing the work

This project was rated **3.7** for identifying and addressing objectives and barriers and for project design, feasibility, and integration with other relevant efforts.

- The project is developing a new design for next-generation solid oxide electrolyzer cell (SOEC) stacks and conducting testing of stacks to verify the designs. The project follows good safety standards; diversity, equity, inclusion, and accessibility standards; and community benefits plan standards.
- Nexceris' approach is a good match for the challenge of developing low-cost electrolyzer stacks. The project team is drawing upon decades of expertise in developing solid oxide fuel cell (SOFC) stacks to make decisions that enable cost reductions in solid oxide electrolyzer stacks by lowering the materials and processing costs of the cells and stacks. The described safety approach is very thorough, detailing the plans and culture, as well as the $93,500 invested in safety in 2023.
- The team understands the objectives and barriers of high-temperature electrolyzers.

Question 2: Accomplishments and progress

This project was rated **3.5** for its accomplishments and progress toward overall project and DOE goals.

- The progress in developing FlatCell alternatives to the standard FlexCell® is encouraging. The performance is very similar, but the cost can be reduced by $20/kW.
- The project team made good progress toward achieving the objective of building low-cost SOEC stacks.
- The team has made progress in stack performance demonstration, but performance still has room to improve. The electrolyzer performance should also be characterized by long-term stability (i.e., how many thousands of hours) and efficiency. In this aspect, steam utilization needs to be considered in the metrics when reporting performance.

Question 3: Collaboration and coordination

This project was rated **3.3** for its engagement with and coordination of project partners and interaction with other entities.

- Stack testing and validation at Idaho National Laboratory (INL) is the best option available for third-party validation of commercial electrolyzer stacks. It is advantageous that Nexceris is making use of INL's resources. Pacific Northwest National Laboratory is another good resource for scanning electron microscopy (SEM) and energy dispersive spectroscopy (EDS) evaluation of cells and stack components and is a valuable partner. The project team at Nexceris is making further efforts to expand collaboration through the DOE benchmarking workshops and H2NEW (Hydrogen from Next-generation Electrolyzers of Water) advisory board participation, as well as by hosting a Solid Oxide Forum in Ohio. Strategic Analysis, Inc., is a broadly knowledgeable resource for techno-economic analysis of electrolysis systems, and Nexceris appears to be making good use of that company's capabilities.
- Nexceris is collaborating with Strategic Analysis, Inc., in conducting system cost analysis, and collaborating with the University of Connecticut, West Virginia University, and Georgia Tech on current and pending DOE and Advanced Research Projects Agency–Energy (ARPA-E) projects. The project team demonstrated good coordination of these efforts.
- During the project review, the project team should have provided additional details on what the partners have done.

Question 4: Potential impact

This project was rated **3.7** for supporting and advancing progress toward Hydrogen Program goals and objectives.

- High-temperature electrolysis is the most electrically efficient method of generating clean hydrogen through splitting water, as the high temperature enables efficient operation. This is important because the electricity cost is the largest contributor to operating expenses for steam electrolysis systems. Efficient use of electricity lowers the levelized cost of hydrogen produced. If the project team lowers stack costs to less than $100/kW, that will also lower the capital expenditures of the clean hydrogen generation system.

- Development of low-cost, high-efficiency SOEC systems supports and advances progress toward achieving the Hydrogen and Fuel Cell Technologies Office's ultimate "1 1 1" goal for green hydrogen production.
- The electrolyte support electrolyzer design has a limitation to achieving higher performance, namely, higher resistance. To overcome this low performance, the electrolyzer needs to operate at higher temperatures, which in turn harms the durability and increases system cost.

Question 5: Proposed future work

This project was rated **3.7** for effective and logical planning.

- The focus on single-cell and stack testing is appropriate. The INL testing will be valuable in validating what Nexceris finds in its own facilities, and the testing may highlight degradation mechanisms or verify the ruggedness of the stacks in an environment that differs from what Nexceris is using for testing. Third-party validations like these are very compelling for potential customers who can trust the data offered by a third party with no commercial interests in Nexceris' stacks. Furthermore, scaling up and reducing costs will continue to be valuable focus areas for this project.
- The project team has identified issues of low performance and poor durability and has laid out a reasonable plan to address these two critical issues.
- The project team has planned logical future development work.

Project strengths:

- The project is focused on solid oxide cell technology that is expected to deliver high-efficiency conversion of clean electricity to clean hydrogen. Nexceris draws upon three decades of experience in this field. The cost and performance values are already compelling and are expected to further improve by the end of the project in September of 2025.
- The project follows many years of successful SOFC and SOEC development by Nexceris. The project has identified a new FlexCell design for a unit cell, which provides an improved platform for stationary high-temperature electrolyzer applications. The improved design for stack assembly was developed in the last year of work.
- The stack design and fabrication capabilities demonstrated by the team are a major strength of the project.

Project weaknesses:

- The cell/stack area remains small (<100 cm^2). Nexceris should analyze how large the cell area can ultimately be built. A small cell will result in the need to build many parallel stacks, where each stack will require multiple balance-of-plant components for flow and power control, which will ultimately lead to a higher system cost.
- More testing is needed for the thin FlatCells to prove out the durability and the stacking.
- The major weaknesses of the project are low performance and poor durability at the stack level.

Recommendations for additions/deletions to project scope:

- The team has developed cell and stack manufacturing processes for solid oxide electrolyzers. To further improve the performance and durability, the team should consider implementing novel materials that can enhance the performance and enable the lower-temperature operation.

Project #P-202: Novel Microbial Electrolysis Cell Design for Efficient Hydrogen Generation from Wastewaters

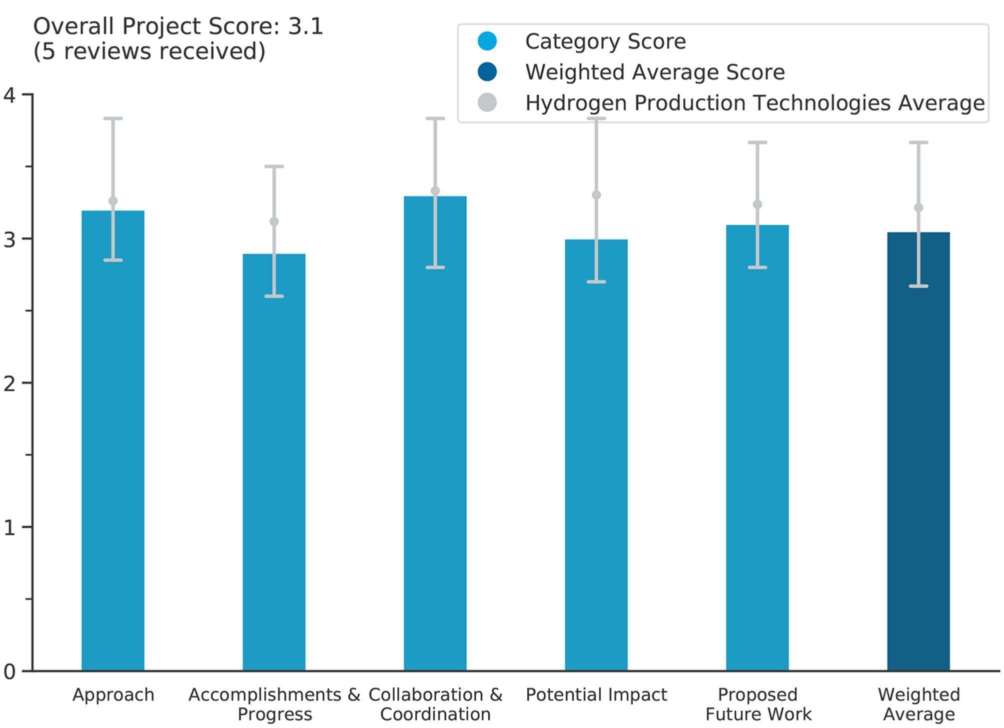
Bruce Logan, The Pennsylvania State University

DOE Contract #	DE-EE0009623
Start and End Dates	9/1/2021–9/30/2024
Partners/Collaborators	Johns Hopkins University, National Renewable Energy Laboratory, Island Water Technologies
Barriers Addressed	• Low cell efficiency • Small current density • High cathode cost and poor hydrogen production

Project Goal and Brief Summary

This project seeks to offer a cost-effective method to generate hydrogen utilizing wastewater as a renewable resource while reducing feedstock costs and environmental impact. The primary objective is to develop a novel design for a zero-gap bench-scale (100 cm^2) microbial electrolysis cell (MEC) that efficiently produces high-rate hydrogen from wastewaters. The innovation involves combining an anion exchange membrane (AEM) and eliminating the use of a liquid catholyte, resulting in improved current density, hydrogen production rates, and pH stability. Activities include testing hydrogen production from various feedstocks and optimizing the fermentation process, as well as validating and optimizing MEC performance. Additionally, researchers will prepare cathodes free of platinum group metals. The ultimate aim is to demonstrate a pathway for hydrogen production at scale using wastewater feedstock, while addressing cost, performance, durability, and scalability challenges.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Hydrogen Production Technologies projects.

Question 1: Approach to performing the work

This project was rated **3.2** for identifying and addressing objectives and barriers and for project design, feasibility, and integration with other relevant efforts.

- The project is developing advances to the MEC process by developing new membranes with OH- conductivity. This promises more stable pH, which is beneficial for a microbial colony. The system can operate at higher current.
- The Pennsylvania State University's (Penn State's) approach to developing MECs addresses the critical barriers to potentially reducing biological hydrogen cost.
- Omission of liquid catholyte seems promising.
- The approach seems fine, but it is not clear what size cell is being used. It is unclear if this approach was developed with the larger cells in mind that are necessary for practical use. The figure in slide 8 shows a cell, which is hard to see. It may be less than 10 mL. If a larger cell must be built for practical application, it is unclear whether the reported results will hold. The approach slide (#8) indicates MEC architecture optimization for scale-up. This suggests scale-up was considered. Factors that went into this optimization were not clear. The approach to research and development, which is to demonstrate the target current density and hydrogen productivity, should be such that the construction of the cell should be possible at larger scale and the cost should be manageable. It is unclear whether the team has any idea of the cost of producing the multicomponent cell as shown in the exploded diagram if built at a cubic meter of anode volume. The cost in $\$/m^3$ is not clear. The National Renewable Energy Laboratory (NREL) approach mentioned different biological buffers. The approach/results did not indicate which buffers. This is critical to MEC technology. The buffer can be an expensive component of MEC operation. It was not clear whether the buffer was reused through the operation of the MECs in the results shown in slide 11. It seems the buffer was changed daily. It may not be economical to change the buffer every day. That will define whether this approach is practical. If practically relevant conditions are not used in determining performance, that result does not carry much meaning. The approach of genetically engineering a microbe to produce acetate only for MEC use seems very problematic. It was unclear whether the engineered microbe may work with any feedstock other than that which was used to develop it. Practical use with wastewater is unclear. There are many questions this approach raises in terms of host robustness and use, which may pose a problem with applications with other feedstocks and can be costly if the strain has to be engineered for each feedstock/use case separately.
- The AEM approach is interesting. The need to process mostly acetate seems like a limit.

Question 2: Accomplishments and progress

This project was rated **2.9** for its accomplishments and progress toward overall project and DOE goals.

- Penn State is making great progress toward achieving its objectives. The project has shown hydrogen production rates and applied current densities to the microbial electrochemical cell that are in family with the highest performance reported to date. The project has demonstrated progress toward meeting the DOE goals but is still about an order of magnitude on applied current density from approaching the hydrogen production cost of $2/kg per consortium economic analysis projections. This project has shown very good work.
- The accomplishments of high current density and productivity look good, but the key is to understand whether this result extends to appropriate cell size, buffer needs, media needs, feedstocks, continuous operation, etc. The cell size was not mentioned in the presentation. It is well-known in the MEC literature that cell size is a huge determinant of the two main parameters reported here (current density and hydrogen productivity). For small sizes, these performance parameters are high, but as size increases, the performance can go down significantly, almost exponentially. It is not clear whether this result will hold for a size suitable for practical deployment. The criteria for choosing the cell size were not clear. The figure in slide 11 indicates a batch mode of operation with current starting at a lower level every 24 hours, so if the media was changed every day, it implies supply of new buffer every day. This may not be practically and economically feasible. The slide does show a four-day run at the end in which current density seems to go down after Day 1 (even before the substrate runs out). The inability to use ethanol, lactate, etc. (fermentation end products other than acetate) seems like a significant drawback of the proposed approach/

work. The solution proposed, which is engineering the fermentation microbe to produce only acetate as byproduct, seems plagued with problems. While the amount of lactate and ethanol produced may be lowered, it will likely not be eliminated completely; so if a continuous process is established, it will require the recycling of media and buffer. Thus, these intermediates will accumulate. This is a significant problem because these chemicals seem to inhibit the ability of electrogens to use acetate as well, so the process cannot be operated for a long term. Additionally, the robustness of the fermentation host is an important consideration if this were to be used for a different feedstock. One of the tasks was to develop a strategy to manage solids. It seems the solution was to remove solids and provide liquid only for MEC experiments. This does not look like a solution to help manage the solids. It was unclear whether the solids will need to be thrown away or how this affects overall conversion of biomass to hydrogen. The impact on hydrogen yield from biomass/waste was not clear.

- The researchers have engineered the fermentation portion with some success. Slide 11 states an 81 L_{H2}/L-d production rate, but those data are not presented on the slide. The 0.95 V with only 20 A/m^2 current density (slide 16) seems low. At 0.95 V, it is unclear whether the current is doing the organic degradation or the microbes are performing degradation. The presentation showed the ability to operate for 42 days, which is good.
- There has been very limited progress from the last year's presentation, apparently owing to the principal investigator's (PI's) changing universities.
- The project delayed some portion of its work from Penn State to John Hopkins University (JHU).

Question 3: Collaboration and coordination

This project was rated **3.3** for its engagement with and coordination of project partners and interaction with other entities.

- Penn State has shown good collaboration and coordination with each of its project partners. Guidance from Island Water Technologies and NREL improves both the project's impact and its likelihood for success.
- It seems to be the right combination of collaborators, with the inclusion of JHU.
- The team seems well-organized. The roles are defined.
- There seems to be a good collaboration between Penn State, JHU, and NREL. The role of industry seems minor. This may be why the size of the cell was so small. It is important to get input from industry on the size of a system needed for this to work.
- Most of the work is conducted by the PI. No significant collaborative effort was discussed.

Question 4: Potential impact

This project was rated **3.0** for supporting and advancing progress toward Hydrogen Program goals and objectives.

- This project is relevant to the DOE cost target for hydrogen production. Penn State is specifically addressing hydrogen production cost; its impact will be on reaching a hydrogen production cost of $1 or $2/kg H_2.
- Wastewater utilization for hydrogen production through the MEC route will have a significant impact on cost reduction.
- Production of hydrogen from organic waste streams is important. The waste streams can have above 1% organics in them, with a large distribution of materials. The low concentrations and the limit on the materials to be fed may limit the impact of this technology. The preference of operating on acetate is a limitation that will limit the potential impact.
- Since the project does not have a techno-economic analysis component (at least in Year 1/2), any advances made without consideration of increased costs in either capital expenditures or operational expenditures are a concern. The use of a small-size cell to claim "largest production rate to date" for hydrogen production hardly translates into an advance, knowing that size has a significant effect on performance metrics (published in MEC/bioelectrochemical systems literature a decade ago). This puts in doubt the potential impact of this project.

- The project is at very low technology readiness level, and it is unlikely that it will be able to reach the DOE cost target in the required timescale.

Question 5: Proposed future work

This project was rated **3.1** for effective and logical planning.

- Penn State's future work will focus on scale-up, durability, and other feeds. The impact of scale-up will be important.
- Proposed future actions are in the right direction.
- Scaling up is a good step. The real biomass fermentation generates effluent with greater complexity than what the project is currently doing. Solving this problem will be a significant challenge.
- The study of cell size from 25 cm^2 to 100 cm^2 is too narrow and limited. It is not clear that a cell size of 100 cm^2 is suitable for practical feasibility. This should be a regular size of cell used for all studies, not a max size to be studied. Results from this size, in themselves, will likely not be suitable for a potential practical application. If the team is going to study the effect of size, it needs to be evaluated with some form of techno-economic analysis or with literature data on identifying size for a study that will have practical relevance.
- The project intends to continue zero-gap cell development. Specified development targets are very brief and not detailed.

Project strengths:

- The project has an engaged end user. The team was able to show long-term operation. The use of the AEM is very creative and has potential to greatly improve this technology.
- The project is developing a novel zero-gap MEC process that promises to provide longer durability operation and lower cost for electrode maintenance.
- The project team is the greatest strength. Island Water Technologies and NREL are providing the guidance required to maximize project success.
- JHU, NREL, and Island Water Technologies are strengths of the project.
- The project has good collaboration between academics and the national lab but not with industry. The work done indicates a design that may have merit, but the use of a tiny cell puts in question the merit of this work for any application.

Project weaknesses:

- There are no apparent project weaknesses in this reporting period.
- The need for engineering a strain to generate acetate as the only product means this technology will have very limited use and will need strain development for every new feedstock that is considered for use as a source of energy. The approach to do genetic engineering vs. advancing the MEC technology to handle multiple substrates may lead to a huge weakness.
- The MEC is limited to acetate. This may limit the technology's applications.
- The cost of produced hydrogen is unlikely to reach the DOE target.
- The time needed to overcome the past delays is a project weakness.

Recommendations for additions/deletions to project scope:

- It is recommended that the project continue testing the fermentation system with real feed and then feed the fermentation effluent to the MEC. It is recommended that the team find a way to improve the MEC to be able to operate effectively on more than just acetate.
- The team may consider reprioritization of efforts in the third year.
- There are no recommendations for additions/deletions to project scope this reporting period.

Project #P-203: Novel Microbial Electrolysis System for Conversion of Biowastes into Low-Cost Renewable Hydrogen

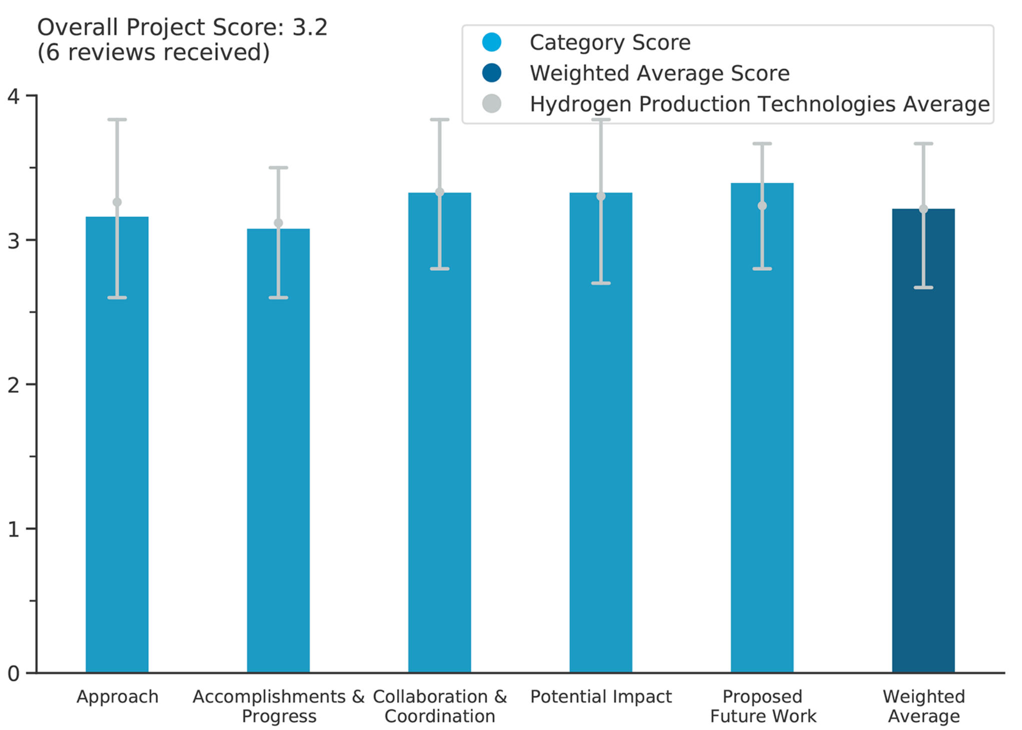
Noah Meeks, Southern Company Services, Inc.

DOE Contract #	DE-EE0009624
Start and End Dates	11/1/2022–10/31/2025
Partners/Collaborators	Electro-Active Technologies, Inc., T2M Global
Barriers Addressed	• Scale-up • Performance • Durability • System/process engineering

Project Goal and Brief Summary

The project aims to identify critical scale-up parameters and develop a microbial electrolysis cell (MEC) stack to achieve target hydrogen productivity (>20 L/L-day). The project also focuses on demonstrating the stability and durability of MEC technology and developing an integrated waste-to-hydrogen system using commercial food waste. The project seeks to enable distributed hydrogen production, increase hydrogen yields in MECs (>40%), and provide a renewable source of hydrogen while abating waste management costs. By the end of the project, the project team will demonstrate an integrated waste-to-hydrogen system using commercial food waste to produce hydrogen with end use in fuel cells.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Hydrogen Production Technologies projects.

Question 1: Approach to performing the work

This project was rated **3.2** for identifying and addressing objectives and barriers and for project design, feasibility, and integration with other relevant efforts.

- Conversion of food wastes that are typically high in chemical oxygen demand (COD) to distributed hydrogen production makes a good deal of sense, as the discharge rate correlates directly with the COD level, so the production cost can be offset by the premium associated with the waste management costs to those generating it. It may be worthwhile for the project to consider or evaluate other or different types of waste streams, as some may have even lower value or better characteristics for MEC operation. Currently, one major barrier for economic biohydrogen production via MEC is scale-up, and much of scale-up is uncharted territory, so one significance of this work is to identify critical scale-up parameters in developing the MEC stacks. It is not clear if a diversity, equity, inclusion, and accessibility (DEIA) plan or a community benefits plan (CBP) is required for this project. It appears that DEIA and CBP are not considered, so it would be important to address these.
- The project objectives are clearly identified as determining the critical scale-up parameters and development of an MEC stack with target hydrogen productivity, demonstrating stability and durability of MEC technology, developing an integrated waste-to-hydrogen system, demonstrating conversion of commercial food waste to hydrogen with end use in fuel cells, and developing a manufacturing plan for product development and market entry. It is not clearly specified, though, how the production target correlates with broader DOE hydrogen strategy.
- Southern Company Services, Inc. (Southern Company) has proposed an effective approach to overcoming the barriers of hydrogen production via an MEC. The project objectives, specifically the plan to commercial entry, could help establish a baseline for how this technology should work in a real-world environment. A milestone schedule could have helped to better assess the approach to performing the work.
- The project approach is in the right direction.
- The project is focused on device development. The electrochemical impedance spectroscopy (EIS) is well-done and allows identification of limits. There is not much focus on electrocatalyst and electrode development.
- The hydrogen production rate is very low. The current density is minimal. High production of biomass is a challenge in that influent material is wasted. There was poor understanding of the EIS step during the presentation. A computational fluid dynamics analysis is apparently missing. The stability of electrodes and other components seems problematic. Anode degradation has not been investigated. There is a lack of understanding of the impact of the biomass pretreatment step on the overall economics and performance of the cell. It is not clear what fraction of hydrogen is generated at the anode compared to the cathode. As in many other projects of this level, there is no interest in understanding the degradation of components.

Question 2: Accomplishments and progress

This project was rated **3.1** for its accomplishments and progress toward overall project and DOE goals.

- Southern Company is making good progress toward achieving the project objectives. The current densities achieved by Southern Company are low compared to what the BioHydrogen Consortium is publishing as required to achieve a cost of hydrogen of $2/kg. Durability is consistent with that demonstrated by similar projects.
- The work has assessed several performance metrics and demonstrated sustained hydrogen productivity over 25 weeks and high cathode efficiency, so there is demonstrated stability, durability, and high COD removal. The current density seems to be low, and it would be ideal if there were some mention of potential pathways to increase the current density. One of the goals was to identify critical scale-up parameters, but it is not clear what progress was made toward that goal. Beyond the set goals, it is not clear if there are any safety considerations for the scale-up of MEC.
- The project made significant progress in demonstrating durability of the MEC process, increasing cellular biomass yield. The current density of the process is very low, though, which is likely to translate into high costs for the process.

- The project has shown 15 weeks of continuous operation. The cathode efficiency remains high and seems fairly stable. The current density is low, which will result in very large cells/reactors being used. This could result in large capital costs. The voltage is not reported, and it should be. The feed should be defined. The test setup should be shown.
- The project is as per the targets.
- It is not clear how the researchers envisioned their way toward \$2/kg H_2. The electrochemical and microbiological understanding of the proposed project seems limited. The EIS scheme proposed has been known for decades.

Question 3: Collaboration and coordination

This project was rated **3.3** for its engagement with and coordination of project partners and interaction with other entities.

- There is good collaboration between the team members in the project.
- Southern Company has good collaboration with its partners. The project team is encouraged to incorporate the BioHydrogen Consortium hydrogen cost models into the work.
- Partners appear to work together toward meeting the goals. It could be beneficial to make connections with or leverage what is already invested in universities and national labs to accelerate advancements in MEC development and scale-up.
- The team is well-defined. The roles are defined.
- Partnering with industrial partners is a good step.
- There seems to be good synergy between the different partners. T2M's global role is not clear.

Question 4: Potential impact

This project was rated **3.3** for supporting and advancing progress toward Hydrogen Program goals and objectives.

- Southern Company's project is in excellent alignment with the Hydrogen Program's goals. The project is advancing progress toward increasing hydrogen production from MECs, increasing durability, and making transitions to real-world testing. The transition to real-world testing may help assess the status of the cost-effectiveness of hydrogen production via microbial pathways.
- The production of hydrogen while cleaning up wastewater can have a significant impact. The team needs to report on the feed composition, cell design, and construction to better evaluate the potential impact. The project is planning a techno-economic analysis (TEA), which will help with the impact.
- The developing MEC technologies and the proposed goals appear to align with Hydrogen Program and DOE objectives. It appears to be a novel and niche hydrogen production pathway in converting aqueous waste streams high in COD into hydrogen. Enabling economic scale-up for MECs in stacks is highly relevant.
- Potential pathways to reach the hydrogen production cost target of \$1/kg or less than \$2/kg of H2 produced need to be shown.
- The project is developing a pathway to distributed hydrogen production while utilizing waste resources. Waste abatement in the process should lead to low cost of hydrogen production. The project is designing a pilot plant to demonstrate the process operation under realistic conditions.
- There is proper effort for cost reduction and waste management. Using waste for hydrogen production is a plus. The economics behind the proposed approach compared to fermentation toward valuable chemicals are not clear.

Question 5: Proposed future work

This project was rated **3.4** for effective and logical planning.

- The project is currently building the pilot test model and planning on module testing. Clear plans for TEA work are outlined.

- The future work includes TEA/LCA (life cycle analysis), which should be very informative. The components in wastewater can vary significantly, even if the wastewater is coming from the same source. It is recommended that the project test different sources of wastewater to understand the impact.
- The future work proposed by Southern Company builds on past progress and is focused on scale-up and demonstration. The project is logically planned. The decision points could not be accurately assessed, as a timeline was not available to review. Risk analysis and mitigation may be part of the business plan being developed but could not be assessed during this reporting period.
- The project's proposed future work is a logical extension of the work accomplished. As a remaining barrier and proposed future work, it would be relevant and important to conduct TEA to have a clear understanding of the cost drivers for scale-up. Additional gaps, such as how scale-up will impact MEC operations/performance, need to be addressed, as well as how the MEC technology has a pathway to $1/kg of H_2.
- The scale-up phase seems to be proceeding too slowly.
- The proposed future work was not given in the presentation material provided.

Project strengths:

- The project has clear objectives that are relevant, and the overall vision and approach to convert heterogeneous food waste into hydrogen are in good alignment with DOE research, development, and demonstration goals. The project showed reasonably good progress in demonstrating sustained hydrogen production at high cathode efficiency over 25 weeks.
- The project demonstrates MEC operation under realistic conditions and will identify critical process parameters that may lead to lowering the cost of hydrogen production.
- The project's strength is moving microbial-based hydrogen production to real-world applications.
- The team has a motivated end user. The team has demonstrated the MEC's ability to operate continuously for over one month without degradation.
- The project addressed current density limitations in biological hydrogen production through MECs. The use of EIS is a strength.
- The methodology is a project strength.

Project weaknesses:

- There are no major project weaknesses in this reporting period.
- The use of TEA for such an early-stage project can be misleading. Current and hydrogen production rates are low; there seems to be no clear advancement toward the $2/kg as claimed by the proposers. The applied voltage is too large, and it seems that no investigation has been carried out to determine the stability of the electrolyzer component over time. Biomass production is a challenge in that input material is wasted to generate biomass rather than producing electrodes.
- There is no mention of a safety plan. It is not clear that the project takes DEIA into consideration. There is a lack of description of how this type of project can benefit communities. There are ongoing DOE investments in national labs and universities to improve MEC at various fronts, and it would be beneficial to leverage these efforts and cross-inform to make research dollars even more effective.
- The current density is lower than expected. The EIS data has identified which electrode is limiting. The project needs to improve the cells' performance.
- The current density in the process is very low.

Recommendations for additions/deletions to project scope:

- Additional gaps need to be addressed, such as how scale-up will impact MEC operations/performance and how the MEC technology has a pathway to $1/kg of hydrogen. The technology should also assess the energy cost associated with scale-up and compare that with the incumbent and with emerging technologies.

- The current density is lower than expected. The EIS data have identified which electrode is limiting. The team needs to improve the cells' performance. The project should test the system with waste from other locations.
- No additions or deletions to the current project scope are recommended this reporting period.

Project #P-204: Hydrogen Production Cost and Performance Analysis

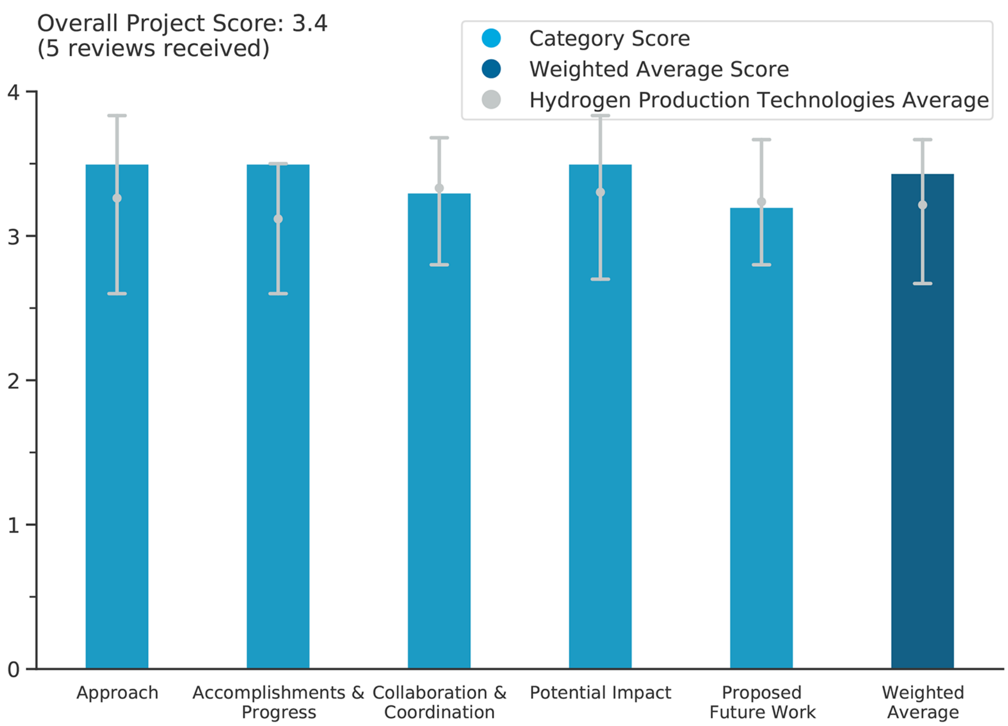
Brian James, Strategic Analysis, Inc.

DOE Contract #	DE-EE0009629
Start and End Dates	10/1/2021–9/30/2024
Partners/Collaborators	National Renewable Energy Laboratory, Idaho National Laboratory
Barriers Addressed	• Hydrogen generation by water electrolysis: • Capital cost • System efficiency and electricity cost • Manufacturing

Project Goal and Brief Summary

The project aims to conduct a techno-economic analysis of various hydrogen production pathways, including electrolysis and photoelectrochemical methods, to evaluate the cost of hydrogen production. The project utilizes Design for Manufacture and Assembly (DFMA®) techniques, heat and mass balances, and Hydrogen Analysis (H2A) discounted cash flow models. The goal is to estimate the cost of hydrogen production based on state-of-the-art technology at central production facilities (50–500 tons per day) and measure the cost impact of technological improvements in hydrogen production technologies. The project will provide a comprehensive pathway analysis, identify cost drivers, guide research and development efforts, and support the Hydrogen Shot goal of achieving $1/kg hydrogen production cost. The approach involves collecting data, conducting cost analysis of proton-conducting solid oxide electrolysis, and collaborating with experts and research institutions to ensure transparency and accuracy.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Hydrogen Production Technologies projects.

Question 1: Approach to performing the work

This project was rated **3.5** for identifying and addressing objectives and barriers and for project design, feasibility, and integration with other relevant efforts.

- The project conducts techno-economic analysis of various technological hydrogen production pathways to evaluate and compare the cost of hydrogen production ($/kg) consistently, allowing for comparisons of prospective outcomes of a broad range of technologies. The project is extremely important in directing agency funding toward the technologies that show the greatest potential for achieving the ultimate cost targets.
- The analysis shown was very thorough. The presentation included the best approach to getting at very difficult cost data for the analysis of high-temperature electrolysis (HTE). A good combination of capital and manufacturing costs are captured for current and future scenarios. Accurate process flow diagrams are used to capture all cost elements.
- This project is conducting an important analysis to understand the overall component costs, project costs, and levelized cost of hydrogen (LCOH). Last year, the overall LCOH numbers (slide 15) looked extremely ambitious; this year, they are still very ambitious, even at a 1 GW/year annual electrolyzer manufacturing rate. However, the numbers are getting better as they are being validated and as the community is learning more about the larger projects.
    - In slide 17, one of the reviewers asked the project team to verify the numbers with vendors (equipment capital expenditures) and engineering, procurement, and construction companies (EPCs) (installed cost). The presentation did not include a slide that summarizes which vendors and EPCs were contacted over the past 2.5 years of the project and their overall inputs on the cost model. Instead, the presentation mentioned reports by third parties. It would be valuable for the remainder of the project to actually verify these numbers with project developers, EPCs, and vendors to provide a realistic cost picture. Naming them directly would boost the confidence on assumptions made in the model.
    - If $30/MWh electricity cost was assumed, it is unclear if this is a basis number and what the cost of delivered energy is, including transmission and distribution. If $30/MWh is the total energy cost, it is unclear where would such projects need to be located. They are certainly not in the United States.
    - It is not clear which alkaline vendors have been considered in this analysis. Alkaline technology is mature and deployed in gigawatts across the world, including high-pressure alkaline. It is unclear how technology readiness level (TRL) 10 technology can be at similar or higher cost when compared to early-stage proton exchange membrane (PEM) electrolysis. The largest PEM project deployed and operational to date is 40 MW and located in the United States. The team is asked to provide a tabulated summary of vendors, EPCs, and project developers the team has reached out to and show numbers/costs provided by those parties, and then reflect a true industry-fed analysis into the cost model. This would benefit the model for future use.
    - If the model is too optimistic and the goal is to share it with industry and the wider community, the dose of reality would strike very quickly and potentially provide a lack of confidence in the tool. Perhaps a more conservative approach should also be considered to understand the range of potential LCOH, as the uncertainty behind treasury guidance is still a massive risk and not included in the model.
    - Remaining questions include what the plan is for this model funded fully (100%) by DOE, whether it be open to public, and how we can access the full model so we can experiment with it and understand the full set of assumptions behind it.
- The reviewer thanks the team for the hard work and looks forward to seeing the implemented changes summarized above.
- The approach is similar to what has been done on other electrolyzers. Most solid oxide electrolyzer cells (SOECs) will be integrated into chemical or other processes that have waste heat. The team did not look at the case in which the SOEC is integrated into a system that provides "waste steam" at 101°C and slightly over 1 bar. This would increase the system efficiency from ~73%, which is what is currently used, to about

80%–85% and significantly change the LCOH. The speaker was careful to use “cost” and “price” terminology correctly.

- The project contributes to an understanding of HTE.

Question 2: Accomplishments and progress

This project was rated **3.5** for its accomplishments and progress toward overall project and DOE goals.

- HTE models are updated with current information. The project is conducting complete system analysis, with the majority of system costs and balance-of-plant (BOP) costs included. Electrical BOP is well-defined and, as a significant cost contributor, is important to capture as part of the total cost of hydrogen. In the reported period, the project conducted bottom-up cost analysis of high-temperature water electrolysis systems and compared results with other previously analyzed pathways for hydrogen production. Guidance was issued for selection between proton-conducting SOECs (p-SOECs) and oxygen-ion-conducting SOECs (o-SOECs).
- The system efficiency seems reasonable, and a thorough job was done to develop it. Most SOECs will be integrated into chemical or other processes that have waste heat. The team did not look at the case in which the SOEC is integrated into a system that provides “waste steam” at 101°C and slightly over 1 bar. This would increase the system efficiency from ~73%, which is what is currently used, to about 80%–85% and significantly change the LCOH. It is assumed that this will be captured in the sensitivity analysis (noted in Future Work). The alkaline and PEM future efficiencies seem very optimistic. The experience with industry using the electrolyzers in the field is resulting in lower efficiencies than are used here for “current.” The fixed operating and maintenance costs for the low-temperature electrolyzers show dramatic decreases from current to future, but the SOEC shows a very modest ($0.01/kg H_2) decrease. It is unclear why that is. The reviewer is looking forward to the sensitivity analysis.
- Significant progress has been made, contributing to overcoming some barriers. Proton-conducting HTE is a distant development objective and should be de-emphasized. The team needs to redirect to Nexceris and OxEon Energy.

Question 3: Collaboration and coordination

This project was rated **3.3** for its engagement with and coordination of project partners and interaction with other entities.

- Strategic Analysis collaborates with a broad range of academic institutions, government labs, and industrial companies to collect the cost and performance data for various hydrogen production technologies. The company’s analysis results are widely respected and used by all the partners developing hydrogen production systems.
- The project has great use of national labs to support and confirm the approach. Engagement with DOE managers through bi-weekly calls helped to guide the direction of work and provide input to modeling efforts. Including an industry partner greatly improves confidence in the quality of the data used and results presented.
- The roles seem well-defined. The lead organization has a history of excellent collaboration and seems to be continuing that in this project.
- The project works well with many other organizations. The project needs to redirect to Nexceris and OxEon Energy.
- There is a lack of first-hand information from vendors, EPCs, and developers. There is certainly room for improvement.

Question 4: Potential impact

This project was rated **3.5** for supporting and advancing progress toward Hydrogen Program goals and objectives.

- This project is critical for achieving progress toward the project’s specific performance targets and the Hydrogen Program goals and objectives, as the work allows for evaluating and comparing the cost of hydrogen production through different pathways and provides valuable insight on the key cost reduction opportunities for each of the production technologies.

- The analysis provides insight as to the parameters and highest cost contributors for HTE. The modeling work can be used to guide developmental efforts toward key areas of research to focus cost reductions in an effort to meet DOE targets.
- Electrolyzers are key for a low-carbon future. This work can be very important for aiding in directional development.
- The focus should be on near-term o-SOEC HTE, which would have a greater possible impact on the Hydrogen Program.

Question 5: Proposed future work

This project was rated **3.2** for effective and logical planning.

- The project will continue analysis of HTE cell technology. Strategic Analysis will conduct cost analysis of additional hydrogen production pathways, collaborate with DOE on system design and operation, and provide estimates of total installed capital cost and resulting LCOH of hydrogen production systems of interest.
- The future work includes sensitivity analysis. The future work should include the impact of integration into a chemical or other system in which steam will be provided to the SOEC. This is the most likely scenario for both types of SOEC.
- Future work is well-defined and shows what areas will be refined to improve the model. Recognizing it is very difficult to get costs from industry, it would be nice if the results and approach could be verified or validated by additional companies working in this space to provide further confidence in the model.
- Proton-conducting HTE is a distant development objective. The near-term focus should be on established vendors such as FuelCell Energy and Bloom Energy. The project should redirect to Nexceris and OxEon Energy.

Project strengths:

- The important strength of the project is in its ability to produce bottom-up cost estimates for a broad range of technologies using a similar set of techno-economic assumptions and, thereby, provide an apples-to-apples comparison of the cost of hydrogen produced by different technologies that may be at very different TRLs.
- The project has a very thorough analysis that covers all aspects of the system. Estimates are being updated as new information becomes available. The team comprises experts in the field to provide confidence in the model. The inclusion of an industry partner is a strong addition to the work.
- The project has a very strong and experienced team with the right tools and approach. The project has buy-in and trust from the industry, so the industry is willing to share information.

Project weaknesses:

- There are no significant weaknesses.
- Both o-SOEC and p-SOEC will most likely be used in conjunction with sources of excess thermal energy such as a chemical plant, fertilizer plant, nuclear plant, or others. The “free” steam will likely increase the efficiency. This scenario needs to be evaluated. The efficiencies for the alkaline seem overly optimistic.
- Through no fault of the principal investigator, the model relies on estimates and available information through literature searches, which can be limited. While tremendous effort has been undertaken to get detailed cost information, the difficulty in getting industry numbers might put some large error bars on some of the inputs used.

Recommendations for additions/deletions to project scope:

- The sensitivity analysis should include the potential for higher efficiency. The p-SOEC full stack lifetime is questionable such that even a four-year lifetime is a stretch. The sensitivity analysis should include very short lifetimes (approximately one year).
- Proton-conducting HTE is a distant development objective. The project should focus near-term and redirect to Nexceris and OxEon Energy.

Project #P-205: Metal–Organic Framework-Based Heterostructure Electrocatalysts with Tailored Electron Density Distribution for Cost-Effective and Durable Fuel Cells and Electrolyzers

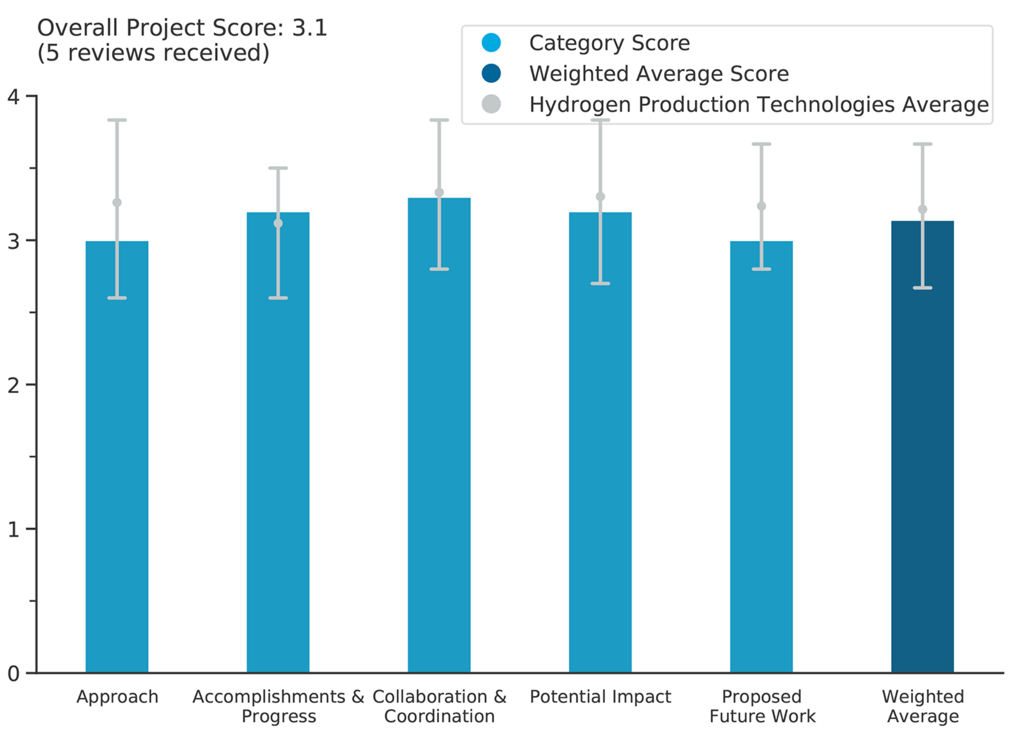
Sreeprasad Sreenivasan, University of Texas, El Paso

DOE Contract #	DE-EE0010431
Start and End Dates	8/1/2023–7/1/2025
Partners/Collaborators	University of Texas at El Paso Functional Quantum Materials Lab, University of Puerto Rico at Cayey, National Renewable Energy Laboratory, Los Alamos National Laboratory, Argonne National Laboratory
Barriers Addressed	• Use of precious Pt-, Ru-, and Ir-based catalyst benchmarks in electrolyzers and fuel cells • Low atomic utilization of alternate catalyst and lower efficiency • Inferior electron dynamics in alternate framework-based catalysts

Project Goal and Brief Summary

This work will advance hydrogen and fuel cell technologies by creating high-performance and cost-effective catalysts for low-temperature reversible fuel cells. The project is developing heterostructure, metal–organic framework (MOF)-based catalysts that are low-cost and free of platinum group metals (PGMs). The catalysts contain fullerene and MXene (a class of graphene). The project aims to demonstrate outstanding oxygen reduction and evolution reaction (ORR and OER) activity and to achieve DOE targets for round-trip efficiency and durability in low-temperature reversible fuel cells.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Hydrogen Production Technologies projects.

Question 1: Approach to performing the work

This project was rated **3.0** for identifying and addressing objectives and barriers and for project design, feasibility, and integration with other relevant efforts.

- The project is taking a different and relatively high-risk approach but, if successful, could have a significant impact.
    - The approach of pursuing bifunctional OER and ORR activity in a single catalyst should be deemphasized. Achieving a breakthrough on either OER or ORR would be a major contribution; trying to simultaneously improve OER and ORR decreases the likelihood of succeeding with either reaction. Overall, based on the published preliminary work on ORR and the concerns about durability in harsh OER environments with concentrated potassium hydroxide (KOH), the ORR aspect of the project appears more valuable.
    - Issues related to the electronic conductivity of MOF catalysts should be addressed and clarified. Although conjugation can provide some conductivity, the MOFs will have conductivity far lower than that of typical carbon-supported ORR catalysts. Quantitative measurements of conductivity are recommended to assess the severity of the problem and shed more light on the need for conductive additives.
    - The particle size of the MOFs appears to be on the micron scale. At this size, there are concerns about transport inside the MOF particles. Specifically, for ORR, there is a need to transport O_2, H^+, H_2O, and electrons; the first three are challenging due to the small pore size, while the last is challenging due to the low conductivity. All these transport problems are exacerbated by the micron-scale size. To address this issue, there is a need to develop the MOFs in a nanoscale form factor. Also, integration into continuous and uniform electrodes will be challenging with such large particle sizes, further necessitating a transition to nanoparticle form factors.
    - The approaches of pursuing lattice strain and undercoordinated sites are promising and should be further pursued.
- The objectives and barriers were clearly identified; the project aims to eliminate the use of precious metals in low-temperature reversible fuel cells by using an alkaline electrolyte and by developing bi-metallic MOF-based catalysts that are active for both oxygen reduction and oxygen evolution. It was unclear from the presentation whether this was targeted for the unitized reversible fuel cell application or for two separate devices, as the researchers were testing the same catalyst compositions for both ORR and OER but requested separate fuel cell and electrolyzer testing from Electrocatalysis Consortium (ElectroCat) core labs. If indeed the same catalyst will be used for both reactions, this is an extremely challenging project. The MOF structures will be oxidized to form oxides of the constituent transition metals during OER, and these oxides will not be very active for ORR. Also, the biggest challenge to using the as-prepared MOFs as electrocatalysts is their low electronic conductivity (as identified in the “Remaining Challenges and Barriers” slide). The bimetallic MOFs, however, could be interesting precursors for forming bimetallic TM1-TM2-N-C ORR electrocatalysts (where TM indicates transition metals).
- Designing innovative MOF materials for bifunctional ORR and OER catalysts in alkaline media is interesting. This could provide new knowledge and an approach to advancing PGM-free catalysts for clean energy storage and conversion. However, the intrinsic stability and electrical conductivity of MOFs may mitigate their application in real water electrolyzer/fuel cell environments.
- The presented approach is generally good; however, several reviewers raised a concern on the stability of MOF under harsh conditions for OER/ORR. The principal investigator has an alternative way to resolve that issue, which potentially can reduce the risks associated with stability.
- The project takes a reasonable approach; there should be more learning from the reasonably extensive work done on this topic previously.

Question 2: Accomplishments and progress

This project was rated **3.2** for its accomplishments and progress toward overall project and DOE goals.

- Given that the project just started last August and only a small fraction of the total DOE budget has been spent, the progress is very good. There has been excellent use of advanced characterization techniques for structural and chemical composition of the catalysts. The initial OER activity is promising, most likely because cobalt oxide is formed from the MOF. The ORR activity demonstrated thus far is very low.

- The team has demonstrated the feasibility of synthesizing different MOFs with viable metal sites and organic ligands. The initial catalytic activities in alkaline solutions were studied. Importantly, doing two ligands to modify the local structures of metal sites in MOF structures effectively improves intrinsic OER activity.
- The project just started, and for the current period of performance and funds spent, progress is good.
- There is some progress on rotating disk electrode (RDE) testing of OER and ORR activity of novel MOF catalysts, but most of the results seem to be from fairly simple monometallic MOFs, based on the results shown so far. Bimetallic MOFs were also pursued, but there is not much evidence so far indicating that bimetallic MOFs provide any advantage over monometallic. Furthermore, since the metal sites are substantially separated within the MOF architecture, there is some question about the degree to which bimetallic MOFs would provide substantially different active sites compared to their monometallic cousins.
    - Good characterization was performed, including x-ray diffraction (XRD), infrared (IR) spectroscopy, scanning electron microscopy (SEM), and x-ray absorption spectroscopy (XAS). Brunauer–Emmett–Teller (BET) and pore size analysis should be shown as well.
    - The OER performance is reasonably encouraging, but durability concerns may be a showstopper.
    - The ORR performance is far lower than that shown in the same group's previous work on Co-Cu MOF based on 1,2,4,5-benzenetetramine and benzene-1,3,5-tricarboxylic acid. The mechanism of high performance in the earlier work, which could have suffered from high electronic resistance, is not very clear. However, given the concerns about the durability in OER environments, focusing on ORR and trying to reproduce or even improve on the pre-project work would be more valuable.
    - Membrane electrode assembly (MEA) testing has not begun yet but will be critical to the success of the project. RDE results are known to have weak correlation with MEA performance, particularly for ORR.
- There has been an impressive amount of work; there is a need for more electrochemical measurements, especially for any measure of stability.

Question 3: Collaboration and coordination

This project was rated **3.3** for its engagement with and coordination of project partners and interaction with other entities.

- The coordination with the University of Puerto Rico is valuable. The planned collaborations with national labs will be even more valuable but do not appear to have started yet.
- The project is partnering with the University of Puerto Rico at Cayey and has plans to partner with ElectroCat labs for characterization and evaluation in devices.
- The proposed collaboration is well-thought-out and quite comprehensive.
- There is good collaboration for such a small project.
- The collaboration between two teams was presented but does not generate sufficient synergy.

Question 4: Potential impact

This project was rated **3.2** for supporting and advancing progress toward Hydrogen Program goals and objectives.

- If successful, the project will have good impact on the implementation of PGM-free materials for production of green hydrogen, as well as utilization through fuel cells.
- This project is highly relevant and valuable for the Hydrogen Program's goals.
- The project is aligned with DOE goals.
- The project is tackling two catalytic challenges that are difficult on their own and trying to tackle both with one material. The synthetic approach to forming well-controlled dispersion of monometallic and bimetallic sites in one material allows for an immense range of tunability of the catalytic sites. However, the stability of the MOF backbone under the oxidizing conditions of the fuel cell cathode and especially the electrolyzer

anode is a concern. It is likely that the oxides of the constituent transition metals will be formed. However, this may be a means for forming bimetallic oxides with high dispersion for ORR. Likewise, the bimetallic MOFs could be pyrolyzed to form TM1-TM2-N-C ORR catalysts that could be highly active. If the MOF materials do remain intact in the fuel cell or electrolyzer environments, lack of electronic conductivity is also an issue.

- MOFs have been widely studied as catalysts for fuel cell and water electrolyzer technologies. However, because of the MOFs' stability and relatively low electrical conductivity, viable applications in practical energy devices are questionable. On the other hand, elucidating the correlation between MOF structures and their intrinsic activity is crucial for understanding active site and reaction mechanisms.

Question 5: Proposed future work

This project was rated **3.0** for effective and logical planning.

- The proposed future work is very relevant to the goals, targets, and barriers to be solved.
- Future work should focus on understanding active site structures and their dynamic changes during the ORR and OER. Importantly, it is critical to examine MOF catalyst performance and durability in fuel cells and electrolyzers to study their effectiveness in the early stages.
- The proposed future work was presented at a very high level. Understanding the changes in the chemical composition and structure of the catalysts induced by the electrochemical environment and potential should be one of the highest priorities.
- Focus on OER makes sense, but the team needs to ensure observed performance is real and not corrosion of carbon through cycling.
- The future work is good but is missing conductivity studies, examination of particle size effects, and surface area and pore size analysis.

Project strengths:

- There is potential for implementation of PGM-free catalysts for reversible alkaline exchange membrane fuel cells and water electrolysis. The project has a great combination of theoretical and experimental work. There are several approaches to minimize the risks associated with materials to be developed.
- The strengths of the project are the synthetic skills of the principal investigator and his team and the immense tunability of the composition and structure of the MOF materials.
- Tuning metal sites and organic ligands to design MOF-based catalysts is innovative. The team has strong expertise in designing and synthesizing MOFs.
- The team has done an impressive amount of work, synthesis, and characterization compared to the timeline and funding level.
- The project is highly innovative, provides high risk–high reward, and attacks key barriers.

Project weaknesses:

- The project plans to improve low electrical conductivity of proposed materials by adding carbon nanotubes (CNTs) and fullerenes. Both these additives are expensive, and in addition, CNTs have a high iron admixture. This approach may not be ideal for this type of MOF catalyst.
- There is no clear reference or leveraging of the extensive background and expertise for these types of materials.
- The work is too scattered between OER and ORR, lacks fundamental understanding of key issues such as electronic conductivity, and is too dependent on RDE (so far).
- The team still lacks a profound understanding of electrochemical ORR and OER in terms of active sites and mechanisms.
- There are issues with stability and low electronic conductivity of MOFs.

Recommendations for additions/deletions to project scope:

- Recommendations include separating the functionality of the catalysts—optimizing one composition for OER and another for ORR—and exploring use of bimetallic MOFs as ORR catalyst precursors, which can be heat-treated to form the active, stable, and electronically conductive form of the catalyst. Also, it is recommended that the project improve understanding of the phase transformations that the MOFs are undergoing in the electrochemical environment.
- Determining catalytic selectivity for the ORR (two vs. four electrons) and OER (oxygen evolution vs. other side reactions) is necessary to understand the reaction mechanism associated with metal sites and local structures. Optimizing catalyst morphologies, such as surface areas and particle sizes, could potentially improve catalytic performance.
- It is recommended that the project concentrate in the next fiscal year on the stability of catalysts, evaluate products of decomposition, and potentially switch to an alternative class of catalysts. Another recommendation is improvement of conductivity with cheap carbons that are free of metal admixtures.
- Recommendations are to focus on leveraging ElectroCat expertise, focus on OER, and account for carbon corrosion in electrolysis at 1.8 V (well above the electrochemical potential for carbon oxidation).
- The project focus should shift to ORR. The work scope on OER should be de-emphasized or removed. There is no good reason to pursue bifunctionality at this point.

Project #P-206: Single-Walled Carbon Nanotubes with Confined Chalcogens as the Catalysts and Electrodes for Oxygen Reduction Reaction in Fuel Cells

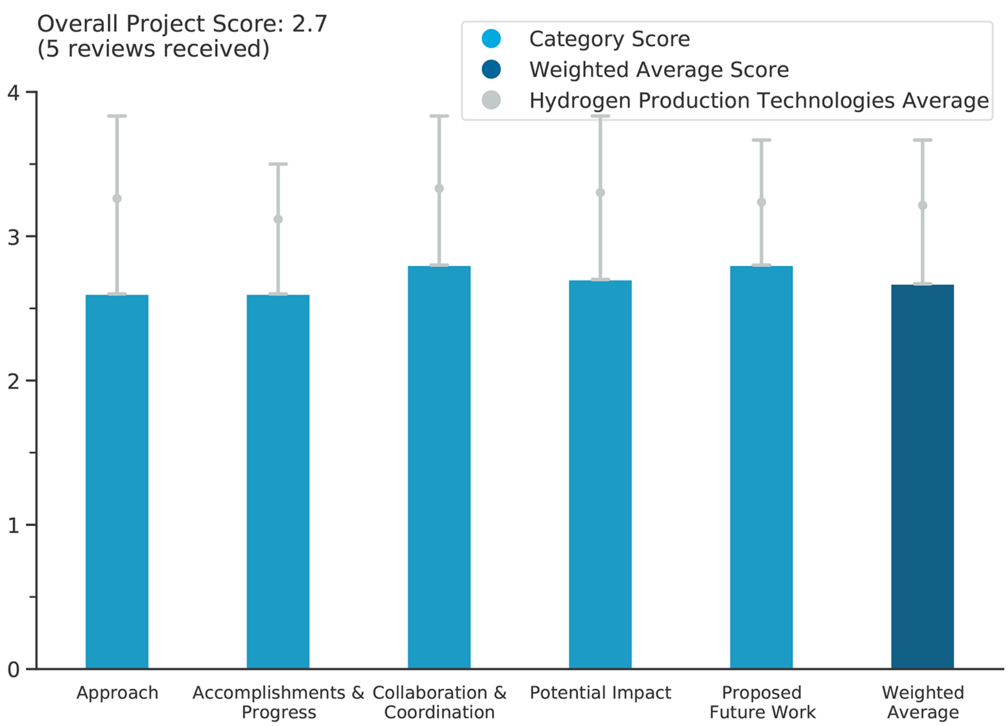
Juchen Guo, University of California, Riverside

DOE Contract #	DE-EE0010432
Start and End Dates	6/1/2023–5/31/2025
Partners/Collaborators	Los Alamos National Laboratory
Barriers Addressed	• Synthesis of effective catalysts free of platinum group metals • Simulation and characterizations of the catalysts • Membrane electrode assembly performance demonstration

Project Goal and Brief Summary

The project is conducting experimental and theoretical investigations on a new type of platinum group metal (PGM)-free catalyst for oxygen reduction reaction (ORR) in proton exchange membrane fuel cell (PEMFC) technology. These catalysts consist of single-walled carbon nanotubes (CNTs) with sulfur and selenium confined in the interior. The project aims to synthesize and investigate the catalytic properties of these catalysts, understand the relationship between electronic structure and catalytic activity, and fabricate and evaluate integrated electrodes. By developing an innovative, PGM-free catalyst that will advance efficiency and cost-effectiveness, the project may generate new knowledge of fundamental materials science, electrochemical catalysis, and PEMFC technologies.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Hydrogen Production Technologies projects.

Question 1: Approach to performing the work

This project was rated **2.6** for identifying and addressing objectives and barriers and for project design, feasibility, and integration with other relevant efforts.

- Exploring alternative catalysts to replace platinum is high-reward research and potentially generates a significant impact on future fuel cell technologies. The project explores a possible synergy between sulfur and CNTs to design iron-free and metal-free catalysts for challenging ORR in acidic media. The work could generate interesting understanding and synthesis methods for catalyst development.
- The concept of using chalcogenides in a confined form to improve ORR activity of carbon-based materials is novel and has not been studied in detail before. Being metal-free, these materials can potentially have higher stability in PEMFC conditions.
- The approach seems reasonable; the team should look into previous work by S.C. Barton and U. Diebold.
- The aim of the project is to develop PEMFC ORR catalysts using sulfur and selenium confined in the interior of single-walled nanotubes. These materials have been suggested by density functional theory (DFT) calculations to have very high ORR limiting potentials; however, no other rationale was given regarding why these materials should be ORR active.
- The project focuses on development of PGM-free ORR catalysts based on sulfur and/or selenium encapsulated in CNTs. There is little evidence or reason to think that these catalysts can be effective for ORR. Indeed, carbon is already known to have poor activity and high overpotential. The idea that sulfur or selenium can induce activity in adjacent carbon is not well-supported or persuasive. Overall, the approach does not seem well-justified, and the project is unlikely to contribute to the DOE Hydrogen Program.

Question 2: Accomplishments and progress

This project was rated **2.6** for its accomplishments and progress toward overall project and DOE goals.

- The project started just last fall, and a very small fraction of the overall funding has been spent. The theoretical calculation aspect of the project is well-developed and has made progress. Initial materials have been synthesized, and preliminary ORR active measurements have been performed. The onset potentials for ORR are very low and could possibly be attributed to residual iron in the nanotubes.
- Theoretical and experimental work performed is relevant to the funds spent. Taking into account that the project is recently started, the accomplishments are good.
- The team has synthesized a few samples and studied their catalytic activity in comparison to state-of-the-art Pt/C catalysts. The progress is reasonable.
- Progress as a new, small project is solid.
- Minimal progress was presented (though spending seems to have been minimal as well). The initial ORR results are discouraging. ORR activity of the CNTs without sulfur and selenium was not reported but should be measured.

Question 3: Collaboration and coordination

This project was rated **2.8** for its engagement with and coordination of project partners and interaction with other entities.

- The principal investigator is collaborating with a theoretician at the University of California, Riverside (UC Riverside) and plans to collaborate with Los Alamos National Laboratory (LANL) for fuel cell testing when promising materials are identified.
- This is a new project with ongoing collaboration. More active collaboration with the Electrocatalysis Consortium (ElectroCat) is highly encouraged, as is following best practices for rotating ring disk electrode as proposed for ElectroCat.
- As the proposed work focuses on development of PGM-free catalysts, it is recommended that the project coordinate with partners from ElectroCat.
- The experimental and theoretical teams have worked together to elucidate the possible synergy and the possible active site structures.

- The collaboration within UC Riverside could be helpful, but the suggestions from DFT that the materials may be catalytically active are not persuasive, especially considering the extremely low ORR activity measured via rotating disk electrode (RDE). The planned collaboration with LANL does not appear to have begun. The principal investigator seems to be new to the ORR and fuel cell field and needs more support from experts to guide the research and assess whether it is able to contribute to the DOE Hydrogen Program.

Question 4: Potential impact

This project was rated **2.7** for supporting and advancing progress toward Hydrogen Program goals and objectives.

- If the materials will have an activity comparable to the state-of-the-art Fe-N-C catalysts developed by ElectroCat and have higher stability, the project will have a substantial impact on substitution of PGMs in fuel cells.
- Based on just what was presented, it is difficult to judge whether this project will be able to achieve the ORR activity and material stability needed for use in a practical device. While transition metal chalcogenides have been explored for ORR and show moderate ORR activities, the chalcogens in the absence of transition metals have not. This is an extremely novel approach and may possibly show promise for tuning the electron density of catalyst supports or of transition metals incorporated into the CNT walls.
- Development of high-performance PGM-free catalysts still faces significant changes to improve their catalytic activity and stability. Current progress and achievement are promising, but the project needs to demonstrate performance and durability under a fuel cell environment.
- If effective, PGM-free ORR can be helpful.
- The project is addressing the important topic of ORR catalysis, but the specific catalytic system being developed is not promising.

Question 5: Proposed future work

This project was rated **2.8** for effective and logical planning.

- The proposed future work is well-aligned with project scope.
- The proposed work was primarily related to catalyst synthesis and DFT. The proposed work should also focus on understanding the stability of the sulfur in the acidic electrolyte, on catalytic activity evaluation, and on incorporating other components into the catalysts if the sulfur and selenium alone do not result in reasonable ORR activity.
- The future work is reasonable based on what was proposed for this project, but it is unlikely to lead to any meaningful advancement because of the lack of catalytic activity of the chosen material set. It would be better to pivot to a more promising research direction.
- It is unclear what strategies and approaches could further advance the catalyst through generating fundamental understanding and designing innovative catalysts with improved performance.
- The project should focus on understanding performance potential rather than structure.

Project strengths:

- Exploring innovative formulations and structures without metal and iron is essential to catalyzing the challenging ORR. Elucidating the possible synergy between carbon nanostructures and inexpensive sulfur could yield interesting knowledge.
- Metal-free, PGM-free ORR catalysts should be tolerant of demetallization, which will positively affect the stability of these materials. DFT calculations will guide experimentalists toward materials improvement.
- The project has a good amount of work for the budget and for a new project.
- The project includes DFT calculations in the approach.
- The concept is different from anything in the DOE Hydrogen Program.

Project weaknesses:

- The team should focus on leveraging ElectroCat expertise and previous work with relevant publications such as U. Diebold on sulfur doping for ORR, S.C. Barton for ampule approach, and G. Woo for nanotubes.
- A clear understanding of possible active sites and reaction mechanisms is still lacking. Rational catalyst design is more desirable. The presenting synthesis procedures require extreme conditions and may generate additional barriers for the possible scale-up.
- The core idea is not well-justified, and the project is not likely to make any meaningful contributions or advance the state of the field. The team appears to lack familiarity with the fuel cell field. The core material appears to have been developed as a sulfur cathode for lithium-ion batteries. The team seems to be searching for a different application and funding source, but fuel cells do not provide a good fit for this material.
- The project weaknesses are the lack of a comprehensive rationale as to why these materials should be ORR active and the lack of a back-up plan if incorporating sulfur and selenium alone does not result in ORR active materials.
- Single-wall CNTs, especially highly purified from iron, have a higher price than PGMs. That may impede implementation of these materials in real fuel cell systems.

Recommendations for additions/deletions to project scope:

- A recommendation would be to explore the possibility of incorporating chalcogenides in cheaper multi-walled CNTs and potentially in multi-layered graphene. That will help to de-risk the project and increase the chances of a successful accomplishment of all targets.
- Introducing the well-studied FeN_4 sites to the current systems may provide a new opportunity to improve catalytic performance. Studying catalyst stability in the early stage is necessary.
- An addition would be exploring incorporation of transition metals and the use of sulfur-modified nanotubes as supports for other ORR active materials, such as Fe-N-C catalysts or chalcogenides.
- Material and electrode conductivity should be added.
- The proposed work is unlikely to contribute to the progress of the Hydrogen Program, so the team should consider a major pivot. For instance, the team could abandon the sulfur and selenium work and instead try creating active sites in the CNTs by doping them with metals and heteroatoms (but not the same metals and heteroatoms being explored already in ElectroCat).

Project #P-208: Non-Intermittent, Solar-Thermal Processing to Split Water Continuously via a Near-Isothermal, Pressure-Swing Redox Cycle

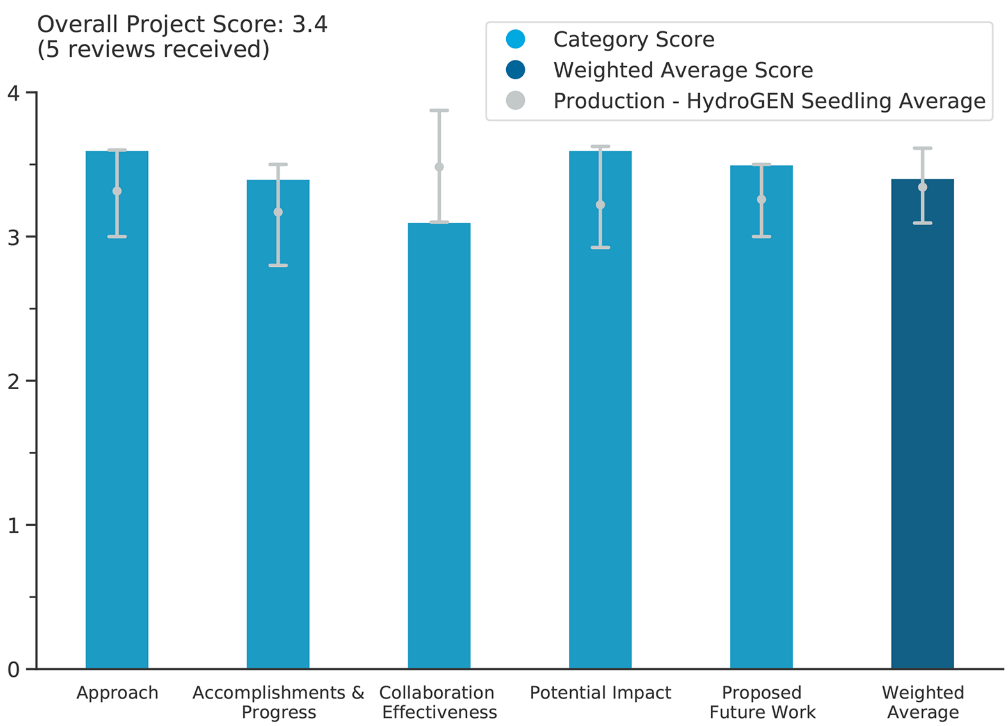
Alan Weimer, University of Colorado, Boulder

DOE Contract #	DE-EE-0010729
Start and End Dates	10/1/2023–9/30/2025
Partners/Collaborators	ETH Zürich, National Renewable Energy Laboratory
Barriers Addressed	• Efficiency and scalability issues that challenge solar thermochemical hydrogen production technologies

Project Goal and Brief Summary

Thermochemical pathways for green hydrogen production, although economically advantageous because of their ability to utilize the entire solar spectrum and potential for volumetric scaling, are not yet efficient enough to meet the DOE cost target of less than $1/kg. This project aims to address this challenge by enhancing the efficiency of thermochemical hydrogen (TCH) production. The approach involves decoupling the reactor from the solar receiver and employing a pressure-swing method to reduce irreversibilities associated with wide temperature swings. The project plans to make TCH production a cost-effective and scalable solution by using established reactor technologies, techno-economic analysis (TEA), and experimental evaluation of iron-aluminate-based materials.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Production - HydroGEN Seedling projects.

Question 1: Approach to performing the work

This project was rated **3.6** for identifying barriers and addressing them through project innovation, as well as for project design and feasibility.

- The main objective of this project is to decouple the solar receiver from the thermochemical reactor that utilizes flowable redox oxide powders to enhance the efficiency and scalability of solar thermochemical hydrogen (STCH) production. It is hoped that this STCH production system will be able to achieve the DOE technical target of $1/kg for a 50,000 kg H_2/day plant. The safety planning and culture for the project appear to be well-established. The project's diversity, equity, inclusion, and accessibility (DEIA) plan involves maintaining partnership with the existing DEIA Center at the University of Colorado, sponsoring university senior capstone design projects, and providing students from underrepresented groups the opportunity to participate in the proposed technology development.
- The project team's approach of decoupling the solar receiver from the reactor by using an intermediate thermal storage system improves the success probability. However, identifying high-temperature material to withstand 1400°C has always been a challenge for STCH technology and has been clearly identified by the project team as a barrier.
- The project team has a clear understanding of the barriers facing STCH hydrogen and has identified objectives to overcome the barriers.
- The overall project approach to the hardware is excellent, and there is excellent preliminary information. The biggest gap is on the specific materials science for the iron aluminate. There would be considerable value in the x-ray diffraction (XRD) of the materials as a function of thermal cycling. Even better would be an operando experiment, as it is not clear how crystalline the materials are or if they are single-phase or if there is significant amorphous content. It would be expected that the Fe is responsible for most of the actual chemistry, so it would be interesting to see how the Mossbauer looked. If you look at the phase diagram, there are many phases at nearly the same temperature. Understanding the Fe redox behavior during cycling may be critical in optimizing the over-cycle.
- This is an innovative approach to overcoming the limitations inherent to conventional technology. The motivation for developing a decoupled reactor–solar-receiver system is well-explained. The project results would contribute to its further development, including the identification and validation of the material that enables a pressure-swing approach, as opposed to a wide temperature swing, reporting the minimum fluidization velocity and demonstrating that system components can operate at the required temperatures. The TEA is also an important component of the approach that could motivate further investment in the technology. The project team did not explain well how the modeling will be utilized for improved reactor design. The safety plan is adequate. The team should include further details on the DEIA efforts, the number of underrepresented minority students from the Broadening Opportunity through Leadership and Diversity (BOLD) Center at the University of Colorado whom the project directly impacted, and how the project directly impacted the students. It is unclear what opportunities this project provided to the students.

Question 2: Accomplishments and progress

This project was rated **3.4** for its accomplishments and progress toward overall project and DOE goals, as well as the HydroGEN Consortium mission.

- Iron aluminate powders of the desired composition have been successfully produced as planned. Additionally, the operating conditions have been computationally optimized to achieve higher solar-to-fuel conversion efficiency than the current state-of-the-art technology. The team has made additional progress toward achieving the targets for the go/no-go point.
- The project team had made considerable progress in the development of the ability to cycle the iron aluminate to evaluate the ultimate process efficiency. The team is on track for its milestones, and overall progress is excellent.
- The milestones have been met, and adequate data was provided to demonstrate that the project is on track.
- The project was started only two quarters ago, and its accomplishments are in line with the timeframe.

- The performance of aluminoferrite is equivalent to CeO_2, but it may have a cost advantage over CeO_2. The performance in the oxidation cycle is under pressure. It is unclear how this will integrate with a low-pressure thermal reduction cycle.

Question 3: Collaboration effectiveness

This project was rated **3.1** for its collaboration and coordination with HydroGEN and other research entities.

- The collaborations among the participants appear to be well-planned, involving the University of Colorado, Boulder; OMC Thermochemistry; ETH Zürich; and the National Renewable Energy Laboratory (NREL). The engagement with the HydroGEN Consortium with appropriate use of nodes (NREL) is well-coordinated.
- Collaboration with other teams is good.
- There are industrial, international, and national laboratory collaborators on the team. It is unclear from the presentation how NREL will play a role.
- Utilization of the HydroGEN node for TEA is a project strength and is well-integrated with the overall project. There is no explicit description of the benchmarking/protocols being utilized. There is no description of data being shared on the Data Hub.
- The project has good interactions for system and TEA development. However, there is very little on the materials science involved. It would be of value to partner with a laboratory expert in oxide synthesis and detailed structural, morphological, and redox characterization. This might suggest solutions to the materials processing—phase stability and even the potential of ternaries.

Question 4: Potential impact

This project was rated **3.6** for supporting and advancing progress toward DOE Hydrogen Program goals and the HydroGEN Consortium mission.

- This project shows considerable potential in the overall validation of the total cost of hydrogen approach. It will provide insight into both the chemistry morphology of the material and, even more so, in practical approaches to TCH at scale. It can have a substantial impact on the field. At present, the cost targets seem unrealistic, but as the project continues, the estimates could become more realistic.
- The project is still in its early stages, but the prospects for significant impact are promising. The impact will be significant if the outlined performance and cost goals are achieved.
- The project identifies the inherent limitations of the current technology and provides a solution. The project's success will advance the development of more efficient STCH processes.
- The material selected by the project team has more promise than current state-of-the-art materials (i.e., ceria).
- The presented aluminoferrite is a new material, but its stable spinel structure may limit the oxygen deficiency level. This can translate to high reduction and oxidation temperatures, like CeO_2, causing durability and cost issues.

Question 5: Proposed future work

This project was rated **3.5** for effective and logical planning.

- The project team's plan to test the new material at another facility is an excellent idea to cross-check the commercial feasibility and gain confidence in the material.
- Overall, the team has an excellent project plan with a tight focus and the potential for considerable impact.
- The delivery and testing of iron aluminates at ETH Zürich is a good plan. This will give independent confirmation of the new material's capability.
- The main task that the project team listed for future work is "experimental demonstrations." It is planned that approximately 2 kg of iron aluminates, produced at a large scale using the optimal spray-drying (or modified Pechini) method, will be transported to ETH Zürich for assessment in the university's solar mini-

refinery system. Providing specific details about the experimental system, such as the operating conditions and target performance metrics, would be beneficial.

- The plan for meeting the Quarter 4 go/no-go is logical and well-described. The end-of-project goal is not defined in the slides and so cannot be evaluated. The demonstration needs additional details, including whether it will incorporate any of the innovations that this project is pursuing, such as decoupling the receiver from the reactor and using a fluidized bed (or clarify whether there will be testing of the material developed under conventional operating conditions).

Project strengths:

- The aluminoferrite redox material is an interesting material for solar thermal hydrogen production. The team has established a lab-scale reactor to vigorously test the material. This testing at bench scale has commercial implications.
- Iron aluminate shows promise and is better than ceria. The project team is capable of completing the project successfully.
- Project strengths are the clear focus, excellent system approach, and attainable milestones. There is great strength in the overall reactor plan.
- The overall project idea is an innovative solution to current technology limitations. One strength is integration of the TEA in the overall project plan.
- The potential of the suggested system, and the initial findings, seem encouraging, yet further concrete results are needed to illustrate the projected improvements in system performance and cost.

Project weaknesses:

- One potential weakness is regarding teaming. There could be a substantial benefit in coordinating with a materials synthesis and characterization team, and better understanding the phase and activity of iron aluminate in the reactor could be valuable. Second, investigating the Fe-Al phase diagram against the reaction cycle could lead to ways to optimize the process.
- The project team did not include an explanation of how system modeling fits into the overall project. It is unclear whether this will impact TEA and how the results will be leveraged to improve the system design.
- It is stated that iron aluminate powders with the desired compositions have been identified and produced. Nevertheless, the process used to optimize these compositions remains unclear, including the strategy for composition screening, essential property descriptors, and performance metrics.
- High-temperature material is always a challenge, and in this case, the gas distributor needs to withstand 1400°C. The project team did not discuss the attrition of iron aluminate through multiple redox cycles.
- The oxygen deficiency of the material might not be sufficient because of the stable thermodynamics of the spinel structure. This would require high cycle temperatures.

Recommendations for additions/deletions to project scope:

- Given that the performance and cost of the proposed system are closely tied to the iron aluminate powders being utilized, it would be advantageous for the project team to ensure that both the microstructure and compositions of these powders are thoroughly optimized.
- The project team should test specific components of the proposed innovations in the solar mini-refinery.
- The project team needs to develop new compositions to increase oxygen deficiency.

Project #P-209: Gallium-Nitride-Protected Tandem Photoelectrodes for High-Efficiency, Low-Cost, and Stable Solar Water Splitting

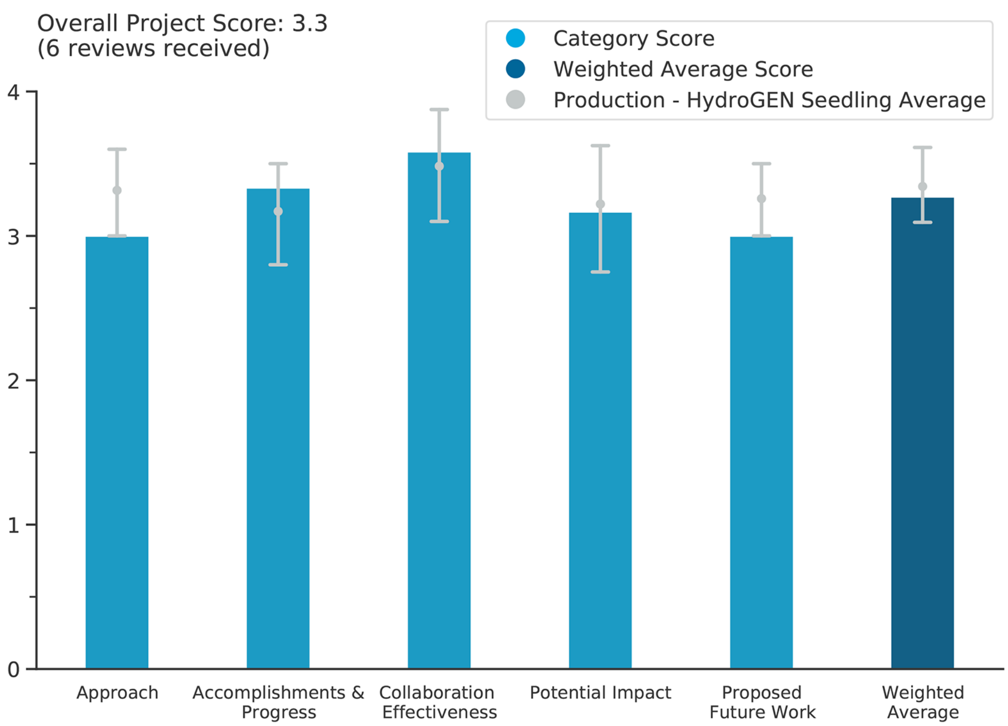
Zetian Mi, University of Michigan

DOE Contract #	DE-EE0010730
Start and End Dates	10/1/2023–9/31/2026
Partners/Collaborators	University of Toledo, University of Michigan–Ann Arbor, National Renewable Energy Laboratory, Lawrence Livermore National Laboratory, Lawrence Berkeley National Laboratory
Barriers Addressed	• Processing compatibility • Low-temperature deposition of ultrathin GaN that does not compromise surface protection and efficiency

Project Goal and Brief Summary

No photoelectrochemical (PEC) device has been able to achieve both high efficiency (>10%) and stable operation (<1,000 h) simultaneously. The main project objective is to prevent photo corrosion and oxidation in these devices, improving their lifespan and performance. The approach involves GaN nanostructures to protect the devices, combined with low-cost, high-efficiency perovskite light absorbers. Concentrated sunlight, obtained through solar concentrator systems, is used to increase the intensity of solar irradiation, significantly reducing the amount of semiconductor light absorber and catalyst materials required. This project aims to achieve a solar-to-hydrogen (STH) conversion efficiency of up to 20% and long-term stability exceeding 1,000 hours, contributing to the DOE target of producing hydrogen at $1/kg by 2030.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Production - HydroGEN Seedling projects.

Question 1: Approach to performing the work

This project was rated **3.0** for identifying barriers and addressing them through project innovation, as well as for project design and feasibility.

- The project is focused on the development of GaN-protected tandem PEC utilizing perovskite/Si and GaInP/InGaAs (indium gallium phosphide/indium gallium arsenide) configurations through the application of a diverse array of synthesis techniques. Addressing key challenges of PEC technology, the team aims to enhance durability by implementing a GaN protection layer and achieve cost-effectiveness by leveraging industry-ready materials for semiconductor photoelectrodes. A systematic approach has been outlined to attain the targeted STH efficiency and durability, with a particular emphasis on optimizing the performance of GaN-protected devices. This strategy demonstrates a comprehensive and methodical pathway toward realizing the project objectives.
- This is one of several seedling projects on PEC generation of hydrogen, including at least a couple efforts that focus on tandem photoelectrodes. The crux of the approach is the use of protective GaN layers on both sides of the tandem system, which appears to have been established by the principal investigator (PI) and his co-workers before the start of this project at the beginning of fiscal year 2024. The approach uses epitaxial growth of an ultrathin layer of GaN, which undergoes oxidation to stable GaON under the conditions of PEC cell operation. If successful, the approach can help to overcome the durability challenge that has plagued PEC generation of hydrogen for decades, generally rendering it not viable for practical applications.
- The primary barrier of processing incompatibility between GaN and the selected photoelectrode is identified. The metrics of STH efficiency and stability provide additional measures of success. The safety plan is appropriate. Diversity, equity, inclusion, and accessibility and community benefits plans show meaningful progress. The team has a strong understanding of the concept and a vision for implementing the GaN protecting layer. Initial tests have proven successful, achieving deposition of a GaN layer on perovskite material and III/V material. Stable operation is shown at over 100 hours. During questions, the PI indicated that next steps include scaling to a larger area while monitoring for pinholes, increasing solar concentration on the cell during testing, and testing longer durability periods. Additional transparency into specific next steps and/or broad timelines would be helpful for gauging appropriateness of the approach. While not technically within the project scope, some acknowledgement of the cost of molecular beam epitaxy and potential challenges of scaling up may be useful in the future and strengthen the long-term vision of the technology.
- The approach of using a robust coating on high-performing photoelectrodes has potential for success. The Hydrogen and Fuel Cell Technologies Office has done several analyses on the most likely PEC pathways to achieve low-cost hydrogen. Those analyses seem to favor the dual-bed approach. The approach selected here of a planar single bed resulted in the highest costs. Adding solar concentrators increases the efficiency but also increases the costs. It is unclear how the team will get the costs down to achieve the hydrogen cost targets. It is also not clear why using concentrated solar light is an innovation (slide 6). This has been looked at in the past and is well-known to increase production rates. The challenge will be achieving high enough performance to offset the cost of solar concentrators. On slide 8, the team stated that solar concentrators will result in lower hydrogen costs, but no analyses were presented that support this claim. The goals are very bold and well-defined.
- The project has identified barriers addressed through project innovation. However, the project has not provided enough detail about the specific project activities to be undertaken for reviewers to determine the appropriateness of the scope of work for the timeline and budget provided. The provided milestones have specific goals, but it is unclear what improvements will be made to meet these goals.
- The project is conceptually valid, with concerns about scalability. The team should address the availability of gallium for global deployment and scale-up plans.

Question 2: Accomplishments and progress

This project was rated **3.3** for its accomplishments and progress toward overall project and DOE goals, as well as the HydroGEN Consortium mission.

- The team successfully demonstrated the feasibility of depositing GaN at low temperatures onto both perovskite and III-V materials. Through this process, it was observed that GaN effectively protected the surface of GaInP/InGaAs, enabling sustained operation without significant degradation for 100 hours at 80°C.
- The initial tests have proven successful deposition of a GaN layer on perovskite material and III/V material. Stable operation is shown over 100 hours. The project is expected to meet go/no-go criteria. The expected upper limit of performance for this technology would be helpful for contextualizing maximum possible success.
- The project started very recently, but the team has shown significant progress toward the budget period (BP) 1 go/no-go milestone.
- It is unclear which results reported by the PI were obtained before the start of this project and which ones predate the effort. It seems that the very idea of protecting semiconductors with ultrathin layers of GaN was published by the PI and his co-workers already some time ago. This applies to the epitaxial growth process, presented as vital for the GaN layer formation. That being said, since the project inception, the authors have met the target of demonstrating a GaN-protected perovskite/Si tandem device, as well as the target for GaN-protected GaInP/InGaAs photoelectrode. The authors have also achieved the photocurrent density, open circuit potential, and durability target established for the go/no-go decision. Together, the presented accomplishments show promise going forward.
- This is a new project, and the team has made solid progress, given the short amount of time. Slide 13 shows the “high-performance” device. It is unclear why the device was tested for only 10 minutes. Even in 10 minutes, there is a slope to the performance line. The slope identifies the materials as “perovskite/Si tandem device.” It is unclear whether the same materials are used in the GaN-protected experiments and, if not, why that is the case. Slide 15 has interesting results. The electrolyte “freshness” seems to impact stability. Perhaps the team should consider flowing the electrolyte rather than using a batch reactor. Slide 15 reports a 17% reduction in photocurrent. However, there seems to be a break-in period of about 45 hours after which the stability increases. It is not clear why the test was stopped after 100 hours. It seems the team really needs to account for a break-in period, but to do so, the tests need to be longer, and there need to be more samples in order to do statistical analysis. These initial results are encouraging.
- The project just started.

Question 3: Collaboration effectiveness

This project was rated **3.6** for its collaboration and coordination with HydroGEN and other research entities.

- The project is inherently multidisciplinary and requires engagement form multiple partners. Participating organizations include the National Renewable Energy Laboratory (NREL), Lawrence Livermore National Laboratory, and Lawrence Berkeley National Laboratory. The project includes computational modeling, materials improvement, microscopy, and large-scale testing. The results from this project can have a positive impact on other projects that can similarly benefit from GaN protection.
- The roles and responsibilities of the team members are well-defined. The team showed strong collaboration with NREL and HydroGEN.
- The team of three university partners (two at the University of Michigan) and three national laboratories appears to be well-integrated, with technical contributions in the review period coming from all participants. No collaborations with other HydroGEN institutions appear to have been established so far.
- The project has a strong team across a number of institutions that have already demonstrated results.
- This is a large team that is leveraging the HydroGEN consortia capabilities.
- The project just started, and some collaboration is already shown. Having so many collaborators on this project is concerning, as the PI stated in a weekly meeting.

Question 4: Potential impact

This project was rated **3.2** for supporting and advancing progress toward DOE Hydrogen Program goals and the HydroGEN Consortium mission.

- The project shows a promising pathway for improving durability while maintaining performance, which is a fundamental barrier to economic success of PEC concepts. The final project should consider how the GaN protection and the scaled-up device would impact project economics, possibly including a target levelized cost of hydrogen (LCOH). Ideally, a consistent LCOH method would be used to compare different PEC concepts within this cohort of PEC projects presented in the 2024 Annual Merit Review. GaN protection has some generalizable aspects that can be used for other photoelectrode materials.
- There have been many efforts over the past several decades to make PEC generation of hydrogen truly impactful, with progress stemmed by inferior durability and, ultimately, lower overall efficiency relative to that of combining solar cells with water electrolysis technologies. However, if successful, the presented approach promises to be transformational. This may require accelerating progress in long-term materials durability relative to what is currently assumed, especially in BP 2.
- The PEC goals are reasonable; the concern is about stability testing and global supply of Ga for this low-powered approach, but using concentrated light addresses this, if it works.
- The project has successfully demonstrated the feasibility of enhancing the durability of tandem PEC devices, addressing a major barrier to the widespread adoption of the technology. However, to truly impact low-cost PEC hydrogen production, the proposed solution needs to be scaled up and made applicable to a wider range of semiconductor materials.
- Water splitting is an important area of development to achieve the DOE clean hydrogen targets. PEC is one of the advanced pathways. It seems the intent is to use solar concentrators for this work, which will increase the cost and complexity of the system. It is not clear whether this system will be able to meet the DOE hydrogen cost targets.
- There is a significant question of the potential scalability of the approach.

Question 5: Proposed future work

This project was rated **3.0** for effective and logical planning.

- During questions, the PI indicated that next steps include scaling to a larger area while monitoring for pinholes, increasing solar concentration on the cell during testing, and testing longer durability periods. Additional transparency into specific next steps and/or broad timelines would be helpful for gauging appropriateness of the approach. There are no concerns as to whether future work will be appropriate.
- The focus on further performance improvement is appropriate and reasonable. However, providing more specific details on how these improvements will be achieved would strengthen the approach. Additionally, clarity is required regarding the materials and catalysts used or intended for use in the hydrogen evolution reaction (HER) and oxygen evolution reaction (OER). While there have been claims of catalytic activity for GaN/GaOH in these reactions, recent publications from the team (*Nature* 613 [2023] 66, *Nature Communications* 14 [2023] 179) indicate the application of platinum and rhodium as catalytic components.
- The team has very robust milestones. On slide 6, the team reports using solar concentrators for the system. It is unclear if the team will be using solar concentrators as part of the tests to achieve the STH durability targets.
- The work proposed for BP 2 ("further improve the design, synthesis, integration, and performance of […] photoelectrodes") sounds vague, looking like a wish list rather than a well-thought-out research plan. The durability targets assumed for that budget period should be closer to the targets set for BP 3.
- The team needs to include reproducibility and stability and use a flow cell.
- The team did not provide adequate information about future activities to evaluate the strength of the future plans.

Project strengths:

- The project places a strong emphasis on enhancing the stability and durability of perovskite and III-V tandem photoelectrodes. According to the team's publications, the proposed PEC devices exhibit the capability to operate effectively with seawater and tap water. This is particularly noteworthy considering that low-temperature electrolyzers—such as proton exchange membrane, alkaline, and anion exchange membrane water electrolyzers—are typically sensitive to water quality and require deionized water for operation. This achievement highlights the potential of the project's PEC technology to offer a more versatile and practical solution for hydrogen production, capable of utilizing a broader range of water sources compared to traditional electrolysis methods.
- The PI and supporting teams and organizations are experts in developing PEC materials and technologies. Early results are promising, and additional progress is likely to happen relatively quickly, since there are no major barriers currently identified.
- The team is combining a durable layer with high-performing PEC cells. The team is very strong. The GaON has been shown to work well.
- There is a focus on durability and concentrating light as a mitigation for low availability of Ga.
- The project has a strong team with significant progress early into the project.
- The team is strong and off to a good start in this project.

Project weaknesses:

- The operation of the proposed PEC devices necessitates elevated temperatures and concentrated sunlight, which introduces the need for a cooling system, thereby adding complexity to the overall design. This aspect requires clarification or further elaboration to provide a comprehensive understanding of the challenges and considerations involved. Moreover, the team should offer more specific details regarding the applied catalysts for the HER and OER. Clarifying the choice of catalysts will enhance transparency and aid in better understanding the performance and efficiency of the PEC devices. Additionally, the project should address or discuss scale-up strategies to effectively transition from lab-scale prototypes to larger-scale implementations. Exploring and outlining potential strategies for scaling up production processes are essential for realizing the practical viability and commercial potential of the technology.
- The cost of the proposed approach may make this technology unfeasible. High-level techno-economic assessment may be helpful for understanding potential end game economics.
- The researchers are not sure of the GaON stability at high temperatures. It is not clear that a pinhole-free protective layer can be scaled up.
- The project provided minimal information about the specifics of future activities that prevent independent evaluation of the project activities.
- The project needs to address heat, electrolyte concentration, and durability issues.
- The large gap between milestones in the last and the preceding year of the project is a weakness.

Recommendations for additions/deletions to project scope:

- One recommendation is a Gantt chart indicating how the project activities of each project partner feed into each other. For improvements between BP 2 milestones of STH >15% and >200 hours maintaining 80% of the initial STH to STH >20% and STH >500 hours, it is unclear what activities and learnings are going to make these improvements achievable. Such information will significantly aid evaluation of planned work.
- The team should consider involving additional HydroGEN partners and organizations external to the consortium. Performance targets for the second year should be revised to reduce gaps to those established for the end of the project.
- It is not clear that the GaON has been tested at 160x concentrated sunlight or what the thermal stability of the GaON is. It is recommended that the team perform some of these tests, as the researchers have stated that their intention is to test the device under concentrated sunlight.
- Additional clarity of near-term and long-term next steps would be helpful. Basic cost modeling may be helpful.

- The cost of fabrication and scale-up of the GaN protection layer should be assessed.
- Durability and reproducibility should be established early.

Project #P-211: Inverse Design of Perovskite Materials for Solar Thermochemical Water Splitting

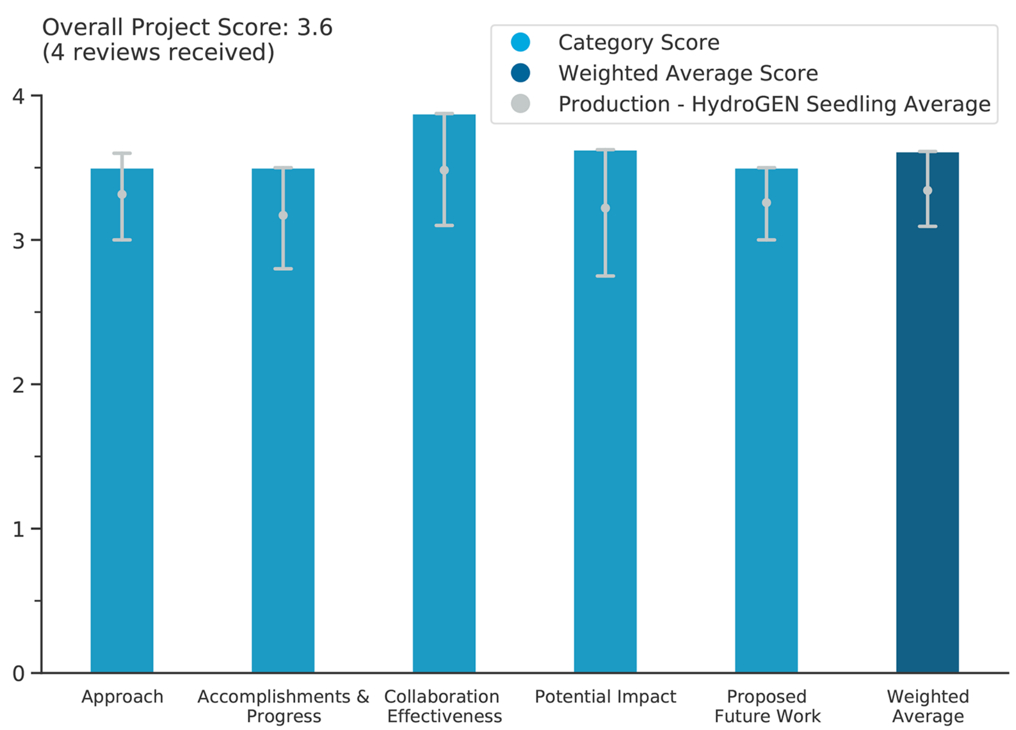
Christopher Muhich, Arizona State University

DOE Contract #	DE-EE0010732
Start and End Dates	10/1/2023–9/30/2026
Partners/Collaborators	University of Munich, Valparaiso University, National Renewable Energy Laboratory, Sandia National Laboratories, Idaho National Laboratory
Barriers Addressed	• Ideal reduction–oxidation materials thermodynamics unknown • Composition that matches ideal thermodynamics unknown • Reactor configuration that maximizes production unknown

Project Goal and Brief Summary

Achieving cost-effective solar thermochemical hydrogen (STCH) production requires identifying materials with optimal reduction–oxidation (redox) properties. This project aims to discover perovskite compositions that meet the ideal thermodynamic criteria for efficient hydrogen production. The team will identify quinary perovskite materials capable of producing hydrogen at a cost of less than $1.5/kg by utilizing inverse design and high-throughput materials development. The goal is to demonstrate these materials' stability and efficiency in a reactor configuration that maximizes hydrogen yield, providing a pathway to achieving hydrogen production costs of less than $1/kg at scale.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Production - HydroGEN Seedling projects.

Question 1: Approach to performing the work

This project was rated **3.5** for identifying barriers and addressing them through project innovation, as well as for project design and feasibility.

- The objective of the project is to computationally identify perovskites with high oxygen deficiency and stability to address the current barriers. Diversity, equity, inclusion, and accessibility (DEIA) and community benefits plan activities are planned.
- The project provides an innovative approach to identifying novel STCH materials and optimum reactor design. The project is well-designed, and the scope of work is reasonable and logical for achieving the end goal. If successful, the project will advance the field. A safety plan was not required, but the project's safety culture explanation is reasonable. The research group is diverse, but the DEIA plan is weak. It is unclear what the goals of the outreach events are or what is expected to be achieved with these events.
- The project approach has ambitious goals. It is a very good approach, using analysis to identify thermodynamic fingerprints (TFPs) and to select a composition. It gives an opportunity to down-select promising compositions prior to experimental evaluation. It is not clear whether the approach includes evaluating stability properties through thermodynamic calculations.
- The project approach is a bit mixed. The density functional theory (DFT) portion is very good. It may be worth validating the model of some simpler materials to get the correspondence between theory and experiment. It is interesting to think about how this model can learn from the existing materials and knowledge in the field. The project team should think about the methodology for high-throughput materials; there is extensive literature on high-throughput materials diagnostics. It would be of considerable value to assess techniques such as pulsed laser deposition or sputtering for their ability to create isolated libraries of composition or thickness gradient samples. There are several approaches that can be seen in the high-throughput literature. Also, it may be worth developing some design rules based on the TFP. It seems reasonable to map against the nearest phases to evaluate the ultimate stability of the calculated phase.

Question 2: Accomplishments and progress

This project was rated **3.5** for its accomplishments and progress toward overall project and DOE goals, as well as the HydroGEN Consortium mission.

- Identification of a large set of compositions through computational screening is impressive.
- This project started only recently, but initial milestones have been met, and the project is on track for meeting future milestones.
- This is a new project with progress observed in computational screening of new perovskite materials using TFP and compound energy formalism (CEF) and high-throughput reactor design.
- The number of possible candidates is huge, and it seems difficult in the time available to reach closure on a set of meaningful candidates. There needs to be a clear focus on a small number of viable candidates that can inform the model. The high-throughput characterization seems flawed versus the state of the art. If there were a more defined set of guidelines for decisions, maybe there could be a more rapid focus to test the model. There have been several computational approaches to thermochemical hydrogen (TCH) materials. This approach seems novel and valuable—but only if demonstrable.

Question 3: Collaboration effectiveness

This project was rated **3.9** for its collaboration and coordination with HydroGEN and other research entities.

- Broad collaboration is exactly what is needed for this project. The team includes several universities and three national laboratories.
- The project has close collaborations with national laboratories for materials characterization and techno-economic analysis (TEA).
- The project has a very good team across the spectrum of the project milestones in both materials and analysis. It may be worthwhile to work with a group that has expertise in combinatorial materials development.

- Collaborations with HydroGEN nodes are strong, and node choices are logical for completing the proposed project. This is a strong team. Benchmarking protocols were not mentioned, but based on the team, it can be assumed that these will be integrated into the experimental component of the project. The project does not state what will be saved to the Data Hub.

Question 4: Potential impact

This project was rated **3.6** for supporting and advancing progress toward DOE Hydrogen Program goals and the HydroGEN Consortium mission.

- The project specifically targets the HydroGEN program goals and DOE hydrogen production goals.
- If new high-performing redox materials are identified, it will make a significant impact on the current DOE solar thermal hydrogen program.
- The combination of analytical and experimental work increases the chance of success.
- The project is clearly aligned with the potential for next-generation TCH materials but may be overly optimistic on reaching Hydrogen Shot goals. Perhaps the TEA will provide a more realistic timeline.

Question 5: Proposed future work

This project was rated **3.5** for effective and logical planning.

- Future work is reasonable, with a planned theoretical prediction and experimental verification approach.
- Overall, the proposed future work aligns with the project goals. It is not clear if a single reactor design will be built and others modeled, providing a pathway for improved efficiency, or if more than one design will be built and tested. This should be clarified.
- Down-selecting the compositions for experimental validation may be very cumbersome. This reviewer expects that many of the compositions from the DFT calculations will exhibit similar performance characteristics. Selecting criteria to screen those compositions will not be straightforward.
- The work seems too broad, and the experimental validation is not enough to demonstrate the validity of the approach to identify new TCH materials competitive with ceria and $BaCe_{0.25}Mn_{0.75}O_3$. During the time that funding is available, it seems very optimistic to have a “solution” but reasonable to demonstrate the methodology with competitive materials.

Project strengths:

- This project provides an innovative solution to identifying efficacious materials for STCH. The highly integrated TEA is a clear strength for evaluating the overall process and will provide valuable information as to the economic feasibility of the technology, as well as a roadmap to TEA of other similar STCH processes.
- Thermodynamic calculations to select perovskite compositions is an excellent approach. The project has team members capable of addressing various analytical challenges.
- Project strengths include atomic-level prediction of material properties and reactor design.
- The project has an excellent computational approach and the potential for materials demonstration at scale.

Project weaknesses:

- DEIA is weak. The material characterization is not well-described. It is unclear what information will be targeted from each technique. It is also unclear how the water-splitting mechanism of down-selected materials will be evaluated (i.e., identifying which cation[s] are redox-active). Often, these materials have stability issues under these conditions, including irreversible secondary phase formation, which was not addressed. It is unclear whether and how this will be considered. The project does not clearly define how the models will be validated.
- Project weaknesses include synthesis, characterization, and success metrics and the ability to demonstrate true success of the computational methodology.

- It is unclear how the theoretical calculations can predict chemical/phase stability under STCH working conditions. It is also unclear what the descriptions for the stability are.
- It is not clear how the compositions will be down-selected for evaluation. It is likely that many may have similar properties.

Recommendations for additions/deletions to project scope:

- The overall project scope is reasonable.
- Experimental validation should be done sooner instead of waiting for the completion of thermodynamic analysis. Initial analysis could be limited to a smaller subset, and experiments would validate the results. This would provide greater confidence in the analytical results.
- It is recommended that the project work with an expert combinatorial laboratory for mixed oxides.
- The project should specify criteria for down-selecting the final candidates for experimental testing.

Project #P-212: Ca-Ce-Ti-Mn-O-Based Perovskites for Two-Step Solar Thermochemical Hydrogen Production Cycles

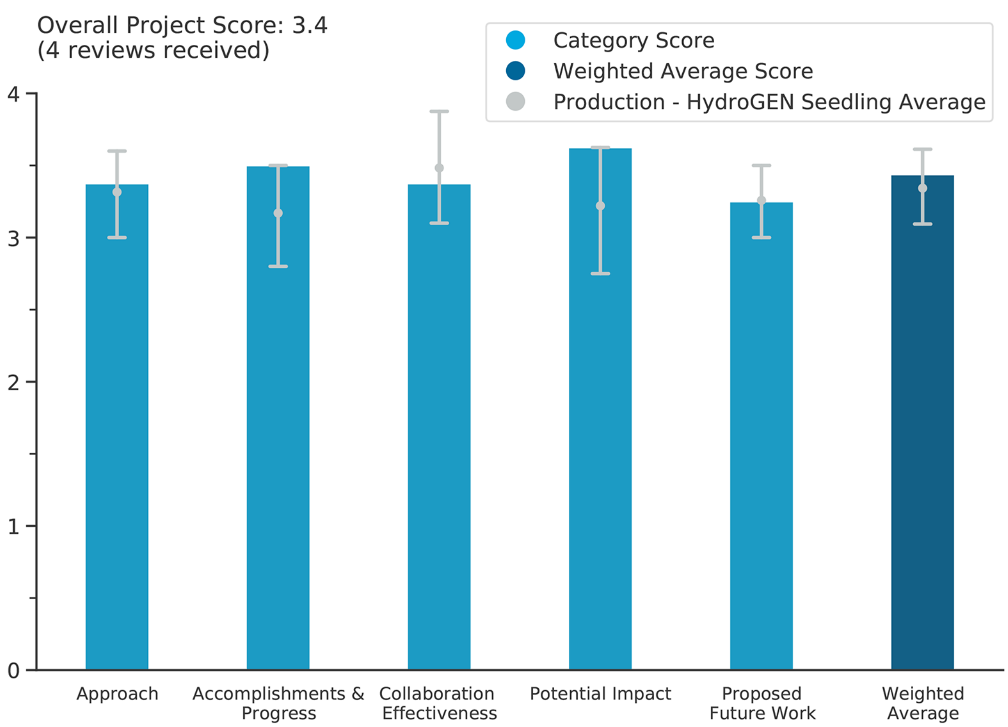
Robert Wexler, Washington University in St. Louis

DOE Contract #	DE-EE0010733
Start and End Dates	9/1/2023–8/30/2026
Partners/Collaborators	Arizona State University, Oregon State University, Sandia National Laboratories, National Renewable Energy Laboratory
Barriers Addressed	• An overly complex thermodynamic model • No accepted receiver/reactor for solar thermochemical hydrogen • Many parameters that go into the cost of $1/kg H_2

Project Goal and Brief Summary

Addressing the challenge of optimizing solar thermochemical hydrogen (STCH) production, this project focuses on enhancing efficiency and stability while maintaining competitive costs. The project aims to optimize Ca-Ce-Ti-Mn (CCTM) compositions by targeting a formation energy range of 3.4–3.9 eV for vanadium oxide. Scaling up synthesis processes and adapting reactors, such as the Labyrinth Reactor, are key steps in achieving 1 g/h hydrogen production on-sun. The project employs innovative approaches to surpass existing technological challenges, ensuring economic viability in hydrogen production.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Production - HydroGEN Seedling projects.

Question 1: Approach to performing the work

This project was rated **3.4** for identifying barriers and addressing them through project innovation, as well as for project design and feasibility.

- The project approach is logical, and each main component of the project (computation, reactor design, synthesis, material characterization, and techno-economic analysis [TEA]) is being led by experts with demonstrated success in the relevant area. Thus, there is a high confidence in project success. The integration of computation with experimental validation of the computational results is a project strength. It will provide confidence in the computational approach, providing the research community with a roadmap to further develop novel materials via similar methods. The diversity, equity, inclusion, and accessibility (DEIA) plan is strong. Redirecting resources when hiring goals were not met is reasonable and will enable an impact to still be achieved. Below are points to clarify during the next Annual Merit Review:
    - How much material is needed for the on-sun demonstration
    - Whether the synthesis method is readily scalable to the needed quantity
    - How the team will determine material cost at scale for the TEA
    - Whether the initial material, which is the basis for material optimization, can be used for on-sun demonstration if a stable, more optimized material cannot be identified
    - How much improvement in performance can be expected from material optimization versus the baseline material
    - How much cost savings will be achieved from material optimization when the balance of plant (BOP) is considered
- There are statements regarding state-of-the-art reactor design as part of this project, but the details of this effort are not clear (there are conflicting statements in the slides). Questions include:
    - Whether a novel reactor will be designed and built or a current reactor will be modified
    - Whether the modifications are for improved STCH efficiency or for enabling use for on-sun testing
    - What modeling or experimental results will be used for reactor design/optimization
    - Whether this is an iterative process
- The project objective is to refine a STCH production system by employing CCTM to attain high efficiency and stability at competitive costs. Key outcomes involve fine-tuning CCTM compositions to enhance efficiency, with a focus on achieving an oxygen vacancy formation energy of 3.4–3.9 eV and scaling up CCTM synthesis to enable high-yield hydrogen production. The criteria for optimizing the CCTM should be more clearly defined, and milestones with quantifiable parameters for material optimization would be helpful. To increase the project impact, the scope of work for validating the technological innovations may need to be adjusted to include the kinetics of the thermochemical hydrogen production processes. For instance, performing theoretical analysis and experimental validation of the rates of surface exchange processes and defect transport within the bulk phase of the oxide would be important. Additionally, evaluating the microstructure and morphology of the redox oxide particles, which may significantly influence these properties, is necessary. The DEIA and community benefits plan (CBP) are reasonable, but no safety plan was included.
- The project objectives are clearly defined to address the barriers identified. DEIA and CBP activities are well-planned.
- Selecting CCTM for optimization through computational prediction, followed by experimental validation, is a sound approach.

Question 2: Accomplishments and progress

This project was rated **3.5** for its accomplishments and progress toward overall project and DOE goals, as well as the HydroGEN Consortium mission.

- The project seeks to identify and demonstrate a more efficient STCH material that supports the DOE hydrogen production goals. Including a strong TEA component will provide a robust evaluation of STCH

feasibility with the material class being pursued. The project is on schedule for meeting milestones. The DEIA plan is strong and does support DOE DEIA goals.
- Some interesting data have been collected to identify promising compositions of redox active metal oxides such as CCTM2112. However, it is not yet clear how to achieve an optimal composition. Overall, it appears that good progress has been made toward the go/no-go criteria. Since the project is still in its early stages, more progress is expected in the future.
- This is a new project with a good start and is on schedule. One promising composition has been identified.
- A promising candidate composition has been identified.

Question 3: Collaboration effectiveness

This project was rated **3.4** for its collaboration and coordination with HydroGEN and other research entities.

- The project principal investigator has chosen effective HydroGEN nodes that will contribute to project success. The members of the project team are leaders in the benchmarking effort, so it is expected that best practices will be incorporated into the project.
- Collaborations are identified with universities and national labs for experimental verification of the new materials and the analysis of potential impact.
- The team initiated discussions with other project partners to coordinate upcoming tasks. The team also began initial interactions with Energy Materials Network nodes.
- Collaborative work is good.

Question 4: Potential impact

This project was rated **3.6** for supporting and advancing progress toward DOE Hydrogen Program goals and the HydroGEN Consortium mission.

- The project is designed to align with DOE objectives. It pairs material optimization and reactor design to increase STCH efficiency and hence lower hydrogen production cost. It is unknown whether the technology can meet the $1/kg target, but the project is incorporating a strong TEA component for evaluating system cost.
- The project aims to identify new high-performance materials for solar thermal production of hydrogen, which is well-aligned with the Hydrogen Program's goals and objectives. If successful, the project can make a significant impact on the solar hydrogen program.
- If successful, this project will contribute to a body of knowledge in the field.
- Preliminary results appear interesting and promising. However, to assess the project's impact, more tangible and measurable accomplishments need to be demonstrated.

Question 5: Proposed future work

This project was rated **3.3** for effective and logical planning.

- The plan for completing density functional theory calculations and synthesizing compositions for evaluation at various partner organizations is a sound approach.
- The team has a logical plan to computationally identify new compositions, followed by synthesis and testing.
- The materials development efforts are centered on thermodynamic properties, such as optimization of the vacancy formation energy of the active redox metal oxide and use of existing thermodynamic models. However, the kinetics of the thermochemical hydrogen production processes may be even more important, as they determine the rate and cost of hydrogen production.
- Overall, the project plan is logical for meeting the end goal, but the details on future work cover only computations, synthesis, and one characterization technique. More information should be provided on next steps for other project aspects, including TEA, reactor design, and computation/model validation.

Project strengths:

- The objective of the project is to optimize a STCH production system using CCTM to achieve high efficiency and stability at competitive costs. The preliminary results appear interesting and promising. It is anticipated that fine-tuning CCTM compositions will further enhance efficiency, leading to high-yield, low-cost hydrogen production.
- The project team is composed of experts in the relevant areas. There is a strong plan for validating the computational predictions with experiment/characterization. The overall project plan integrating computation, synthesis, characterization, and system modeling is well-designed to achieve the project goal of a final demonstration with an improved material.
- This project has a good team, the approach sounds good, and it limits the materials space to a single set of cations to find an optimal composition.
- Materials discovery is computationally guided.

Project weaknesses:

- There are no major weaknesses.
- Investigation of thermal and chemical stability of the material under real-world conditions is lacking.
- In addition to the tasks focusing on the thermodynamic properties of the active redox metal oxide, the kinetics of the thermochemical hydrogen production processes may be even more important, as they determine the rate and cost of hydrogen production. It would be beneficial to gain a more mechanistic understanding of the redox reaction kinetics and the transport of species associated with these reactions.

Recommendations for additions/deletions to project scope:

- It would benefit the research community if additional information could be provided from the TEA (essentially a sensitivity analysis), including (1) the impact of material cost on the TEA versus BOP cost and (2) the properties of the material—such as durability, hydrogen generation per gram of material, etc.—that have the largest impact on the final system cost from TEA. It would also be beneficial to the community for the team to evaluate the impact of material form factor on hydrogen generation efficacy, either through modeling or experimentally. For example, it is unclear whether the form factor impacts the steam flow profile in the reactor and hence the interaction with the material. It is also unclear whether the form factor impacts heat transfer through the material and whether this will impact performance.
- The project has a good plan. No changes are needed.
- The surface reaction kinetics between H_2O and redox material could dominate the hydrogen production rate. The surface reaction kinetics should be at least computationally investigated.
- It would be more productive to include detailed studies on the mechanisms, kinetics, and stability of redox reactions in active metal oxide materials under typical conditions for thermochemical hydrogen production.

Project #P-213: >200 cm^2 Type 3 Photoelectrochemical Water-Splitting Prototype Using Bandgap-Tunable Perovskite Tandem and Molecular-Scale Designer Coatings

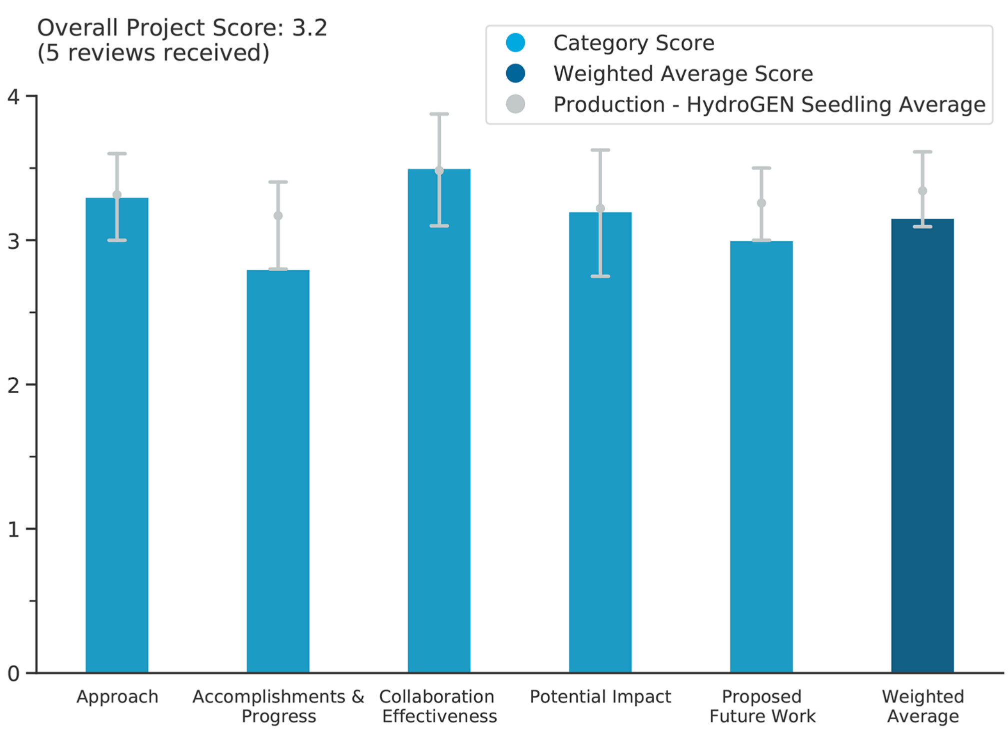
Shu Hu, Yale University

DOE Contract #	DE-EE0010734
Start and End Dates	10/1/2023–9/30/2026
Partners/Collaborators	Lawrence Berkeley National Laboratory, Lawrence Livermore National Laboratory, National Renewable Energy Laboratory
Barriers Addressed	• Unstable hybrid organic–inorganic perovskite under normal growth temperature, forcing use of lower temperature that causes pinholes in coating and undermines protection • Need for large-scale fabrication and assembly of the unit cells and quality control of each unit

Project Goal and Brief Summary

This project's objective is to advance solar thermochemical hydrogen production through integrating innovative technology. By combining low-cost hybrid organic–inorganic perovskite (HOIP) materials with molecularly engineered coatings, the project aims to overcome the limitations of current systems, such as low efficiency and stability, while ensuring cost-effectiveness. Through this approach, the project seeks to achieve a high efficiency of over 18%, exceptional stability for more than two weeks of diurnal operation, and a throughput of 0.12 grams H_2 per hour of >200 cm^2 light capture area.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Production - HydroGEN Seedling projects.

Question 1: Approach to performing the work

This project was rated **3.3** for identifying barriers and addressing them through project innovation, as well as for project design and feasibility.

- The project team identified the primary barrier: instability of HOIP under normal ALD growth temperature (which typically requires a lower temperature), which can cause pinholes in coating and thus requires Al pinhole fillers. The project team also identified a barrier in cost-effectively scaling up the technology. The described metrics of HOIP bandgap targets and tandem perovskite/HOIP bandgap targets provide additional measures of success for the project. The project's safety plan is appropriate, as are the diversity, equity, inclusion, and accessibility (DEIA) and community benefits plans. Continued progress is anticipated. This project is ambitious and will require success across multiple aspects. Team members assigned to those tasks are well-suited to advancing their respective areas, including perovskite performance, coating performance, device development, and final device testing. While not technically in scope of the project, some acknowledgement of the cost of slow atomic layer deposition (ALD) growth and potential challenges of scaling up may be useful in the future and strengthen the long-term vision of the technology.
- The project approach employs a combination of low-cost HOIP materials alongside molecular-engineered ALD coatings, which provide the system protective, conductive, and catalytic functionalities. The project team found that operating the photoelectrochemical (PEC) cell under alkaline conditions enhances the durability of photovoltaic (PV) components, ensuring prolonged functionality. Moreover, the PEC cell design facilitates the separate generation of hydrogen and oxygen, mitigating issues associated with gas phase mixing. To build a 200 cm^2 prototype, the team will adopt a modular approach, allowing for efficient assembly and scalability. This methodological choice seems to be very reasonable for scaling up, paving the way for the development of larger-scale systems.
- The project team's approach of using a tandem PEC cell with a new low bandgap (<1.15 eV) is a logical strategy that can likely achieve both high efficiency and long(er) life. The cell construct is interesting: a central photoanode surrounded by a picture frame anion exchange membrane (AEM) and cathode.
- The proposed HOIP with ALD-growth coatings with multifunctionalities of protection, conduction, and catalysis is a novel and interesting project approach. The technical barriers have been clearly identified. The project goal is clearly set. Below are some questions and comments on the approach:
    - The theoretical value of the voltage of these new materials is unclear (slide 8). The project is target-driven, but knowing the theoretical limits will allow the team to know where the ceiling of these new materials is and guide the project direction. Additionally, it is recommended that the principal investigator propose the hypothesis for the project and make the project hypothesis-driven.
    - Perhaps there are alternatives that do not require two days to grow (slide 12). For future scale-up, a fast coating method is needed to shorten the process.
- The approach seems to have three distinct concepts in novel perovskite materials, TiAlOx coatings, and a novel device design. Each concept seems to be independently interesting, but it is not clear how the three enhance each other beyond the sum of their parts.

Question 2: Accomplishments and progress

This project was rated **2.8** for its accomplishments and progress toward overall project and DOE goals, as well as the HydroGEN Consortium mission.

- The team demonstrated successful deposition of the TiAlOx coating at 85°C with thickness of 100 nm. The project team has shown that for PV fabrication, Ni and TiAlOx can both be coated on the exact same spot with a precisely controlled area using the specially made aluminum cover. This technique streamlines the manufacturing process and ensures accurate placement of materials, contributing to enhanced efficiency and reliability of the PV devices. Furthermore, the team has developed a clear pathway for synthesizing a narrow-bandgap perovskite thin film (Pb-free, $Cs_4CuSb_2Cl_{12}$) with an optical bandgap of ~1.1 eV. The team has met Milestones 1.1 and 1.2.

- Initial tests have shown successful ALD under multiple temperatures and materials. The initial optimized ALD temperature was selected based on supporting information. Performance maintenance from use of the coating is supported by data. Initial steps for manufacturing the device have been shown. The team has identified some candidates for lower-bandgap perovskite materials, although more experimental results are required for validation. Durability testing is quite limited right now (i.e., approximately 10 continuous hours); more testing is required to validate this aspect of the project. The project's demonstration of a full PEC device is still upcoming. The project team has made significant progress to meet go/no-go criteria, but more work is needed on several dimensions. The expected upper limit of performance for this technology would be helpful for contextualizing maximum possible success.
- Progress is good, particularly for being only halfway into the first year. Identification of 55 supercycles of ALD for protection (100 nm) is a significant finding. The project also conducted studies on ALD growth temperature.
- The project made some progress on the fabrication of the ALD-grown coatings for six months of the project. It is strongly recommended that the project team include a table that can clearly show the milestones and progress of each task and the go/no-go decision points.
- The project has just started.

Question 3: Collaboration effectiveness

This project was rated **3.5** for its collaboration and coordination with HydroGEN and other research entities.

- The project is inherently multidisciplinary and requires engagement from multiple partners. Participating organizations include the National Renewable Energy Laboratory (NREL), Lawrence Livermore National Laboratory (LLNL), and Lawrence Berkeley National Laboratory (LBNL). Their work includes computational modeling, materials improvement, microscopy, and large-scale testing. Results from this project can influence the development of similar PEC devices.
- While difficult to assess from a single slide, the incorporation and interaction of five Energy Materials Network nodes on the project appears to be a great arrangement for highly effective collaboration.
- The team showed a strong collaboration, with national laboratories utilizing HydroGEN nodes for characterization, testing, and simulation work.
- There appears to be effective integration with HydroGEN planned.
- The project has very good collaboration with NREL, LBNL and LLNL.

Question 4: Potential impact

This project was rated **3.2** for supporting and advancing progress toward DOE Hydrogen Program goals and the HydroGEN Consortium mission.

- The project's photoelectrolysis of water to produce hydrogen is a very attractive and promising approach for green hydrogen production, which is critical for the reduction of carbon emissions. Photoelectrolysis does not require the use of expensive precious-group-metal catalysts, which makes it economically feasible. The proposed ALD coatings with multifunctionality will help to greatly enhance the stability/durability of the PEC water-splitting devices for at least six months for now—and for even more in the future. The project will also push the efficiency to >18%, which will significantly reduce the cost. Although the project technology has a low technology readiness level (TRL) and is still far away from the practical application, it is a critical renewable hydrogen production that holds a great future.
- The use of tandem cells is a key, and perhaps necessary, way to achieve the high solar-to-hydrogen efficiency needed to enable low-cost PEC hydrogen. Likewise, capture of lower-energy/-bandgap photons is also critical to achieving high efficiency. The technology needs large(r) area cells to reduce manufacturing costs. This project combines all three of the above necessary elements and thus stands a good chance of furthering DOE objectives.
- The introduction of novel narrow-bandgap materials holds great promise for enhancing the solar-to-hydrogen efficiency, thereby making a substantial contribution to hydrogen production. However, it is important to acknowledge that the overall PEC technology remains at a relatively low TRL. To advance toward practical implementation, it is imperative that the project team focus on improving durability.

Addressing durability concerns is essential for establishing the reliability and long-term viability of PEC systems.

- This project shows a promising pathway for high performance while maintaining satisfactory durability, which is a fundamental barrier to the economic success of PEC concepts. The final project should consider how slow ALD and the scaled-up device would impact project economics. The principal investigator has proposed that there may be a chemical alternative to ALD, which should be discussed in more detail in future reports, possibly in supporting information. Future results could include a target levelized cost of hydrogen (LCOH). A consistent LCOH method could be used to compare different PEC concepts within this cohort of PEC projects presented in the 2024 Annual Merit Review.
- The project's focus on creating a large-area device significantly enhances its relevance. A major challenge of the project will likely be scaling its technologies.

Question 5: Proposed future work

This project was rated **3.0** for effective and logical planning.

- The project's proposed future work will focus on the evaluation of fully integrated perovskite PEC devices with emphasis on improvement of solar-to-hydrogen efficiency and durability. The project team's efforts on scale-up seem to be well-planned.
- The project team proposed the following aspects of future work: (1) demonstrate the full PEC device with high efficiency, (2) demonstrate durability, (3) demonstrate larger cell area and larger device area, and (4) demonstrate final device stability with a pressure differential. Given the complexity of these tasks and the need for simultaneous development, it would have been helpful for the project team to provide a basic Gantt chart and a map of potential bottlenecks. The reviewer does not have any concerns regarding the appropriateness of future project work.
- The project's planned future work is reasonable and on point. Characterization at a higher hydrogen compression ratio would supply interesting data that may be used in projecting large system performance and cost.
- The proposed future work of the project is solid and well-organized.
- The proposed future work provides the specific goals of the future work, but little information is provided about the specific activities and efforts that have been allocated to meet those goals.

Project strengths:

- The principal investigator and supporting teams and organizations are experts in developing PEC materials and technologies. The project team's focus on device development and scale-up gives confidence that the team has a clear line of sight to a useful final project that may be ready for commercialization. The project's vision of a device with some level of hydrogen compression further improves the economic viability of this pathway.
- The project focuses on enhancing the durability of perovskite-based PEC systems by implementing ALD-grown coatings. By operating water splitting in alkaline conditions, the project aims to extend the lifetime of the PEC devices while also eliminating the need for critical materials such as Pt and IrOx at the anode and cathode. Instead, the project utilizes a platinum-group-metal-free catalyst, thereby reducing cost and reliance on rare and expensive materials. The project also addresses the challenge of scaling up the production of photoelectrodes.
- The proposed approach is novel: HOIP with ALD-growth coatings with multifunctionalities of protection, conduction, and catalysis. The technical barriers have been clearly identified. The project goal is clearly set. The project team is strong and balanced, with good collaborations with national laboratories.
- The project team's target of >18% efficiency and efforts to develop <1.15 eV bandgap materials are strengths. The approach of alternating layers of TiO and Al is another strength. Finally, the skill sets brought to the project by the team, including two national laboratories and two universities, represent a strength of the project.
- The project is highly innovative.

Project weaknesses:

- The importance and meaning of the ALD growth temperature graphs are not clear. More context or interpretation of results is needed. The two days of ALD deposition is currently a major project weakness, as this may make the cells quite expensive. The data reports only one ratio of Ti to Al, which is a minor weakness, as other ratios may be more optimal. Not further explaining the manufacturing process (other than the photoanode) is a minor weakness. The cell design's use of a picture frame membrane and electrode is a modest weakness, as it creates relatively large distances for electron transport; potentially creates large material scrap (if sheet membrane, mesh, and electrodes are used); and has the potential for high gas leakage (through/around the epoxy seals). The methodology and thinking regarding discovery of the new lower-bandgap materials are weak. The presentation cited density functional theory and machine learning but did not provide further elaboration.
- The project team should thoroughly discuss aspects such as adhesion, compatibility, and potential delamination of the deposited layers, as these factors significantly impact the overall performance and longevity of the PEC devices. Furthermore, careful consideration should be given to the selection of hydrogen evolution reaction and oxygen evolution reaction catalysts, including deposition methods and stability under operating conditions. The team should also consider the durability of the AEM.
- Project success requires meeting acceptable metrics in the following aspects: materials development, coating performance, device manufacturing, and systems testing. The project team must take care to ensure that progress continues to be made simultaneously across all fronts. Scaling up of the cell area appears to be challenging. More testing is needed in this area.
- The low-temperature ALD coating is challenging, and a back-up plan is strongly encouraged.
- For the distinct concepts for the project, it is not clear how much time and resources are allocated to each portion and what dependencies exist that are needed to reach on-sun testing.

Recommendations for additions/deletions to project scope:

- The project needs to conduct a techno-economic analysis to assess whether the ALD deposition time is too long for economic fabrication and to assess the scrap rates of membrane, mesh, etc. The ALD time should be further optimized. Additional Ti:Al ratios should be considered. Performance modeling should be conducted to look at the performance drop-off (if any) in going to a larger cell area. Performance modeling should be conducted to assess the optimal area of membrane and Ni foam for a given area (and dimensions) of photoanode.
- It may be appropriate for the project team to explore alternatives to ALD. The use of a robotic arm to manufacture devices is interesting but does not need to be demonstrated during this project.
- The project would benefit from a cost estimate of ALD and photoelectrode fabrication and from techno-economic analysis.
- The low-temperature ALD coating is challenging, and the project team should develop a back-up plan accordingly.
- The project team should provide more detail regarding planned activities and scheduling.

Project #P-214: Demonstration of a Robust, Compact Photoelectrochemical Hydrogen Generator

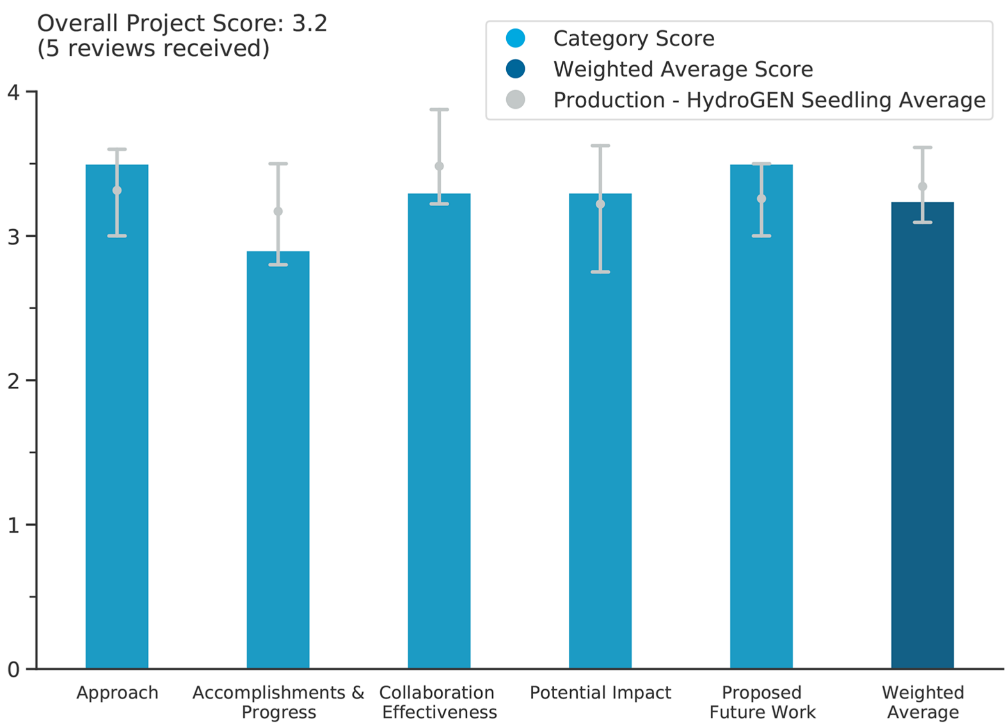
Joel Haber, California Institute of Technology

DOE Contract #	DE-EE0010736
Start and End Dates	10/1/2023–9/30/2026
Partners/Collaborators	National Renewable Energy Laboratory, Lawrence Berkeley National Laboratory
Barriers Addressed	• Increasing solar-to-hydrogen efficiency with product separation >20%, requiring a holistic approach to system design and improvement of light absorbers, electrocatalysts, membranes, and mass transport • Improving the durability of all components using thorough diagnosis of degradation mechanisms

Project Goal and Brief Summary

This project objective is to demonstrate highly integrated, efficient, and durable photoelectrochemical (PEC) hydrogen generators by leveraging high-efficiency, dual-junction organo-halide perovskite/Si photovoltaic (PV) architectures. This approach seeks to advance state-of-the-art efficiency and durability to reduce the levelized cost of hydrogen (LCOH). Additionally, the project aims to diagnose, publish, and address degradation pathways that limit durability, offering valuable insights to the solar hydrogen community. Through collaboration with HydroGEN nodes, the project utilizes a total system design, modeling, testing, diagnosis, and improvement cycle to achieve these goals. This initiative ensures a holistic solution to the challenges of efficiency, durability, and cost-effectiveness in PEC hydrogen generation technology.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Production - HydroGEN Seedling projects.

Question 1: Approach to performing the work

This project was rated **3.5** for identifying barriers and addressing them through project innovation, as well as for project design and feasibility.

- The project is dedicated to the development of a robust PEC hydrogen generator, leveraging high-efficiency, dual-junction organo-halide perovskite/Si PV architectures. Central to this endeavor is a comprehensive understanding and mitigation of degradation pathways that currently limit PEC durability. By conducting water splitting under alkaline conditions, the project aims to enhance durability while potentially obviating the need for costly and scarce Pt and IrO_2 electrocatalysts for hydrogen and oxygen evolution reactions, respectively. The team has systematically identified key technological barriers and proposed a holistic PEC device design aimed at addressing these challenges.
- The primary barriers of building and de-risking the two-terminal, dual-junction Si/organo-halide perovskite PV cell have been identified. Metrics of maximum and average solar-to-hydrogen (STH), as well as target cell size, provide additional measures of success. The safety plan is appropriate, and the diversity, equity, inclusion, and accessibility (DEIA) activities and community benefits plans are appropriate. The project will use decoupling of cell components to conduct discretized testing of individual components, identifying specific degradation rates and mechanisms. While not technically within the project scope, acknowledging potential costs and challenges of scale-up may be useful in the future and would strengthen the long-term vision of the technology.
- Basing the concept on a dual-junction cell is a logical and thoughtful approach. The team's consideration of degrees of integration is a very strong framework, and the team should continually refer back to the diagram as the project progresses.
- The team is well-established, building aggressively on on/off robustness limitations using 25–200 cm^2 areas and pushing the state of the art.
- The approach is well-articulated. However, it is not clear why these specific improvements are sufficient to achieve 25% STH. Analysis supporting this claim would be helpful.

Question 2: Accomplishments and progress

This project was rated **2.9** for its accomplishments and progress toward overall project and DOE goals, as well as the HydroGEN Consortium mission.

- It appears that the project has encountered delays in its research and development efforts following a lengthy contracting process. However, the team has already made significant progress in synthesizing and characterizing hybrid organic–inorganic perovskite (HOIP) PV materials. The researchers are focusing on understanding the effects of electrode area and addressing performance issues. Furthermore, the team has taken steps towards understanding the mechanisms underlying durability and performance degradation by identifying various types and degrees of integration of PV components. This approach demonstrates a proactive effort to tackle challenges and optimize the performance and reliability of the PEC system.
- The hybrid organic–inorganic hybrid perovskite node at the National Renewable Energy Laboratory (NREL) (led by Kai Zhu) has conducted preliminary work to screen optimal cell areas for testing. Since the project has yet to begin, there are no additional data or results to report and discuss. The project team is planning to check for the following potential considerations during data collection: changes in performance due to wetting, catalyst hysteresis, appropriate diagnostic signals for each component, and improving performance while scaling up the cell area.
- The project has not started yet, so there are no accomplishments to report.

Question 3: Collaboration effectiveness

This project was rated **3.3** for its collaboration and coordination with HydroGEN and other research entities.

- The project is inherently multidisciplinary, requiring engagement from multiple partners, including NREL and Lawrence Berkeley National Laboratory (LBNL). The project includes materials improvement, microscopy, and large-scale testing. The results from this project can influence the development of similar PEC devices.

- Collaboration effectiveness is difficult to measure since the project has not yet begun. However, the project team is in contact with and actively monitoring the experimental work at NREL's perovskite PV node, which will be used in the project. The team's participation in the annual Water Splitting Pathways Benchmarking Workshop is both appropriate and important.
- The team is supported by NREL and LBNL through HydroGEN nodes for HOIP synthesis, PV characterization, and some testing and modeling work.
- The team is well-integrated, with established collaborative experience, but the project has not started.
- There is a good degree of partnership with the HydroGEN nodes.

Question 4: Potential impact

This project was rated **3.3** for supporting and advancing progress toward DOE Hydrogen Program goals and the HydroGEN Consortium mission.

- There is a strong deficit in understanding and ameliorating PEC performance degradation. Consequently, advances in understanding the causes of degradation would be a tremendous step forward. Achieving 15% STH efficiency after 1,000 hours of on-sun exposure, particularly at a sizeable 200 cm^2 active area, would be a breakthrough in PEC hydrogen production. While it still has a long way to go to achieve economic competitiveness, this would be a major step forward in achievement of DOE targets.
- The project shows a promising pathway for high performance while maintaining satisfactory durability, which is a fundamental barrier to economic success of PEC concepts. The final project should consider the cost implications of being unable to scale up cell size and should possibly include a target LCOH. Ideally, a consistent LCOH method would be used to compare different PEC concepts within this cohort of PEC projects presented in the 2024 Annual Merit Review.
- The proposed work involves integration and addressing device scaling, which is highly relevant to the Hydrogen Program.
- Overall, the project is complicated and challenging and currently at a low technology readiness level. However, the outcome could pave an additional pathway for hydrogen production alongside direct water electrolysis.
- The project addresses key barriers of durability, cost, and critical materials shortages.

Question 5: Proposed future work

This project was rated **3.5** for effective and logical planning.

- The proposed future work aligns well with the project goal, focusing on studying degradation processes in PEC systems and scaling up the technology. Over the next year, the team plans to concentrate on maximizing the efficiency of devices larger than 0.25 cm^2 by optimizing material properties and characterization techniques. Subsequently, the team aims to scale up components to 25 cm^2, which is a logical progression toward achieving larger-scale implementations of the technology.
- The team has provided a detailed list of activities to perform in the next period that clearly supports meeting the go/no-go milestones.
- Multiple aspects are proposed for future work: testing individual subcomponents, demonstrating durability, and demonstrating larger cell area and larger device area. There are no concerns as to whether future work will be appropriate.
- Extensive plans were presented, but the project has not started yet.
- The project has not started yet, so all work is set for the future.

Project strengths:

- The project has leveraged highly promising HOIP photoabsorbers, along with low-cost, platinum-group-metal-free catalysts for water splitting under alkaline conditions. Operating in such an environment not only enhances the durability of the PV architecture but also eliminates the need for costly and scarce Pt and IrO_2 electrocatalysts. A strategic emphasis is placed on conducting a comprehensive evaluation of degradation mechanisms and developing accelerated stress tests to simulate real-world conditions. This approach highlights the project's commitment to understanding and mitigating degradation processes, ensuring the long-term reliability and performance of PEC systems. By combining innovative materials and catalysts with rigorous evaluation methods, the project is poised to make significant steps toward advancing sustainable hydrogen production through PEC technology.

- Leveraging past work at the Joint Center for Artificial Photosynthesis is a major project strength, as is the use of a "total system design" approach. Achieving the project goal of increasing 1,000-hour STH efficiency from 8% to 15% is a significant step forward (as it is difficult to achieve). The team members are very strong in past experience and expertise in the individual areas of their tasking. Explicit consideration of different levels of component integration is a key aspect of the approach and is a project strength.
- The principal investigator and supporting teams and organizations are experts in developing PEC materials and technologies. The focus on scale-up gives confidence that the project team has a clear line of sight to a useful final product.
- The project is clearly defined and well-planned. The scope of work is clearly aligned with the budget and project timeline.
- The team is well-established, building aggressively on on/off robustness limitations using 25–200 cm^2 areas, pushing the state of the art on key barriers such as durability, cost, and critical materials shortages.

Project weaknesses:

- While achieving 1,000 hours of durability would be a significant improvement over the current state of the art, it still is far short of what is needed for economic competitiveness. The first year's work is not described in much detail. The title of Task 1 refers to "differently integrated devices," so there is confusion as to whether the project is meant to build and test all four of the devices shown in the approach slide. Additionally, the definition and motivation for a "compact tileable device design" should be expanded.
- More clarity on the mitigation of different types of degradation would be beneficial for the project.
- No support is provided for why the project innovations are expected to meet 25% STH and other project goals.
- The loss in performance as cell size increases is a concerning trend that must be addressed.
- The project has not started yet.

Recommendations for additions/deletions to project scope:

- The project is very well-scoped. No additions or deletions are recommended.
- The concept of degrees of integration is a useful framework that could be beneficially applied to other DOE projects. There is no deliverable for understanding degradation mechanisms at the end of the first year. Adding a preliminary report on the first year's findings would strengthen the project.
- A techno-economic analysis would be beneficial for the project to understand the cost of hydrogen generated by the proposed PEC devices.
- It would be appreciated if the team would coordinate materials used with PEC and low-temperature electrochemical water-splitting best practices to reduce catalyst and materials contamination issues.

Project #P-215: Semi-Monolithic Devices for Photoelectrochemical Hydrogen Production

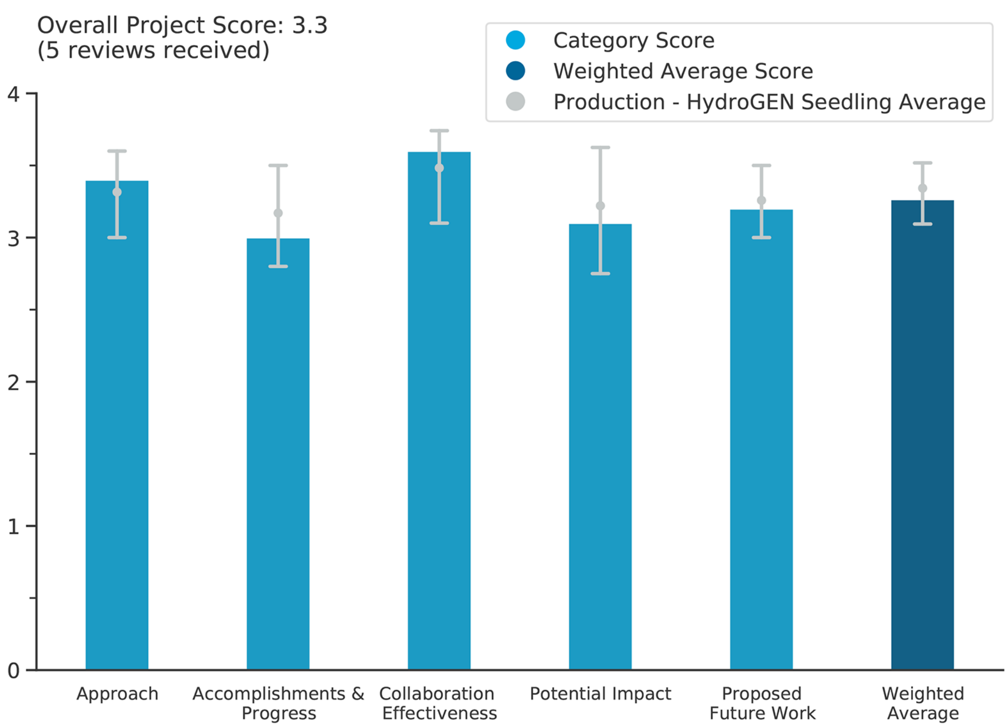
Nicolas Gaillard, University of Hawaii at Manoa

DOE Contract #	DE-EE00010737
Start and End Dates	10/1/2023–9/30/2026
Partners/Collaborators	University of Nevada Las Vegas, Stanford University
Barriers Addressed	• Materials compatibility and integration: room-temperature multi-junction integration scheme based on thin film exfoliation and bonding to combine fully processed subcells while preserving their performance • Materials durability: superstrate multi-junction structure in which the photo-absorbers are sandwiched between a coated glass substrate and a stable catalyst layer

Project Goal and Brief Summary

This project's objective is to strengthen the theory–synthesis–characterization loop to accelerate the development of efficient materials and interfaces for economical photoelectrochemical (PEC) hydrogen production. By combining dissimilar material classes such as chalcopyrites and perovskites into multi-junction (MJ) devices and using x-ray spectroscopy and surface catalysis, the project aims to achieve high efficiency, low cost, and durability in PEC water splitting. Key technical approaches include developing a room-temperature MJ integration scheme based on thin-film exfoliation and bonding to combine fully processed subcells while preserving performance. Additionally, the project involves the development of a superstrate MJ structure, where photo-absorbers are sandwiched between a fluorine-doped tin oxide (FTO)-coated glass substrate and a thick, stable oxygen evolution reaction (OER) catalyst layer to enhance materials durability.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Production - HydroGEN Seedling projects.

Question 1: Approach to performing the work

This project was rated **3.4** for identifying barriers and addressing them through project innovation, as well as for project design and feasibility.

- The approach is to “strengthen the theory–synthesis–characterization feedback loop” to accelerate the development of chalcopyrites and perovskites for PEC hydrogen production. The presentation does a commendable job of communicating how this will be accomplished between the three principal investigators (PIs) and their roles in the project. Materials compatibility, integration, and durability barriers for chalcopyrite–perovskite and all-chalcopyrite devices are identified, and approaches to addressing barriers are clearly defined. The project features excellent safety planning, which includes documents for job safety analysis, risk assessment, development of standard operating procedures, and a what-if analysis. Student training requires reading and understanding the four documents, as well as annual retraining/recertification of workers. The team has engaged the Hydrogen Safety Panel and is in the process of addressing the panel’s feedback. The safety plan ranks among the most comprehensive seen by the reviewer. DEIA and CBPs take advantage of two of the institutions, the University of Hawaii and the University of Nevada, Las Vegas (UNLV), which are minority-serving institutions (MSIs). The plan is to engage at least one student from an underrepresented group in the project and to have one student participate in a summer program with one of the national lab partners. This plan is consistent with what most other projects are undertaking to meet their DEIA/CBP requirements.
- The project targets the development of innovative technologies that integrate dissimilar material classes, specifically chalcopyrites and perovskites, into MJ devices for PEC water splitting. With ambitious goals of elevating the solar-to-hydrogen (STH) efficiency from 3%–5% to over 15% and enhancing durability from 500 hours to beyond 1,000 hours, the project aims to overcome significant barriers in the field. To achieve these objectives, the team has adopted a systematic approach, utilizing a theory–synthesis–characterization loop. By identifying key barriers and addressing them through this iterative process, the project aims to push the boundaries of PEC technology. The proposed approach in the fabrication and characterization of chalcopyrite–perovskite and all-chalcopyrite PEC architectures demonstrates effectiveness in advancing toward the project’s goals. Through innovative material integration and rigorous evaluation methodologies, the project is poised to make substantial contributions to the realization of low-cost, durable, and efficient PEC water-splitting technologies.
- The primary barrier is combining different photoelectrode materials in a mechanically and electrically stable way. Metrics of STH and durability provide additional measures of success. In addition, the project will attempt to improve performance of chalcopyrite materials. The safety plan is robust. A diversity, equity, inclusion, and accessibility (DEIA) plan and community benefits plan (CBP) are part of the project team’s long-term strategy and are ongoing. The project has a comprehensive strategy for characterizing mechanical and electrical stability of the transparent conductive composite (TCC) bridge. In addition, the project team has defined multiple alternative strategies of creating the superstrate in case any one concept fails. The project has taken an initial pass at project economics and levelized cost of hydrogen (LCOH), which increases confidence in the team’s prospects for developing a useful final product.
- The proposed approach is innovative and combines dissimilar material classes, such as chalcopyrites and perovskites, into MJ devices for efficient, low-cost, and durable PEC water splitting. The technical barriers (materials compatibility and integration) have been clearly identified. The project goal is clearly set. However, the microspheres’ size distribution and room-temperature, low-pressure assembly lead to isolated device areas without electrical contacts, per slide 10. It is unclear if there is any plan to improve.
- This project aims to develop an innovative means of combining dissimilar photo-absorber materials classes to form MJ devices to overcome the barriers of efficiency, cost, and durability. Keys to this approach are a room-temperature MJ integration scheme based on exfoliation and bonding and a thick OER catalyst layer for protection of the photo-absorber. This approach is supplemented by a few additional efforts to demonstrate metrics set by DOE, affording time to study and advance the team’s novel adhesive materials approach developed in prior work from a 2017 grant. While this approach is innovative, it does not provide a convincing pathway to hydrogen production at $1/kg H_2 without additional cost reductions in the reactor or installation, as indicated in the techno-economic analysis (TEA). It is strongly encouraged that this group—and DOE, through its future funding opportunity announcements—support the development of innovations that lead to necessary cost reductions. Without them, this approach—like any approach in the

PEC portfolio—will not have its desired impact. Irrespective of this, the safety plan seems sufficient and includes a detailed four-step assessment and analysis plan, which is good. The team has a strong track record of excellence in DEIA that will be continued during this work via annual milestones, and the lead PI and co-PI are located at MSIs.

Question 2: Accomplishments and progress

This project was rated **3.0** for its accomplishments and progress toward overall project and DOE goals, as well as the HydroGEN Consortium mission.

- The team has achieved Milestone 1.1, which validates the electrical and mechanical models describing the processes involved in the deposition of layers and assembly of photovoltaic (PV) devices. This accomplishment demonstrates the team's thorough understanding of the principles governing the fabrication process. Moreover, the team is actively engaged in the fabrication and evaluation of the proposed PEC architectures. By combining theoretical modeling with practical experimentation, the team is well-positioned to make significant contributions toward the realization of efficient and sustainable PEC water-splitting devices.
- The project team has experimentally validated models for understanding the mechanical and electrical performance of the TCC bridge. Additional work is expected to improve the electrical model. STH efficiency is confirmed for perovskite solar cell/$Cu(InGa)Se_2$ (PSC/CIGSe) tandem, which is close to achieving the final project goal of >15%. Durability testing is ongoing and is required for meeting the target of 24 hours. The project is expected to meet go/no-go criteria.
- A mechanical and electrical model and new equipment were reported to predict and evaluate sphere properties in transparent conductive composite adhesive layers. The team also provided the first demonstration of a triple-junction chalcopyrite device. Load-line analysis for the project's Priority 1 device configuration suggests that meeting the go/no-go decision point is likely.
- The project appears to be on track, with the first technical milestone (semi-monolithic integration process development) completed. Other first-year technical milestones/deliverables appear to be on track, as well as meeting the Budget Period (BP) 1 go/no-go criteria.
- The project made some progress on Tasks 1, 2, and 3. It is strongly recommended that the project include a table that can clearly show the milestones and progress of each task and the go/no-go decision points.

Question 3: Collaboration effectiveness

This project was rated **3.6** for its collaboration and coordination with HydroGEN and other research entities.

- There is very strong and clearly defined engagement of HydroGEN expertise and capabilities, with four HydroGEN nodes being identified to aid in developing materials, integrating the photochemical cell with the electrolyzer, developing theoretical models to accelerate development of this technology, and testing and validating the device. There is a strong connection to "2b" benchmarking/protocols efforts, with three PIs having participated in developing PEC standards since 2008 and writing testing and benchmarking protocols for various PEC materials. Benefits to HydroGEN and the PEC community are clearly stated. The project includes the most comprehensive discussion of engagement with HydroGEN of all the projects encountered by the reviewer.
- The Energy Materials Network node collaborators include Zhu (perovskite materials), Muzzillo (chalcopyrite materials), Young (on-sun STH validation), Deutsch (durability), and Ogitsu (theory), which all seem relevant and contributors to results. Moreover, the team has successfully worked together on DOE Office of Energy Efficiency and Renewable Energy (EERE) projects and related efforts for over a decade, including substantial participation in benchmarking/protocols (2b) and opportunities for students from underrepresented groups. The collaborative workflow on this project is clear and strong. A world expert in TEA is missing, but the reported use of the Hydrogen Analysis (H2A) model tool is a good start.
- The project is inherently multidisciplinary and requires engagement from multiple partners. Participating organizations include the National Renewable Energy Laboratory, Lawrence Livermore National Laboratory, Stanford University, and UNLV. Their capabilities include materials improvement, microscopy, and large-scale testing. The project team has a long history of participating in consortiums and

benchmarking activities. Results from this project are generalizable to alternative PEC materials and devices.

- The team demonstrated well-coordinated and close collaboration between the project partners and national labs utilizing available HydroGEN nodes.
- Three university teams have been assembled. The project needs to incorporate the collaboration from national laboratories.

Question 4: Potential impact

This project was rated **3.1** for supporting and advancing progress toward DOE Hydrogen Program goals and the HydroGEN Consortium mission.

- Photoelectrolysis of water to produce hydrogen is a very attractive and promising approach for green hydrogen production, which is critical for the reduction of carbon emissions. Photoelectrolysis does not require the use of expensive precious group metal catalysts, which makes it economically feasible. The proposed new approach and new design have the OER and hydrogen evolution reaction (HER) catalytic layers facing each other, greatly shortening the ion diffusion distance, improving the mass transport of ions compared with traditional PEC cells (in which OER and HER catalyst layers are coated on either side of the device). Additionally, the thick OER catalyst layer shields the solar absorbers from the electrolyte, greatly improving durability. Although this technology is at a low technology readiness level and still far away from the practical application, it is a critical renewable hydrogen production, which holds a great future.
- Durability, efficiency, and cost are critical factors in achieving the DOE goal for hydrogen production costs of $1/kg through PEC water splitting. The project's focus on these key aspects makes it relevant to the field of hydrogen production. If successful, the project has the potential to contribute significantly to the diversification of hydrogen generation pathways.
- The proposed technology develops a "superstrate device architecture," where the thick OER catalyst layer shields the solar absorbers from the electrolyte, which helps to prolong operational lifetime. Models that can predict the properties of solar absorbers (optical absorption, thermodynamic stability, defect chemistry) and interfaces (band-edge offsets) for economical renewable PEC hydrogen production are valuable.
- The project shows a promising pathway for high performance while maintaining satisfactory durability, which is a fundamental barrier to the economic success of PEC concepts. The project team has developed an LCOH model for the technology; the model identifies cost drivers and areas of ongoing need for cost reduction. Ideally, a consistent LCOH method would be used to compare different PEC concepts within this cohort of PEC projects presented in the 2024 Annual Merit Review.
- Presentation of a cost sensitivity tornado plot provides what seem to be realistic TEA outcomes, which predict hydrogen production cost that barely surpasses $2/kg H_2 with exceptional STH efficiency, lifetime, and material cost. This candid output using the H2A tool is a plus, but it is unclear whether a stable membrane is included in this design (as there is a disparity in the presented figures as to whether one is included), though it must be, unless a PEC-specific innovation is being developed in that space as well. The sensitivity analysis indicates that reactor and installation costs would need to be drastically reduced to make up for the cost disparity with $1/kg H_2, but sadly, no pathways were presented to meet this need. Identifying a means to this end is critical to validating the general PEC approach and, therefore, is strongly encouraged as part of this project. Irrespective, the variability in TEA details across the PEC portfolio suggests that DOE should oversee an apples-to-apples comparison of proposed approaches and strongly up-/down-select projects based on that critical metric.

Question 5: Proposed future work

This project was rated **3.2** for effective and logical planning.

- The proposed future work appears to be aligned with meeting the remaining Year 1 milestones/deliverables and the BP 1 go/no-go decision points. Proposed future work on perovskite–chalcopyrite and all-chalcopyrite extensively leverages the HydroGEN nodes to validate the STH performance of the perovskite–chalcopyrite MJ PEC device and increase the performance of the wide E_G chalcopyrites.

Advanced characterization techniques will be employed to improve materials performance and to create models to guide future materials selection for higher efficiency and durability for PEC water splitting.

- The proposed future work is both reasonable and aligned with the project goals, aiming to fabricate and enhance perovskite–chalcopyrite and all-chalcopyrite PEC devices, with the primary focus being on enhancing durability and increasing the STH efficiency of these devices.
- Multiple aspects are proposed for future work: improvement of chalcopyrite materials, assembly of full PEC devices, testing of all-chalcopyrite devices, and evaluation of device durability. This is a complex set of goals, and care must be taken to make progress on all elements. There are no concerns regarding whether future work will be appropriate.
- Planned future work to increase STH efficiency from several device architectures and enhance durability follows logically from the current work, outcomes, and the overall work plan.
- The proposed future work is solid and well-organized.

Project strengths:

- The team members' utilization of their robust material synthesis skills to tackle the material compatibility and integration barriers for perovskite–chalcopyrite and all-chalcopyrite PEC architectures is commendable. This expertise ensures a comprehensive approach to addressing critical challenges in PEC device development. Furthermore, the strong collaboration with HydroGEN nodes enhances the project's capabilities and facilitates knowledge exchange, thereby accelerating progress toward achieving project goals. Leveraging this collaborative network strengthens the project's potential for success. Additionally, the provided TEA serves as a valuable tool for assessing the economic feasibility of the proposed PEC devices.
- There is excellent integration of theory–synthesis–characterization to accelerate materials discovery toward achieving the required STH to meet DOE hydrogen production cost targets. The use of a transparent conductive composite to bond new host substrates to chalcopyrite devices and maintain electrical contact is innovative. TEA analysis shows the required performance metrics—in terms of PEC device efficiency, lifetime durability, and cost metrics for the materials cost, reactor, and installation—that need to be achieved to reach the $1/kg H_2 ultimate target. In conclusion, the significantly higher efficiency makes the investigation of MJ devices a relevant route to meet the DOE hydrogen production cost target.
- Evaluating the properties of previously (more than five years ago) patented transparent conductive composite adhesive layers is good. Also impactful is the reasonable TEA that was conducted using the DOE H2A tool and shared via a technical backup slide. This should be the standard for all projects in the PEC portfolio, with guidance from world experts in TEA of hydrogen technologies.
- The PI and supporting teams and organizations are experts in developing PEC materials and technologies. There is a clear path to 15% efficiency. Focus on scale-up and final project economics instills confidence that the project team has a clear line of sight to a useful final product.
- The proposed approach is innovative and combines dissimilar material classes, such as chalcopyrites and perovskites, into MJ devices for efficient, low-cost, and durable PEC water splitting. The technical barriers (materials compatibility and integration) have been clearly identified. The project goal is clearly set.

Project weaknesses:

- No major weaknesses were noted.
- Providing more clarity on the water-splitting components of the PEC device, particularly the HER and OER catalysts, would be beneficial for the project. By elucidating the specific catalyst materials, their deposition methods, and their stability under operating conditions, the project can offer valuable insights into optimizing PEC device performance. Additionally, detailing any advancements or innovations in catalyst development can inform future research directions and contribute to the broader scientific community.
- Notwithstanding thick OER catalysts, conductive layers to adhere photo-absorbers is a PV challenge, and thus the main focus of this project might be best suited for PV research and development. In addition, there

was no mention of the proposed study of large-area devices, which should be seriously considered in a DOE EERE PEC project.

- Durability is a significant concern with a multi-material device. Stability of TCC under high solar conditions and high temperatures is a risk factor.
- No national lab collaboration was established. It is strongly recommended that the project establish such a collaboration.

Recommendations for additions/deletions to project scope:

- It is recommended that the team collaborate with world experts in TEA to conduct a thorough analysis, and only with a legitimate pathway to \$1–\$2/kg H_2 that is agreed upon by PV and electrolysis experts should an effort be supported by DOE EERE. As work from this project suggests, this may reveal that what limits attaining a \$1/kg H_2 cost target is the entire reactor design, which resembles a PV coupled to an electrolyzer with cost predictions beyond this value, calling into question the logic of a PEC approach. If, however, innovative enclosures are identified that move beyond plexiglass, their study should be added to the scope of this project. However, one must also be transparent in this regard, in that innovations in enclosures may benefit all PV and hydrogen technologies, thus also decreasing their projected costs.
- TEA analysis suggests that STH of 25% is required to achieve a production cost of ~\$2/kg. The project's end goal is to demonstrate STH at an expectant value of >15%. Although not part of this project, it would be good to know how the team envisions achieving the 25% STH.
- While showing a possible pathway to \$1/kg is good, it may be prudent not to show unproven cost reductions such as reactor cost reductions. Unrealistic LCOH numbers can reduce cost modeling credibility.
- The scope of the project is reasonable.

Project #P-216: Scalable Halide Perovskite Photoelectrochemical Cell Modules with 20% Solar-to-Hydrogen Efficiency and 1,000 Hours of Diurnal Durability

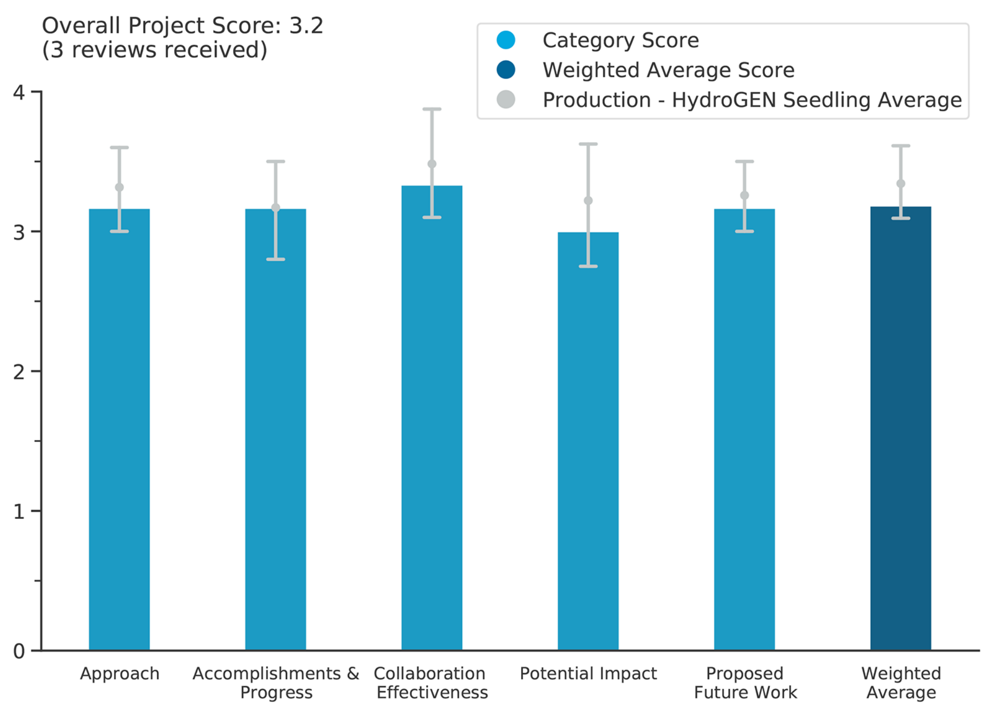
Aditya D. Mohite, Rice University

DOE Contract #	DE-EE0010738
Start and End Dates	10/1/2023–9/30/2026
Partners/Collaborators	National Renewable Energy Laboratory, Lawrence Berkeley National Laboratory
Barriers Addressed	• Integration with proton exchange membrane and alkaline water electrolysis reactors • Stability of Si–perovskite tandems • Acquisition of Si–perovskite tandem

Project Goal and Brief Summary

This project's primary objective is to develop halide–perovskite-based tandem photoelectrochemical (PEC) modules with an area of 200 cm^2, demonstrating an unassisted solar-to-hydrogen (STH) efficiency of 20% and 1,000 hours of diurnal operation. Key technical approaches include exploiting high-efficiency three-/two-dimensional (3D/2D) perovskite solar cells and Si–perovskite tandem solar cells, utilizing a conductive adhesive barrier (CAB) to address integration barriers, and designing reactors to integrate hydrogen evolution reaction and oxygen evolution reaction catalysts with CAB in low-gap configurations. The project aims to overcome technical challenges related to integrating the CAB and Si–perovskite with a proton exchange membrane (PEM) or alkaline water electrolysis reactor, conducting deposition of catalysts on porous surfaces, translating photovoltaic (PV) J_{SC} (short-circuit current density) in an integrated PEC, and optimizing heat transfer from solar cells to catalysts through protective barriers. The milestones include demonstrating stable water-splitting with 250 hours, starting with 20% STH and achieving 1%–2% STH gain via thermal integration to accomplish 25% STH and diurnal operation of 500–1,000 hours.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Production - HydroGEN Seedling projects.

Question 1: Approach to performing the work

This project was rated **3.2** for identifying barriers and addressing them through project innovation, as well as for project design and feasibility.

- The team has a novel approach using Si–perovskite tandems. The initial STH efficiencies are very promising, using Si–perovskite tandems with 21.7% efficiency demonstrated. The barriers identified are related to this specific technology and address some of the major technical challenges such as improving STH efficiency, addressing durability/stability issues through the development of a protective barrier technology, and integrating the materials into a polymer electrolyte or alkaline water electrolyzer. The project targets a relatively high STH efficiency of >24.5%, which represents a significant improvement over the current 20.8% efficiency. The safety plan appears adequate in that it provides training to students for working with hydrogen and ensures that students are wearing the proper personal protective equipment. The plan also states that the team will develop safety protocols and work with industry and national labs to verify the protocols. However, it does not appear that the Hydrogen Safety Panel was engaged. Instead of developing new safety protocols, the team should reach out to the Hydrogen Safety Panel and take advantage of the Panel's collective expertise to ensure that the project's safety training, planning, etc., follow well-established protocols. The team has undertaken very commendable diversity, equity, inclusion, and accessibility (DEIA) and community benefits activities, collaborating with Dr. Graham Thomas at Texas Southern University (TSU), a historically Black college/university (HBCU), and identifying four students from TSU to join the project. Two students are being retained to work on the project and supported for a visit to Lawrence Berkeley National Laboratory (LBNL) or National Renewable Energy Laboratory (NREL). Presumably, these students will be from underrepresented or disadvantaged groups.
- This project aims to develop silicon/halide–perovskite tandem PEC modules to overcome the barriers of efficiency, diurnal stability, and large-area devices. The key aspects to this approach are a patented conductive adhesive barrier; use of low-cost, high-surface-area catalysts; tandem photoabsorber designs; and device integration for effective heat transfer. While these metrics seem important, based on the information supplied, it was unclear whether the scope of work would be suitable to evaluate the project's technology innovation with a convincing pathway to hydrogen production at \$1–2/kg H_2. Irrespective, the safety plan seems sufficient for benchtop-scale experiments, but if large amounts of hydrogen are to be generated and collected, a more detailed plan must be adopted. The team included suitable DEIA efforts with annual milestones.
- The project approach seems solid and well-considered.

Question 2: Accomplishments and progress

This project was rated **3.2** for its accomplishments and progress toward overall project and DOE goals, as well as the HydroGEN Consortium mission.

- The team has made good progress to date toward meeting the Budget Period 1 go/no-go criteria. The team met both Milestone 1.1 (i.e., demonstrated stable water-splitting with <75 mV overpotential change of 200 hours) and Milestone 1.2 (i.e., demonstrated an electrolyzer with <50 mV overpotential over 1,000 hours). There has been a good effort to identify catalyst delamination from the planar surface as a major contributor to instability in device performance and then to develop and demonstrate the carbon-form process for minimizing delamination. The project appears on track to meet its DEIA and community benefits plan (CBP) milestones, with two students from TSU identified as having been onboarded to the project.
- A new PEC reactor was designed for two-electrode measurements, and modest increases in STH efficiency and stability were reported, which is on track to meeting the go/no-go decision point. PV performance of larger-area photoabsorbers was also reported. Notwithstanding, reporting enhanced stability at a smaller operating current density may be misleading if degradation is a Faradaic process, and thus stability (as J_{op}) should also be reported as a function of total charge passed.
- The project managed to progress, despite supply chain limitations for key materials. The refocus on sealing as the key metric for observed degradation seems appropriate.

Question 3: Collaboration effectiveness

This project was rated **3.3** for its collaboration and coordination with HydroGEN and other research entities.

- The team has strong engagement with HydroGEN, working with the following people: Todd Deutsch at NREL on on-sun testing of the integrated reactor system, STH benchmarking, and techno-economic analysis (TEA); Joel Agers and Rangachary Mukundan at NREL on polymer electrolyte and alkaline water electrolyzer design and degradation studies; and Berry and Kai at NREL on Si–perovskite tandems. The defined engagements leverage the capabilities and expertise of the HydroGEN team, targeting a number of the technical challenges in developing this technology. The project should be expected to greatly benefit from these engagements. The project appears to be well-engaged with HydroGEN, based on the activities identified in the presentation.
- The project's collaboration seems appropriate to the timeline and scope.
- Energy Materials Network node collaborators include Deutsch (on-sun testing and STH benchmarking), Agers and Mukundan (reactor designs and degradation studies), and Berry and Kai (Si–perovskite tandems at scale), which all seem relevant and contributors to results. However, the team is missing a world expert in TEA. There is a significant collaboration with TSU, an HBCU, but there was no mention of benchmarking/protocols participation.

Question 4: Potential impact

This project was rated **3.0** for supporting and advancing progress toward DOE Hydrogen Program goals and the HydroGEN Consortium mission.

- The TEA identifies the major cost contributors that need to be addressed to meet the DOE interim hydrogen production cost target of <$2/kg H_2. Based on the initial TEA and roadmap, production costs of around $2/kg appear to be achievable, but a significant reduction in panel costs coupled with a significant increase in STH efficiency will be required to meet the ultimate cost target of $1/kg H_2 without production tax credits. The team's progress to date suggests that the project is on track toward meeting the efficiency and materials durability targets to achieve the $2/kg H_2 target.
- This project aims to address the key barrier to durability of PEC.
- The project aims to advance this PEC approach from a technology readiness level of 3 to 7, with a TEA that predicts a hydrogen production cost of $1–$2/kg H_2. This is surprising because the use of stable membranes alone often leads to cost projections beyond this range, but it is unclear if a membrane is included in this design (i.e., there is disparity in the presented slides as to whether one is included), which it must be unless a PEC-specific innovation is being developed in that space as well. The presented TEA includes optimistic, but attainable, values for efficiency, lifetime, and panel cost but with no indication of being able to attain $2/kg H_2 from the tornado plot, yet the previous slide indicates $1/kg H_2 at the same panel cost, so those inconsistencies must be reconciled. As such, the innovation, relevance, or potential impact in this approach is unclear. Since the state-of-the-art demonstrations show 20.7% STH efficiency, 100 hours of stability, and 1 cm^2 device, a TEA must be presented that shows a clear path to $1/kg H_2. Then this project should hone in on milestone demonstrations to achieve that. A >25% STH efficiency does not seem to be the key lever to break the cost scaling relationship, nor is increasing the stability from 100 hours to 1,000 hours. This seems important, but it is somewhat incremental in the scope of DOE targets. Irrespective, the variability in TEA details across the PEC portfolio suggests that DOE should oversee an apples-to-apples comparison of proposed approaches and strongly up-/down-select projects based on that critical metric.

Question 5: Proposed future work

This project was rated **3.2** for effective and logical planning.

- The project team's planned future work to increase STH efficiency, diurnal stability, and device area follows logically from current work, outcomes, and the overall work plan.
- The project's focus on addressing the greatest barrier of sealing and stability of semiconductors is appropriate. The team should look to PEM water electrolysis and alkaline electrolyte membrane (AEM) water electrolysis work on optimal catalysts (e.g., IrO_2 and RuO_2 for PEMs), catalyst poisoning (primarily

on the cathode), catalyst degradation (possibly due to sealant solvents), and anode current collector and support (i.e., platinum-coated titanium for PEMs to withstand carbon corrosion, Ni or stainless steel for AEMs).

- A significant focus of the future work seems to be to reduce the iridium loading in the PEM electrolyzer to lower the cost of the electrocatalyst by investigating iridium alloys. It is unclear whether this is appropriate or if effort would be better spent on addressing technical challenges and barriers associated with the photoelectric cell. Demonstration of large-area photoanodes is critical for scaling up the device to meet the 25 cm^2 end-of-project goal. Looking at the milestones table, there appear to be a number of significant milestones coming up in months 12 through 24, such as demonstrating 1%–2% STH gain via thermal efficiency and fabrication of CAB–catalyst and halide–perovskite PVs with 200 cm^2. The reviewer expected future work to focus on achieving these milestones. The principal investigator may have stated it during the presentation, but this information was expected on the future work slides.

Project strengths:

- The team has made very good progress to date in identifying and addressing issues associated with catalyst durability and designing and developing the new PEC reactor, showing performance improvements toward meeting the Budget Period 1 go/no-go criteria. The project has good engagement and leveraging of HydroGEN expertise and capabilities. The DEIA efforts and CBP were well-defined and -executed, engaging faculty and students from an HBCU, including providing support for at least two of the students to visit NREL or LBNL. The DEIA milestones were clearly defined. The reviewer appreciated that the TEA began in the early stage of the project. The TEA identifies the major cost drivers and should help focus the research and development (R&D) efforts to address the major technical challenges that drive cost in order to meet the ultimate DOE production target.
- The team's work to progress the design and development of halide–perovskite PVs to couple in tandem with technologically advanced silicon photoabsorbers could be scalable.
- The project focuses on key limitations.

Project weaknesses:

- The project team should try to leverage partners and their available understanding about electrode structure and materials from PEM water electrolysis and AEM water electrolysis. It is unclear if the issue of using a highly constrained supply chain can be solved.
- The project has too much focus on reducing the iridium loading for the PEM electrocatalyst. The team should leverage what is being done by the PEM R&D community to reduce the iridium loading and hence cost of the electrocatalyst. It is unclear what the goal/objective of the statistics study on five devices is, since it appears that the parameters were varied on the five reported trials. Looking at the data presented, it is unclear what to make of the data and what conclusions to draw.
- The team reported insufficient TEA details to support a pathway to \$1–\$2/kg H_2, and results must be compared on equal footing with TEAs for grid-scale electrolysis.

Recommendations for additions/deletions to project scope:

- The project's proposed future work focuses on reducing the iridium loading in the electrocatalyst for the PEM electrolyzer. Significant R&D efforts are being conducted to reduce the iridium loading and hence the cost of the PEM electrocatalyst, both domestically (funded primarily by the Hydrogen and Fuel Cell Technologies Office) and internationally. The project team should take advantage of what is being done by others to reduce the cost of the PEM electrocatalyst and focus more on improving the STH efficiency and materials durability of the photoelectric cell, as well as integration of the photoelectric cell with the electrolyzer. The team listed optimizing heat transfer from the solar cells to catalysts through the protective barriers as a technical challenge, and the team should provide greater detail on the issue, why this is important, and how the project would accomplish this to achieve a 1%–2% gain in STH.
- The project team should try to leverage partners and available understanding about electrode structure and materials from PEM water electrolysis and AEM water electrolysis (including adhesives).

- For future Annual Merit Review presentations, the project team should leave enough time to present all slides, especially the most important details of the TEA, which were skipped because of insufficient time. The team should replace all acronyms on all slides with words and include details on every slide as to the materials' composition, experimental conditions, etc. used in each experiment and analysis. Without that information, a detailed peer review is impossible. The team should also collaborate with world experts in TEA to conduct a thorough analysis, and only with a legitimate pathway to \$1–2/kg H_2 that is agreed upon by PV and electrolysis experts should an effort be supported by DOE Office of Energy Efficiency and Renewable Energy.

Project #P-217: Scalable Solar Fuel Production in a Reactor Train System by Thermochemical Redox Cycling of Novel Nonstoichiometric Perovskites

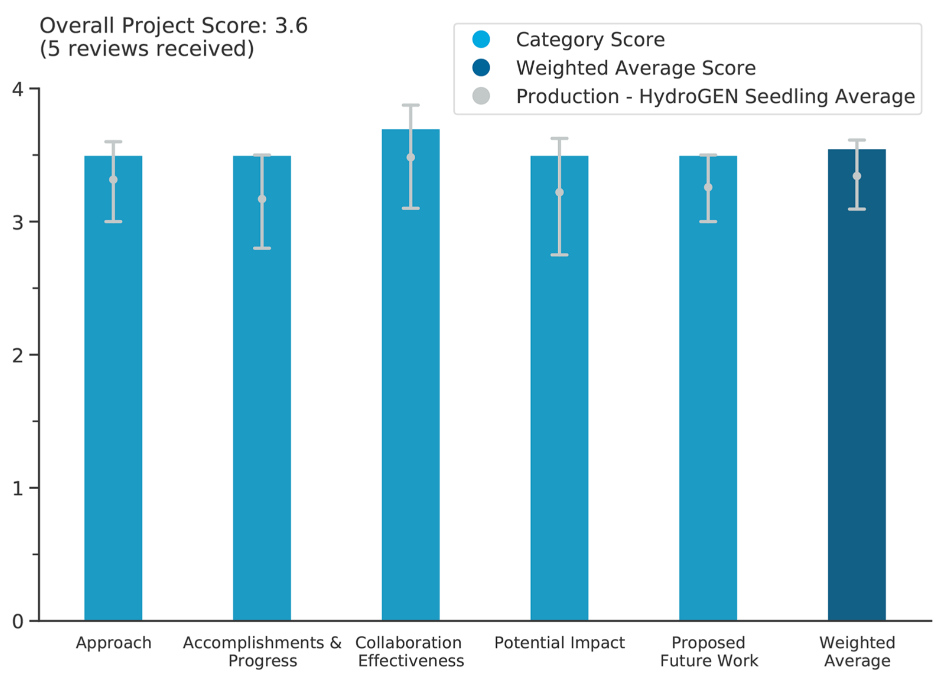
Xin Qian, Saint-Gobain

DOE Contract #	DE-EE0010739
Start and End Dates	10/1/2023–9/30/2026
Partners/Collaborators	Northwestern University, Massachusetts Institute of Technology
Barriers Addressed	• Phase stability, thermodynamic and kinetic properties: identify phase stability boundary with favorable thermodynamic and kinetics • Microstructure engineering: fabricate materials ensuring porosity and defect-free microstructure • Reactor train system (RTS) single reactor construction: design, model, and construct an RTS reactor enabling durability for on-sun testing and ≥20% efficiency • On-sun testing: integrate the RTS into a solar furnace or tower, ensuring stable solar thermochemical hydrogen operation under realistic solar radiation

Project Goal and Brief Summary

The project's focal point lies in developing a scalable reactor train system (RTS) capable of producing hydrogen fuels efficiently. Furthermore, the project will identify perovskite compositions achieving a hydrogen productivity of ≥12 mL/g for ≥20 cycles, accompanied with an RTS boasting ≥20% efficiency and demonstrating scaled hydrogen production rates ≥1 g/h. Technical innovations include modifying perovskite compositions, optimizing microstructure, and designing high-flux solar reactors. Through safety planning; diversity, equity, inclusion, and accessibility (DEIA) initiatives; and collaboration with HydroGEN nodes, the project sets out to deliver impactful advancements in solar fuels technology, bridging the gap between laboratory-scale research and commercial viability.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Production - HydroGEN Seedling projects.

Question 1: Approach to performing the work

This project was rated **3.5** for identifying barriers and addressing them through project innovation, as well as for project design and feasibility.

- This methodical sintering study allows for the selection of optimal balance of surface and bulk reactions. Combining the COMSOL model with experimental reactor design is a good approach.
- The project objectives are clear, and the team identified barriers. DEIA and community benefits plan (CBP) activities are planned.
- The approach of the project to further improve Saint-Gobain's CTM55 series of perovskite materials is sound. The starting material has a high fuel productivity and production rate, but further improvements may be possible. The stability of the phases and the microstructure are also considered. Testing this in an RTS will validate the performance in real on-sun experimentation that can highlight performance and degradation phenomena that could be missed in more controlled lab testing. The safety plan is adequate. The CBP provides an actionable level of detail to have impact.
- The project approach is based on optimizing current promising technologies (material and reactor) to meet DOE targets. The material optimization approach of changing Ti:Mn and evaluating the impact of porosity is logical, based on previous work demonstrating that the B-site cation chemistry impacts redox activity and that the reaction is surface-kinetic and gas-phase-limited. It is not clear how the sintered material will be integrated with the reactor. Details on the electrochemical thin approach are missing. The team should provide details on how the materials with different cation ratios will be evaluated for stability. For example, it is unclear whether x-ray diffraction (XRD) be used to identify secondary phase formation from cycling. It is not clear how the CBP will support DEIA principles. There are no specific milestones listed that require hiring from underrepresented groups, and there is only one mention that the team will recruit from underrepresented groups. It is unclear how the team will recruit from these groups. Details and descriptions of successes or challenges should be provided in the next Annual Merit Review.
- This is a very tightly focused project with an excellent team. This has potentially good material and a novel reactor design. Overall, this is an excellent project, but the team could do more XRD analysis (operando, if possible). The morphology characterization is good but potentially needs more than an empirical model to have true value. It is unclear if grain, grain boundary, or surface reactivity is key, but theory could help here.

Question 2: Accomplishments and progress

This project was rated **3.5** for its accomplishments and progress toward overall project and DOE goals, as well as the HydroGEN Consortium mission.

- Overall, the project team has made outstanding progress, particularly in its materials choice and approach to characterization of the overall thermochemical hydrogen (TCH) potential.
- All tasks and milestones that are currently due have been completed. The initial materials microstructure characterization looks reasonable, and the reactor design communicated seems adequate to meet the requirements of the effort.
- The project team has made good progress in modeling and microstructural engineering. Planning the reactor design at an early stage is an excellent approach.
- The project is only six months into its three-year timeline, but thus far, it is on track with meeting milestones.
- This is a new project that has not generated many results. The project appears to be on schedule.

Question 3: Collaboration effectiveness

This project was rated **3.7** for its collaboration and coordination with HydroGEN and other research entities.

- The team at Saint-Gobain is collaborating with very effective partners. The team at Northwestern University has been a leader in solar thermochemical hydrogen (STCH) materials for many years, and Heliogen, Inc., brings expertise in concentrated solar reactors, supplemented by the team at the Massachusetts Institute of Technology. The team at Sandia National Laboratories brings the on-sun testing capabilities. Overall, this project benefits from an incredibly well-suited team to solve the technical and scaling challenges the tasks require.

- The project team collaborators (including the nodes, academic partners, and industry partners) are very well-chosen for their expertise, previous successes, and capabilities.
- The project team's interaction with partners appears to be well-planned to combine the potential contributions.
- The project includes multi-level collaborations with academia and national laboratories. National laboratory nodes (TEA and surface kinetics modeling) have been used for the project.
- The core team is very good. It is not clear how the team will manage six national laboratory efforts or whether the time constant for those will affect the overall project timeline. A clear management and communication strategy is needed.

Question 4: Potential impact

This project was rated **3.5** for supporting and advancing progress toward DOE Hydrogen Program goals and the HydroGEN Consortium mission.

- The potential impacts of solar-thermal technologies have a difficult time competing with more conventional methods of generating clean hydrogen. A true advantage, however, is that solar-thermal technologies can operate using nearly entirely thermal power, with minimal electrical input. This could help reduce the costs of clean hydrogen because the cost of electricity is the primary operational expense contributor for membrane-based electrolysis technologies. The project's goal of improving the efficiency of STCH materials and reactors will further enhance the possibility that the systems can deliver cost-effective clean hydrogen at scale.
- This project is a very good test case for the ability to improve TCH performance by materials engineering and can therefore affect the whole field.
- The project has the potential to advance water-splitting technologies, both in materials development and in reactor design. The goals of the project align well with the HydroGEN mission.
- The project has good potential, if it is successfully implemented.
- The redox material of the project was developed by the principal investigator's previous work in the lab. There is no direct comparison with CeO_2 in terms of oxygen deficiency. Therefore, it is still too early to conclude the potential of this material.

Question 5: Proposed future work

This project was rated **3.5** for effective and logical planning.

- The future work activities present a strong approach in material and reactor improvements, along with validation testing.
- The plan outline is good in bringing the partners together.
- The proposed future work is logical for meeting the project objectives.
- The project proposal by the core team is excellent and well-thought-out. The national laboratory integration may need some work.
- The future activities are well-planned, but there seems to be a disconnect between Saint-Gobain and Northwestern University work. The new material that Saint-Gobain will engineer also depends on the materials characterization and recommendations from the team at Northwestern University.

Project strengths:

- The TEA evaluating the use of electrical energy as opposed to concentrating solar-thermal is valuable for determining the economic feasibility of using concentrated solar. The team members are well-chosen for their expertise, thus increasing the potential for project success. If the project is successful, the partners are well-positioned to leverage the prototype results into larger-scale demonstrations and potentially move to commercial viability.

- The project brings together an excellent team led by Saint-Gobain, which has the capabilities to scale this material up for commercial manufacture at meaningful scales from commercially obtainable feedstocks. This process starts with a material that is already high in production capacity and rates and seeks to improve it.
- One strength of the project is its multidisciplinary approach to materials selection, ceramic processing, reactor design, and testing.
- The project has a clear focus, potentially excellent materials, and control of materials properties. The team has created a novel reactor design using SiC expertise.
- The project has a strong team with diverse expertise to solve both scientific and engineering problems.
- Project weaknesses:
- Overall, this is a strong project with no glaring weaknesses.
- The only identified weaknesses are the typical high-temperature (1600°C) material needs and the ability to cool the reflectors.
- Whether the material can meet the STCH application requirements is still an unknown. The project team's use of "g/h" to express the hydrogen production rate is confusing. It is unclear that this should be dependent on redox material mass. A 1 g/h production rate for hydrogen is too aggressive. On slide 4, the time for cumulative hydrogen production should be provided. It is unclear what the relationship is between cumulative hydrogen production (mL/g) and the hydrogen production rate (g/h).
- The main weakness of the project is shared with other STCH approaches in that the conversion efficiencies are relatively low and require an inexpensive and robust solar concentration option to make them reliable and cost-effective.
- No description was provided of how reactor design modeling will be validated. Perhaps this will be an iterative approach.

Recommendations for additions/deletions to project scope:

- The plan is good.
- It would be useful to compare the cost of hydrogen generated from thermochemical redox cycling using electricity versus high-temperature and low-temperature electrolysis (which also require electrical energy input). This would provide insight into whether thermochemical redox cycling will be competitive with the more mature electrolysis technology.
- The project team should show at a bench scale that the perovskite material can stably produce O_2 and H_2 for many cycles. The team should also unify the metrics to represent the performance of the hydrogen production rate.
- The project could benefit from work with a computational group looking at the surface energy and morphology effects on high-temperature chemistry.

Project #P-218: All-Perovskite Tandem Photoelectrodes for Low-Cost Solar Hydrogen Fuel Production from Water Splitting

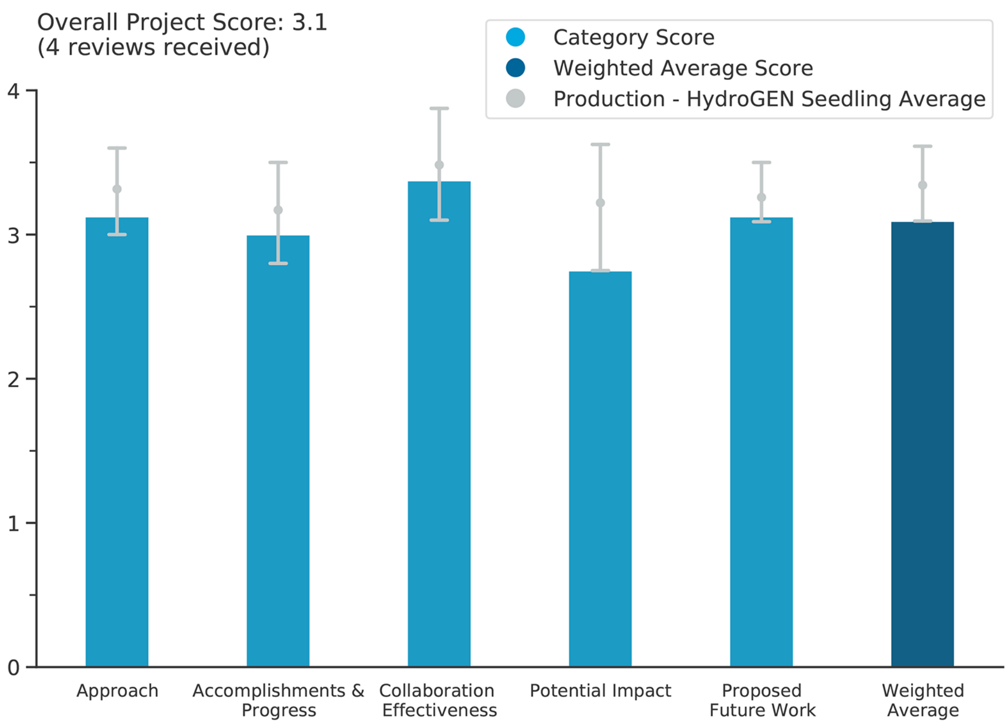
Yanfa Yan, University of Toledo

DOE Contract #	DE-EE0010740
Start and End Dates	10/1/2023–9/30/2026
Partners/Collaborators	National Renewable Energy Laboratory, Lawrence Livermore National Laboratory
Barriers Addressed	• Phase segregation in wide-bandgap perovskites • Sn^{2+} oxidation in narrow-bandgap perovskites • Scale-up of tandem device production • Photoelectrode panel assembling • On-sun photoelectrochemical testing

Project Goal and Brief Summary

The project's approach involves the design, fabrication, and testing of all-perovskite tandem photoelectrodes. Leveraging wide-bandgap (1.7–1.8 eV) and narrow-bandgap (1.2–1.5 eV) perovskites, the main objective is to optimize absorbers for efficient tandem cells, suppressing halide segregation and utilizing mixed two-dimensional/three-dimensional and all-inorganic perovskites. This project endeavors to demonstrate high efficiency and stability in all-perovskite tandem devices and pave the way for sustainable solar hydrogen production.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Production - HydroGEN Seedling projects.

Question 1: Approach to performing the work

This project was rated **3.1** for identifying barriers and addressing them through project innovation, as well as for project design and feasibility.

- The team is focusing on the design, fabrication, and testing of all-perovskite tandem photoelectrodes and panels to achieve low-cost, durable, and unassisted photoelectrochemical (PEC) water-splitting systems with high solar-to-hydrogen (STH) efficiency. This project is a continuation of the previous initiative, P-191, which began in 2019. The project has a good approach for the development of inexpensive perovskite PEC leveraging production capabilities at the University of Toledo, modeling efforts, and collaborative work with the national laboratories.
- The technical barriers have been clearly identified. Effective approaches have been proposed, which cover both wide bandgaps and narrow bandgaps, greatly increasing the efficiency. The project goal is clearly set: achieving production of hydrogen at a rate of 0.1 g/h for diurnal operation over two weeks.
- The project aims to develop a solar photoelectric cell based on integrating a wide-bandgap perovskite top adsorber with a narrow-bandgap perovskite bottom absorber with the potential to achieve STH efficiencies of >22% and meet the DOE cost target of $1/kg hydrogen. Barriers related to issues in both the wide- and narrow-bandgap materials are well-defined. Barriers associated with scaling up production and photoelectrode panel assembly are not as well-defined. The safety plan seems adequate for a project of this size and scope in terms of the amount of hydrogen to be generated/used in experimental work. The principal investigators (PIs) engaged the Hydrogen Safety Panel and incorporated its comments and recommendations into the experimental safety plan. Students will receive laboratory safety training, and the university's safety staff will conduct periodic inspections. Diversity, equity, inclusion, and accessibility (DEIA) and community benefits plan (CBP) activities have focused on hiring female graduate students, hiring two female post-docs, and ordering materials from Kurt J. Lesker Company, which is identified by the PI as a woman-owned and woman-operated company. Unfortunately, the DEIA plan does not address engaging underrepresented minority or disadvantaged groups such as Blacks or African Americans, Hispanics or Latinos, Native Americans, etc., which should be the focus of the DEIA and CBP.
- This project aims to develop all-perovskite tandem PEC photoelectrodes and panels to overcome the barriers of efficiency, long-term stability, and large-area devices. Keys to this approach are to overcome perovskite instabilities, including halide phase segregation, by reducing defect density and tin oxidation through development of alternative hole-transport layers (HTLs). While these metrics seem important, based on the information supplied, the reviewer could not adequately determine whether the scope of work would be suitable to evaluating the project's technology innovation with a convincing pathway to hydrogen production at $1–$2/kg. Irrespective of this, the safety plan seems sufficient, and sharing near-misses is a good standard practice. Reported DEIA efforts are minimal.

Question 2: Accomplishments and progress

This project was rated **3.0** for its accomplishments and progress toward overall project and DOE goals, as well as the HydroGEN Consortium mission.

- Overall, the project team has made good progress. The team has successfully demonstrated an STH efficiency exceeding 15% (Milestone 2.1) and achieved J_{SC} (short-circuit current density) = 16 mA/cm^2 for all-perovskite tandem cells (Milestone 1.1). It should be noted that commercial catalysts, Pt (hydrogen evolution reaction), and IrO_X (oxygen evolution reaction) were utilized for the water-splitting process. Additionally, the team's investigation into interface degradation in Sn-Pb perovskite has provided valuable insights, enabling the development of strategies to enhance durability.
- The project met two of the early milestones demonstrating a current density, J_{SC}, of >16 mA/cm^2 and an STH efficiency of 15%. The project appears to be on target to meet its first go/no-go decision point—an STH efficiency of 16% while retaining 90% of the initial efficiency for at least 300 hours of operation. The project states that at least five devices show the milestone target efficiency and stability and that the report was sent to DOE. Density functional theory (DFT) calculations appear to have provided some insight into the interface degradation mechanisms for the Sn-Pb perovskite subcells, finding that deprotonation from the HTL is the cause of the interface degradation. The DFT calculations also appear to have provided a rationale for selecting the HTL.

- The project reported enhanced stability in Sn-Pb perovskite subcells using a less acidic HTL, which seems like an important discovery that will affect long-term stability. Other efforts that the project predominantly focused on were reproducing prior results with a new cohort of researchers. Project progress has already been sufficient to meet the go/no-go decision point, although the replicable data were not shown directly even though they should have been.
- The milestones have been met and progress is on schedule. It is not clear why the carboxylic acid (-COOH) group is more suitable for the HTL of Sn-Pb perovskites (slide 11). There are also questions about the source of the voids and cracks, the gaseous iodine and methylamine, and the tin oxidation state.

Question 3: Collaboration effectiveness

This project was rated **3.4** for its collaboration and coordination with HydroGEN and other research entities.

- The team showed a strong collaboration with national laboratories and the HydroGEN community via characterization of the materials, theoretical modeling, and benchmark measurements of PEC performance.
- The project has good collaboration.
- The project has strong engagement and collaboration with HydroGEN Energy Materials Network (EMN) nodes; EMN collaborators include Dr. Deutsch (National Renewable Energy Laboratory [NREL]) for PEC benchmarking, Dr. Zhu (NREL) for investigating stability of wide- and narrow-bandgap perovskites, and Dr. Ogitsu (Lawrence Livermore National Laboratory [LLNL]) for providing theoretical understanding of the wide- and narrow-bandgap perovskites. The project's engagement with the HydroGEN EMN addresses several critical issues for developing this technology—in particular, evaluating the stability of wide- and narrow-bandgap perovskites and understanding them from a theoretical perspective. While these engagements address important technical issues, they also seem to require a significant amount of work on the part of the national laboratory collaborators. It is unclear what the expectation is regarding the amount of effort from the national laboratory collaborators.
- EMN node collaborators include Dr. Zhu (materials synthesis and characterization), Dr. Ogitsu (theory and modeling), and Dr. Deutsch (PEC testing and benchmarking). All seem relevant and are contributing to results. The project is missing a world expert in techno-economic analysis (TEA). The project team is working with a minority business enterprise, and the team participated in benchmarking/protocols meetings. However, the project team indicated difficulties in identifying minority-serving institutions (MSIs), which were seemingly necessary for compliance with the funding opportunity announcement. Information on MSIs is freely available from government sources.

Question 4: Potential impact

This project was rated **2.8** for supporting and advancing progress toward DOE Hydrogen Program goals and the HydroGEN Consortium mission.

- Photoelectrolysis of water to produce hydrogen is a very attractive and promising approach for green hydrogen production, which is critical for the reduction of carbon emissions. Photoelectrolysis does not require the use of expensive precious-group-metal catalysts, which makes it economically feasible. Although this technology has a low technology readiness level (TRL) and is still far away from practical application, it is critical to renewable hydrogen production, which holds a great future.
- The project demonstrates a promising approach in the application and fabrication of cost-effective materials for photovoltaic (PV) architecture; however, achieving a truly low-cost PEC system requires that the team explore substituting more economical alternatives for expensive catalysts such as Pt and IrO_X. Additionally, addressing the limited durability of perovskite-based PEC devices under acidic conditions and scaling up cell area beyond the current size (<1 cm^2) are crucial steps to advancing the project's TRL.
- The project has defined targets for increasing STH efficiency and improving the long-term stability/ durability of the proposed materials; however, without a TEA to understand the material costs, it is unclear whether these targets are sufficient to demonstrate that the proposed materials can eventually meet the ultimate DOE cost target of <$1/kg hydrogen. Currently, the PI has not provided any information/analyses to suggest that these materials could have the potential to meet the cost target. The collaborations with the HydroGEN EMN nodes to address critical technical issues leverage the expertise and resources of HydroGEN very well.

- The project aims to advance this PEC approach with a TEA that predicts a hydrogen production cost of \$1/kg by 2031. This is surprising because the use of stable membranes alone often leads to cost projections beyond this range, and so many more details of the TEA must be made clear. If devices were proposed as membrane-free, a PEC-specific innovation in that space must be presented. Perovskite PVs are not projected to attain ultra-low-cost grid-scale electricity, so it is surprising that they are projected in this project to surpass the cost of PV-driven electrolysis, even with the aim of a 1/1000th reduction in cost from III-V photoabsorbers. Without additional details, the innovation, relevance, or potential impact of this approach remains unclear. Irrespective of this, the variability in TEA details across the PEC portfolio suggests that DOE should oversee an apples-to-apples comparison of proposed approaches and strongly up-/down-select projects based on that critical metric.

Question 5: Proposed future work

This project was rated **3.1** for effective and logical planning.

- Planned future work to increase STH efficiency, stability, and device area follows logically from the current work, outcomes, and overall work plan.
- Scaling up the photoelectrode area and building panel reactors are important and reasonable activities to perform.
- The proposed future work is appropriate. Although the project is target-driven, the project may need to spend some effort on the fundamentals that determine the performance of the photoelectrolysis and should attempt a hypothesis-driven, instead of trial-and-error, approach.
- Proposed future work for Fiscal Year (FY) 2024 focuses on enhancing the stability of perovskite subcells and tandem photoelectrodes and meeting the first go/no-go milestone, which is to demonstrate >300 hours of continuous operation with an STH efficiency >16%. Few details are provided on how the project team will address the stability issues. The project appears to be on target to address the go/no-go milestone. Proposed future work for FY 2025 focuses on scaling up the tandem photoelectrode to areas >1 cm^2. It is unclear whether there will be efforts focused on addressing the stability issues and improving the STH efficiency toward >18% to meet the end-of-project goals. While these efforts may be inferred, they were not stated. If they are not pursued, there will be concern about meeting the end-of-project goals in FY 2026.

Project strengths:

- The project focuses on low-cost photoelectrochemical materials such as perovskites, which is highly beneficial for both the PV and PEC communities. The demonstration of an STH efficiency surpassing 15% over 300 hours for the proposed PEC device is a significant achievement with strong potential. Scaling up is crucial, as it not only validates the technology but also opens doors for practical implementation on a larger scale.
- The project team is strong and balanced and has good collaborations with national laboratories. The project is strengthened by good modeling-guided approaches. Proposed continuous investigation on enhancing the stability of perovskite subcells is a plus.
- This project builds upon prior work that demonstrated 18% efficient tandem photoelectrodes. The project has made good progress to date to meet all Budget Period 1 milestones and deliverables.
- This project provides an optimistic viewpoint that all-perovskite tandem designs, such as those proposed herein, may lead to a reduced cost of green hydrogen in comparison to other approaches.

Project weaknesses:

- The performance degradation mechanism needs to be investigated so that the stability of the system can be improved, guided by the fundamental understanding.
- The project currently relies on costly commercial Pt and IrO_X catalysts for water electrolysis. To pursue the cost-effectiveness of the PEC system, the team should explore alternative catalyst options. Additionally, referring to the schematic of the PEC cell presented on slides 2 and 15, the team needs to address the challenge of separating the generated hydrogen and oxygen gases, which mix in the gas phase. It is crucial for the safety of the system that the project implement efficient separation techniques.

- The presentation states that the project will impact design and fabricate all-perovskite tandem devices with comparable STH efficiency with the state-of-the-art III-V tandem photoelectrodes but at 1/1000 of the cost. The basis for the 1/1000 cost reduction is unclear. The cost it is compared to is unclear. There appears to be no effort to perform a TEA, so it is difficult to understand how the project team came to this conclusion. The presentation states "capable of meeting <$1/kg hydrogen cost" under Accomplishments, but no data or information is provided to support this statement in the presentation. While the project has end targets for STH efficiency (>18%) and durability (>80% retention of initial activity for >500 hours), the project needs to demonstrate that these targets, as well as the current density, are sufficient to show that these materials can eventually meet the DOE hydrogen production cost targets. In essence, the project needs to demonstrate what material costs, STH efficiency, durability, current density, etc. are required to meet the DOE targets. These targets may not be achievable with this funded project, but if this technology can be transferred to industry, it is important to understand what these target values are and show that work is being performed toward these targets.
- Almost zero TEA details were included to support the mentioned pathway to $1/kg hydrogen. The TEA details must be compared on equal footing with TEAs for grid-scale electrolysis. This must be reported for a DOE Office of Energy Efficiency and Renewable Energy project—and in sufficient detail for critique.

Recommendations for additions/deletions to project scope:

- The project should consider conducting a TEA to justify the stated cost reduction target. Both NREL and LLNL have extensive experience in conducting TEAs and can help. Furthermore, a TEA can help identify where research and development efforts should focus to meet cost targets. Without a TEA, it is difficult to understand how this technology will meet the DOE cost targets of <$2/kg by 2026 and <$1/kg by 2031. Project end goals are all-perovskite tandem photoelectrodes with an STH of >18% while retaining 80% initial efficiency for more than 500 hours and a demonstrated hydrogen production at a rate of 0.1 g/h for diurnal operation for two weeks. Presumably, the second goal will require a system efficiency of >18%. The project should focus on engaging a student who represents an underrepresented or disadvantaged group, either from the University of Toledo student body or from an MSI or minority business enterprise (MBE). According to information online, the University of Toledo student population consists of 8.74% Black or African American, 5.07% Hispanic or Latino, and 3.64% who identify as two or more races. There are several online sites that identify MSI/MBE institutions. Numerous U.S. government agencies (such as NASA) have websites identifying MSI/MBE institutions.
- The project team should collaborate with world experts in TEA to conduct a thorough analysis. DOE EERE should support only an effort with a legitimate pathway to $1–$2/kg hydrogen that is agreed upon by PV and electrolysis experts.
- The project needs to consider a TEA.
- A plan for investigating the degradation mechanism of perovskite subcells is encouraged. This will help to guide the project on a hypothesis-driven basis.