IEA HYDROGEN TASK 35
RENEWABLE HYDROGEN PRODUCTION

FINAL REPORT
for
INTERNATIONAL ENERGY AGENCY (IEA) HYDROGEN TECHNOLOGY COLLABORATION PROGRAMME (TCP)

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EXECUTIVE SUMMARY

The past several years have witnessed significant progress in fuel cell technology advancement and cost reduction. As a result, rollouts of fuel-cell vehicles by major automotive manufacturers are scheduled in upcoming years. With these rollouts, enabling technologies for the widespread production of affordable renewable hydrogen become increasingly important. Near-term utilization of current reforming and electrolytic processes is necessary for early hydrogen markets, but transitioning to industrial-scale renewable hydrogen production remains essential to the longer term. Central to the long-term vision are renewable hydrogen conversion processes, including, for example, the photoelectrochemical and thermochemical water splitting, as well as photo-assisted electrochemical water-splitting. The long-term viability of such hydrogen production pathways needs to be assessed using broader techno-economic analytic approaches to help identify key materials- and system-level cost drivers with the associated research and development (R&D) needs. The IEA-Hydrogen Technology Collaboration Programme (IEA-HTCP) Renewable Hydrogen Production Task 35 brought together leading world experts covering a broad spectrum of key renewable hydrogen technologies in a well-organized network to facilitate progress toward needed solutions.

The objective of the Renewable Hydrogen Task 35 was to create an international network of experts in all the renewable hydrogen pathways to leverage developments in critical technology areas with cross-cutting importance to all such pathways. To achieve this objective, Task 35 established such a network to improve communication and dissemination among the leading experts within the international community; and to establish a direct information link with the IEA-HTCP Executive Committee for conveying concise summaries of the most important and promising technical progress in all of the renewable hydrogen pathways. The Renewable Hydrogen Task 35 network has allowed cutting-edge research from around the world to be shared amongst peers, thus accelerating the development of high efficiency and low cost materials and systems for the deployment of all renewable hydrogen technologies.

The report includes technology overviews of the primary renewable water splitting pathways of electrolysis, photoelectrochemistry, and solar-thermochemistry covered in Task 35, including status and research needs in each of the technology pathways. It also includes information on some of the major international agencies that have supported early-stage applied research and development (R&D) in areas directly relevant to the pathways covered in the Task as well as cross-cutting technology issues. Detailed summaries of various research projects and initiatives, including those involving Task 35 Expert participation, are provided, along with summaries of important meetings and special projects involving Task 35 Experts in areas relevant to all the major water-splitting pathways.

An important outcome of this Task has been the reinforcement of the strength and enthusiasm of the ever-growing R&D community in the water splitting technologies key to renewable hydrogen production. Through Task 35, this R&D community has clearly articulated the critical need to maintain an open-source international network allowing for continued coordination and potential collaboration among leading technical experts across all the water splitting pathways. New opportunities to move forward in this direction are being developed. An example of a common interest already being pursued is the establishment of standardized experimental, validation and reporting protocols for the water splitting technologies, such as current activities under the U.S. Department of Energy’s HydroGEN Consortium as well as the IEA Advanced Fuel Cell Technology Collaboration Programme’s Annex 30.
**TASK DESCRIPTION**

**Motivation**

Research innovations are needed to push forward the state-of-the-art in all of the renewable hydrogen production technologies toward practical viability. The objective of the Renewable Hydrogen Task 35 was to create an international network of experts in all the renewable hydrogen pathways to leverage developments in critical technology areas (such as thermodynamics, catalysis, membranes/separations, metrics and standards, techno-economic analysis, etc.) with cross-cutting importance to all such pathways. Task 35 established such a network to improve communication and dissemination amongst the leading experts within the international community (e.g., through the organization of conference symposium and joint publications in relevant renewable hydrogen production technology areas); and to establish a direct information link with the IEA-HTCP Executive Committee for conveying concise summaries of the most important and promising technical progress in all of the renewable hydrogen pathways. The Renewable Hydrogen Task 35 network has allowed cutting-edge research from around the world to be shared amongst peers, thus accelerating the development of high efficiency and low cost materials and systems for the large scale deployment of all renewable hydrogen technologies.

This approach leverages the complementary R&D needs among the different technology options for renewable hydrogen. The overarching Task structure, comprised of Subtasks dedicated to specific renewable hydrogen pathways, relied on the skillful management of motivated Operating Agents (also serving as Subtask leaders) to provide effective networking of leading Experts in the individual technology pathways, as well as cross-cutting networking opportunities among the Experts in all the important renewable hydrogen fields. The reporting of this Task to the IEA-HTCP has provided an invaluable source of the best and most up-to-date information on the emergence of renewable hydrogen options in the international framework.

**Sub-Tasks**

The Task and Subtask structure of the Renewable Hydrogen Task is shown in Figure 1. Key emerging technologies for large-scale, renewable hydrogen production are represented in the Subtasks, initially set up as follows:

- **SUBTASK 1: Renewable Electrolysis** (Subtask Leader, Everett Anderson, USA) This Subtask was planned as a ‘shared’ Subtask with the IEA-Advanced Fuel Cells Implementing Agreement, providing further cross-cutting opportunities for leveraging synergies among related technology Experts.

- **SUBTASK 2: Photoelectrochemical Water Splitting** (Subtask Leader, Wilson Smith, The Netherlands).

- **SUBTASK 3: Solar-Thermochemical Water Splitting** (Subtask Leader, Christian Sattler, Germany). This Subtask was planned to be a ‘shared’ Subtask with the IEA SolarPACES, providing further cross-cutting opportunities for leveraging synergies among related technology Experts.

As shown in Figure 1, each Subtask is managed by a Subtask Leader (also acting as a Task Co-Operating Agent) in conjunction with an appointed Steering Committee. For each technology area, the Subtask Leader with the Steering Committee act as liaisons with world-leading Experts participating
in the major R&D hubs, centers, projects, etc. across the globe; key objectives are the organization and coordination of appropriate meetings and technical symposia at relevant international conferences, as well as collection of the key information and data from such meetings and symposia for compilation into summary reports to the IEA-HTCP Executive Committee. An additional objective of the Subtask Leaders and the Steering Committees is to identify opportunities to explore cross-cutting R&D topics (for example, in catalysis, membranes/separations, technoeconomic analysis, etc.) amongst themselves, and to coordinate relevant collaborative activities, meetings, etc. as deemed appropriate.

Figure 1: Task, Subtask & Administration Structure of Renewable Hydrogen Task

REPORT CONTENTS

This is the final report of the IEA-HTCP Task 35 on Renewable Hydrogen. The report includes technology overviews of the primary renewable water splitting pathways covered in Subtasks 1-3, including status and research needs in each of the technology pathways. It also includes information on some of the major international agencies that have/are supporting early-stage applied research and development (R&D) in areas directly relevant to the pathways covered in Subtasks 1-3 as well as cross-cutting technology issues. Detailed summaries of various research projects and initiatives, including those involving Task 35 Expert participation, are provided, along with summaries of important meetings and special projects involving Task 35 Experts in Advanced Electrolysis, Photoelectrochemistry, Solar-Thermochemistry, and cross-cutting issues relevant to all the major water-splitting pathways.
RENEWABLE HYDROGEN TECHNOLOGY OVERVIEWS

Major Pathways

This section presents technology overviews including status of different approaches as well as remaining technical challenges and research and development needs for the following pathways:

- **WATER-SPLITTING ELECTROLYSIS (INCLUDING LOW- AND HIGH-TEMPERATURE ELECTROLYSIS):**
  - Task 35 Subtask 1 Focus

- **PHOTOELECTROCHEMICAL (PEC) SOLAR WATER SPLITTING:**
  - Task 35 Subtask 2 Focus

- **SOLAR THERMOCHEMICAL HYDROGEN PRODUCTION (STCH):**
  - Task 35 Subtask 3 Focus
Water-Splitting Electrolysis

The emergence of commercially-viable electrolyzer technologies for hydrogen production represents one of the key recent enablers for H2@Scale. Electrolysis is the process of using electricity to split water into hydrogen and oxygen. This reaction takes place in a unit called an electrolyzer. Electrolyzers can range in size from small, appliance-size equipment that is well-suited for small-scale distributed hydrogen production to large-scale, central production facilities (MW scale and above) that could be tied directly to renewable or other forms of electricity production. Electricity feedstock cost is the dominant cost component (up to 75%) of the H₂ production cost via the electrolysis H₂ production pathway. Based on the sensitivity studies from the techno-economic analysis described below, this pathway starts to become cost competitive with natural gas steam methane reforming for H₂ production when the electricity cost drops below ~$0.01-$0.03/kWh. Similar to fuel cells, electrolyzers consist of an anode and a cathode separated by an electrolyte. Different electrolyzers function in slightly different ways, mainly due to the different type of electrolyte material involved.

**Polymer Electrolyte Membrane Electrolyzers**

In a (PEM) electrolyzer, the electrolyte is a solid specialty plastic material.

- Water reacts at the anode to form oxygen and positively charged hydrogen ions (protons): \( 2\text{H}_2\text{O} \rightarrow \text{O}_2 + 4\text{H}^+ + 4e^- \)

- The electrons flow through an external circuit and the hydrogen ions selectively move across the PEM to the cathode.

- At the cathode, hydrogen ions combine with electrons from the external circuit to form hydrogen gas: \( 4\text{H}^+ + 4e^- \rightarrow 2\text{H}_2 \)

![Figure 2: Electrolysis Schematic](image)

PEM electrolyzers are a commercial technology which have been used for years at scales up to 100’s of kW. Newer materials and manufacturing methods are emerging to support higher efficiency and lower cost system development. With increasing demand for electrolyzers at the MW-scale and up, the industry is currently significantly scaling up its manufacturing capacity. Commercial products in this range have recently been introduced to the market by several suppliers.

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**Alkaline Electrolyzers**

Alkaline electrolyzers operate via transport of hydroxide ions (OH⁻) through the electrolyte from the cathode to the anode with hydrogen being generated on the cathode side. Electrolyzers using a liquid alkaline solution of sodium or potassium hydroxide as the electrolyte have been commercially available for many years. Newer approaches using solid alkaline exchange membranes as the electrolyte are showing promise in research experiments at the bench scale.

**Solid Oxide Electrolyzers (High Temperature)**

Solid oxide electrolyzers (SOEC) typically use a solid ceramic material as the electrolyte that selectively conducts negatively charged oxygen ions (O²⁻) at elevated temperatures. Water at the cathode combines with electrons from the external circuit to form hydrogen gas and negatively charged oxygen ions; and the oxygen ions pass through the solid ceramic membrane and react at the anode to form oxygen gas and generate electrons for the external circuit. SOEC operates at temperatures high enough for the solid oxide membranes to function properly (~700°–800°C, compared to 70°–90°C for PEM). With the ability to effectively use heat available at these elevated temperatures (from various sources, including nuclear energy), SOEC electrolyzers can maintain high H₂ production rates with high electrical efficiencies, and with low/non-PGM catalysts. This technology is still primarily at the R&D stage, though commercial products are being planned for the near future.

**Electrolysis Cost Status**

Baseline cost projections from H2A analyses for H₂ production via PEM and SOEC electrolysis are shown in Table 1, including stakeholder-vetted results based on current electrolyzer technologies as well as future advanced electrolyzers. The untaxed cost projections, which assume economies of scale, include an average electricity pricing of ~$0.065/kWh derived from the Energy Information Administration’s (EIA) Annual Energy Outlook (AEO).

<table>
<thead>
<tr>
<th>Costs based on average electricity pricing of ~6.5¢/kWh</th>
<th>PEM Baseline ($/kg H₂)</th>
<th>SOEC Baseline ($/kg H₂)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Current Projections Technology</td>
<td>$5.12</td>
<td>$4.95</td>
</tr>
<tr>
<td>Future Technology Projections</td>
<td>$4.20</td>
<td>$3.83</td>
</tr>
</tbody>
</table>

Cost sensitivities for the baseline cases represented in Table 1 are shown in the tornado plots in Figures 3 and 4 for PEM electrolysis and high-temperature SOEC, respectively. As electrolyzer technologies continue to mature and start to achieve economies-of-scale through widespread market adoption, the cost of hydrogen produced by electrolysis starts to become cost-competitive with incumbent SMR production (<$2/kg H₂) at electricity pricing <$0.01/kWh.
**Additional Value Propositions**

Electrolytic hydrogen production may be particularly useful for load-leveling of the electricity generated from wind turbines, reducing fluctuations in capacity or augmenting capacity during periods of peak electricity demand. It may be feasible to negotiate favorable electricity rates by operating the electrolyzers during off-peak periods. Electrolyzers potentially have a secondary use for grid stabilization (e.g., by mitigating frequency disturbances). In Europe, electrolysis is being pursued as a means of grid stabilization through hydrogen storage, where, for example, excess wind energy, which would otherwise not be utilized, produces H₂ via electrolysis which is then injected into the natural gas grid as a means of storage and renewable gas production.
**Ongoing Research Needs**

Important ongoing research in electrolysis focuses on stack and system-level improvements in efficiency (to reduce electricity usage), reductions in capital costs, and exploration of alternative chemistries and operating regimes offering potential for cost reductions. For example, the platinum group metal (PGM) catalysts needed in PEM electrolysis remain a cost challenge. New catalysts and membranes (such as the alkaline exchange membranes which significantly reduce the need for PGM catalysts) are being developed to address this challenge. Advanced electrode structures and manufacturing methods leveraging PEM fuel cell technology can also reduce the need for PGM catalysts in PEM electrolysis systems, as well as reducing manufacturing costs. The high temperature operations of SOEC electrolyzers increase the stack electrical efficiency, but continued R&D is needed to enhance durability under these conditions (e.g., in the development of corrosion-resistant materials, improved seals, etc.). High pressure electrolysis (as high as 10,000 pounds per square inch gauge (psig), compared with typical electrolyzers currently generating H₂ up to 400 psig) is also being explored, particularly in support of the fuel cell electric vehicle sector where the requirement of hydrogen compression for 10,000 psig operations is a significant cost component.

Additional balance-of-plant and system integration R&D is also needed to improve the economics of water electrolysis. For example, water electrolyzers operate on DC power, and similar to batteries, are comprised of stacked cells, each requiring ~1-5-2 volt (V) power input. Depending on the stack configuration, electrolyzers can efficiently utilize up to ~1000V DC. With conventional power electronics, grid AC power can be converted to appropriate DC levels; alternatively, advanced DC-DC power electronics (based, for example on new wide bandgap semiconductor devices currently under development) offer the potential for higher efficiency through direct DC coupling between renewables and electrolyzers.

Table 2 lists critical technology needs for water electrolysis hydrogen production. Discussion of these efforts follows. Note that a single R&D activity may address more than one barrier or multiple R&D activities may be needed to address a single barrier.

**Table 2 Water Electrolysis | Critical Technology Needs and Solution Strategies**

<table>
<thead>
<tr>
<th>Barrier</th>
<th>Strategies</th>
</tr>
</thead>
<tbody>
<tr>
<td>Capital Costs</td>
<td>+ Materials with improved corrosion resistance and conductivity, and lower costs</td>
</tr>
<tr>
<td></td>
<td>+ Low PGM and PGM-free catalysts with improved durability and activity</td>
</tr>
<tr>
<td></td>
<td>+ Optimized membrane electrode assemblies and porous layer transports</td>
</tr>
<tr>
<td></td>
<td>+ Novel, integrated system architecture, including efficient thermal integration</td>
</tr>
<tr>
<td></td>
<td>+ Lower cost balance of plant components</td>
</tr>
<tr>
<td></td>
<td>+ System optimization to manage variable demands</td>
</tr>
<tr>
<td></td>
<td>+ DFMA/high-volume equipment manufacturing</td>
</tr>
<tr>
<td>Operations and Maintenance Costs</td>
<td>+ Automated process control</td>
</tr>
<tr>
<td></td>
<td>+ Improved reliability</td>
</tr>
<tr>
<td></td>
<td>+ Improved system efficiency</td>
</tr>
<tr>
<td></td>
<td>+ More efficient H₂ quality control/hydrogen drying</td>
</tr>
<tr>
<td></td>
<td>+ Efficient water conditioning</td>
</tr>
<tr>
<td></td>
<td>+ Increase capital utilization</td>
</tr>
<tr>
<td></td>
<td>+ Strategies for operation only at times of low electricity costs</td>
</tr>
</tbody>
</table>
Photoelectrochemical (PEC) Hydrogen Production

The PEC water splitting process uses semiconductor materials to convert solar energy directly to chemical energy in the form of hydrogen. The semiconductor materials used in the PEC process are similar to those used in photovoltaic solar electricity generation, but for PEC applications the semiconductor is immersed in a water-based electrolyte, where sunlight energizes the water-splitting process.

PEC reactors can be constructed in panel form (similar to photovoltaic panels) as electrode systems or as slurry-based particle systems, each approach with its own advantages and challenges. To date, panel systems have been the most widely studied, owing to the similarities with established photovoltaic panel technologies, however different possible implementations of both the panel and slurry reactor concepts are under investigation. Both approaches are still at a laboratory scale and require significant development at both the reactor and system level to achieve commercialization.

Figure 5. Two different approaches to PEC solar hydrogen production reactors: (a) electrode systems similar to flat-plate photovoltaic panels; and (b) slurries comprised of PEC semiconductor particles.

In panel reactors (illustrated in Figure 5a), the PEC water-splitting process begins with the absorption of a solar photon by the semiconductor device to form an excited electron-hole pair. The electron and hole are separated by an internal electric field, established by the semiconductor–electrolyte interface or by solid-state junctions buried within the semiconductor. The separated electron and hole are then collected at different surfaces, where they drive the hydrogen- and oxygen-evolving reactions, respectively. PEC systems can incorporate a single photon-absorbing semiconductor, or multiple absorbers in a higher-efficiency tandem device.

PEC hydrogen production may also be accomplished through the illumination of light-absorbing, semiconductor photocatalyst particles dispersed in water. Hydrogen and oxygen are evolved from separated H₂ and O₂ photocatalyst particles, as shown in Figure 5b. The overall water-splitting reaction is coupled by an intermediate ionic species “X” in solution (such as Fe³⁺), which is reduced by the O₂ photocatalyst (e.g., to Fe²⁺) and re-oxidized by the H₂ photocatalyst in a continuous closed-loop process.

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**Technical Challenges**

PEC water splitting is a promising solar-to-hydrogen pathway for hydrogen production at semi-central and central scales, offering the potential for high conversion efficiency at low operating temperatures using cost-effective thin-film and/or particle semiconductor materials. Yet much research is still necessary to improve energy conversion, material durability, material cost, large-scale implementation, and integration.

**Conversion Efficiency**

PEC semiconductor efficiency is limited by light absorption, charge separation and charge transport in the bulk, and by energetics and charge transfer at the solid–liquid interface. Further development is needed for materials systems, such as tandem configurations, with appropriate bandgap for light absorption (e.g., <2.2 eV), with band-edges aligned energetically for hydrogen and oxygen evolution, with low-loss charge separation and transport in the solid state, and with interfaces kinetically favorable for the photoelectrochemical water-splitting half reactions. Technoeconomic analysis has indicated that meeting DOE cost targets will require durable PEC semiconductor material systems that provide a STH efficiency of >25% (photo-electrode configuration) or >10% (photo-particle configurations) (as a point of reference, PEC efficiencies in excess of 30% STH are possible under ideal circumstances.) Standardized theoretical, synthesis, and characterization methods in materials discovery and screening are important tools in the basic understanding of the bulk and interface loss mechanisms that limit efficiency.

**Materials/Interface Durability**

PEC semiconductor/electrolyte junctions are prone to both dark- and light-induced degradation due to corrosion reactions that compete with water-splitting half-reactions at the interfaces. Durable materials with the appropriate characteristics for high-efficiency PEC hydrogen production are still under development. Even these more durable materials have not been tested to typical electrolyzer lifetimes. For example, the high-efficiency materials currently available are prone to corrosion, while the most durable materials studied to date have demonstrated substantially lower STH conversion efficiency. Discovery of stable and efficient materials would be an ideal solution to this barrier, but such a finding represents a significant challenge. Promising alternative approaches focus on modification of surfaces through coatings or dispersions that stabilize the interface (energetically or kinetically) and protect the bulk. The use of PEC theory, synthesis, and characterization methods can facilitate a better understanding of corrosion mechanisms for development of mitigation schemes to enhance durability.

**Materials Cost**

Cost of the PEC semiconductor material system has a direct impact on capital costs and, thus, the cost of hydrogen. High-efficiency crystalline III-V materials systems are being developed to meet efficiency and durability requirements, but the cost of these materials could be prohibitive to large-scale deployment. Solar concentrator schemes to reduce the semiconductor footprint and new synthesis technologies are possible approaches for overcoming the cost barriers to utilizing crystalline semiconductors in PEC reactors. Lower-efficiency materials systems based on lower-cost thin-film or particle semiconductors are also being developed. Improved efficiencies are needed in these material systems.

**Auxiliary Materials**

In addition to the semiconductor absorber materials, auxiliary materials for integrated PEC devices include surface treatments, interface/linking materials (including soluble, transparent redox mediators for the particle-based systems) and separators that insure safe gas separation. Techniques are needed to synthesize these integrated device configurations while maintaining each component material’s
integrity, and appropriate manufacturing techniques based on these synthesis routes will be needed to scale device configurations to commercial scales.

**Integrated Devices**
Achieving ultimate targets in PEC solar hydrogen production requires efficient and stable integrated devices combining the best available PEC semiconductors, surface treatments and auxiliary interface and separator materials. These can be planar-integrated devices for photo-electrode reactor configurations or functionalized particle devices for photocatalyst reactor configurations. Integrated device designs that combine functionalized materials optimized for light absorption, charge transport and interfacial catalysis could simultaneously address issues of durability and efficiency. Even with the best available semiconductor absorber materials with properties consistent with efficient PEC solar water splitting, integration into optimized high-efficiency devices requires specific applied and engineering R&D efforts.

**System-Level Considerations**
Determination of the most cost-effective reactor configurations will require rigorous technoeconomic analysis, taking into account materials performance and cost parameters in addition to O&M costs. Technoeconomic models to compare the cost-effectiveness of different PEC reactor approaches need to take into account the system-level costs and the performance and cost parameters of the PEC materials systems under development. Reactors and systems must be designed to account for such elements as diurnal operation, water purity, ion transport (e.g., cell resistance), and gas handling (including drying and compression); and these systems must be evaluated based on costs of commodity materials of construction and system components. In addition, the overall cost sensitivity of hydrogen must be estimated as a function of these various engineering parameters.

**Ongoing research needs**
Continued improvements in efficiency, durability, and cost are still needed for market viability. Ongoing research and development of PEC materials, devices, and systems is making important strides, benefiting from strong synergies with contemporary research efforts in photovoltaics, nanotechnologies, and computational materials. Making PEC technically viable will require long-term, fundamental and applied research efforts. The technology is not expected to meet DOE’s cost targets in the next several years; however, the potential opportunity to harvest this clean energy resource makes the risk acceptable at this time.

Table 3 lists the critical technology development needs for PEC hydrogen production. R&D activities within these categories that address the critical technology barriers to the ultimate commercialization of PEC solar hydrogen generation include the materials research underway in the U.S. Department of Energy’s HydroGEN Advanced Water Splitting Materials Consortium.

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### Table 3: Photoelectrochemical Hydrogen | Critical Technology Needs and Strategies

<table>
<thead>
<tr>
<th>Barrier</th>
<th>Strategies</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Materials and Device Challenges</strong></td>
<td>→ Development of light-absorbing semiconductor materials systems compatible with high STH efficiency devices (&gt;25% for photo-electrode configurations and &gt;10% for photo-particle systems, typically requiring material system bandgap less than 2.0 eV for absorbing a high percentage of the solar irradiance)</td>
</tr>
<tr>
<td></td>
<td>→ Develop Redox mediators for photo-particle PEC that are stable and transparent to visible light</td>
</tr>
<tr>
<td></td>
<td>→ Improved catalytic/protective surface coatings compatible with operating conditions of high-efficiency STH devices</td>
</tr>
<tr>
<td></td>
<td>→ Improved methods of fabrication that yield photo-electrode/ photocatalyst materials at target costs and target STH efficiencies</td>
</tr>
<tr>
<td><strong>Supporting Scientific and Engineering Methodologies</strong></td>
<td>→ Advanced theoretical models of PEC semiconductor bulk and interface properties</td>
</tr>
<tr>
<td></td>
<td>→ Advanced theoretical models of particle PEC that provide estimates of system efficiency as a function of particle size, bandgap, and rate of back reactions (i.e., with the redox mediator)</td>
</tr>
<tr>
<td></td>
<td>→ Comprehensive portfolio of standard and advanced characterization tools for evaluating PEC materials and interfaces</td>
</tr>
<tr>
<td></td>
<td>→ Wide portfolio of state-of-the-art techniques for synthesis of PEC materials and devices</td>
</tr>
<tr>
<td></td>
<td>→ Theory-guided screening tools for discovery and development of novel PEC materials systems</td>
</tr>
<tr>
<td></td>
<td>→ Experimental combinatorial synthesis/rapid screening tools for discovery and development of novel PEC materials systems</td>
</tr>
<tr>
<td></td>
<td>→ Standardized protocols for evaluation and reporting of PEC materials and device physical and operational parameters</td>
</tr>
<tr>
<td><strong>System-Level Technoeconomic Analysis</strong></td>
<td>→ Perform detailed technoeconomic models of photo-electrode–based PEC reactor systems, including sensitivity analysis of prime contributing factors to hydrogen production cost</td>
</tr>
<tr>
<td></td>
<td>→ Perform detailed technoeconomic models of photo-particle–based PEC reactor systems, including sensitivity analysis of prime contributing factors to hydrogen production cost</td>
</tr>
<tr>
<td></td>
<td>→ Prioritization of fundamental and applied R&amp;D needs for addressing the critical factors for reducing hydrogen production costs to meet DOE cost threshold targets</td>
</tr>
</tbody>
</table>
Solar Thermochemical Hydrogen Production (STCH)\(^5\)

Thermochemical water splitting uses high temperatures—from concentrated solar power or from the waste heat of nuclear power reactions—and chemical reactions to produce hydrogen and oxygen from water. The chemicals used in the process are reused within each cycle, creating a closed loop that consumes only water and produces hydrogen and oxygen. This is a long-term technology pathway and calls for producing hydrogen in semi-central and central facilities. Numerous solar thermochemical water-splitting cycles have been investigated for hydrogen production, each with different sets of operating conditions, engineering challenges, and hydrogen production opportunities. In fact, more than 300 water-splitting cycles are described in the literature.\(^6\) STCH offers a potential technology for clean, sustainable, high volume hydrogen production with current R&D priorities focused on materials development for both the reactive material as well as the reactor material and design.

Broadly, the STCH processes can be divided into “direct” cycles, which use only the concentrated solar thermal energy, and “hybrid” cycles, which additionally incorporate an electricity-driven electrolysis step as part of the water-splitting cycle. Typically, the direct thermal cycles offer lower complexity but require higher operating temperatures. With the energy added to the electrolysis step in hybrid cycles (typically less energy-consumptive than direct water-splitting electrolysis), these cycles can operate at relatively lower temperatures, offering practical advantages for reactor design and durability. Disadvantages of the hybrid systems include added complexity and extra requirement for electric input (which perhaps could be generated on site using waste heat from the STCH reactor). Examples of direct thermal and hybrid STCH cycles are, respectively, the simple two-step cerium oxide thermal cycle and the hybrid copper chloride cycles, as shown in Figure .

![Diagram of cerium oxide and copper chloride cycles](image_url)

**Figure 6** Examples of Solar Thermochemical Cycles for Hydrogen Production.


The high temperatures necessary to split water via the “direct” STCH processes require the use of concentrated solar power. One approach is the deployment of a central STCH reactor in a solar receiver tower surrounded by heliostat fields (fields of sun-tracking mirrors) of a suitable size. Another approach is the use of multiple smaller-scale STCH reactor modules, each coupled to a tracking dish concentrator. Both approaches are illustrated in 7. Each approach has unique advantages and disadvantages; however, both can incur significant capital expense because of the solar resource’s diffuse nature, requiring large areas and infrastructure for efficient collection and concentration.

![Diagram of solar receiver and STCH reactor with heliostats](image1)

![Diagram of parabolic dish concentrator](image2)

**Figure 7** Two mirror-based approaches for focusing sunlight on a thermochemical reactor to produce temperatures up to 2000°C are illustrated: (a) a field of heliostat mirrors concentrates sunlight onto a central reactor tower; and (b) dish mirrors focus sunlight.

Independent of the solar concentration approach, STCH cycles face obstacles that include high-temperature operations, highly corrosive chemicals, difficult separations of chemicals during sequential cycle steps, multiple reaction steps necessary to close the cycle, or side reactions with stable products that poison the process upon recycling. Many of these barriers can be overcome, but generally at the expense of energy efficiency, consumption of feedstocks other than water (e.g., electricity in the hybrid cycles), and possibly extremely high temperatures to drive reactions to completion. All of these measures add cost to the product, inhibit acceptable production rates, or prevent the realization of plant designs with acceptable lifetimes.

With solar radiation as the driving energy source, overcoming these barriers is made even more difficult, primarily because of the source’s transient nature and relatively low power density. The low power density characteristic of solar power requires large collector areas and efficient concentrators to drive energy-intensive processes such as water splitting. Additionally, reactors must endure daily cycling from low to high temperatures resulting from the sun’s day/night cycles, as well as weather effects. One option is decreasing reactor cycling by storing the thermal energy in salts or other materials to enable continuous production. A combination of thermal storage and/or backup power might be needed to ensure continuous operation.
STCH reactor systems have the potential to achieve high theoretical STH efficiencies.\textsuperscript{7, 8} Based on boundary level technoeconomic analyses, STH efficiencies >25\% would be needed in order to ultimately reach the hydrogen cost goal. However, bench-scale demonstrations of full-cycle STCH solar hydrogen production to date have been limited to <5\% STH owing to materials, receiver and reactor losses.\textsuperscript{9}

Making STCH technically viable will require long-term, fundamental and applied research efforts. The technology is not expected to meet DOE’s cost targets in the next 10 years; however, the potential opportunity to harvest this clean energy resource makes the risk acceptable at this time.

**Technical Challenges**

DOE’s research activities are being driven by specific barriers identified in the MYRD&D\textsuperscript{10}, as well as others identified by the U.S. DRIVE Partnership’s HPTT.

**Thermochemical Cycle Selection**

The literature has over 300 thermochemical cycle candidates, and new cycles continue to emerge. The most promising cycles need to be identified for further development. The complete set of criteria for selection, described in recent publications,\textsuperscript{11} include thermal efficiency, operation temperature (lower temperatures are desired), minimal numbers of steps, and low raw materials costs, among others. In order achieve the DOE MYRD targets, the projected thermal-to-chemical efficiency will need to exceed 35\%, and the complete solar-to-hydrogen efficiency will need to exceed 25\%.

**Materials Development**

The solar thermochemical cycles require high reaction temperatures, sometimes in excess of 1500°C for the high-temperature reaction step. Many of the materials for the reactants, reactor, seals, catalysts, and supports do not possess adequate thermal, physical, or chemical stability at these temperatures and rapid temperature transients. Thermal compatibility in reactor components, seals, etc., can also be problematic considering the wide temperature swings entailed by STCH. Reactant materials need to be developed not only with sufficient thermal and chemical stability but also with optimized heat exchange and surface kinetics for efficient thermal-to-chemical conversion efficiency.

Materials must endure extreme heat and corrosive and reactive environments, posing major challenges for development of durable, inexpensive materials for reactants, reactor, receiver, and any included thermal/chemical storage. Moreover, these materials would have to be easy to manufacture and capable of enduring extreme thermal shock. Some of the chemical cycles may require catalysts and/or supports, which will also need to endure aggressive environments. The materials will need to endure daily cycles and severe thermal temperature cycling. Ceramics that can endure high temperatures have issues with the cycling and with seals. Metals, such as Hastelloy steel, have better cycle life and fewer seal issues but have a lower usable temperature.

Hybrid STCH cycles also require materials R&D for major components of the electrolysis step. These materials include membranes, catalysts and support structures. Important materials parameters require optimization to achieve low-voltage–high-efficiency operations as well as long operational lifetimes with minimum contamination and/or cross-over degradation and materials durability.

**Chemical Reactor Development**
At the hydrogen production scales of interest, STCH chemical plants are expected to be capital-intensive. STCH chemical reactor designs need to be efficient and inexpensive and entail minimal BOP to meet the DOE cost targets. High-temperature operation necessitates extreme thermal management to achieve high efficiencies. Thermal losses result from inefficient process flow and a lack of integration among unit operations. Heat recuperation is vital to attaining the conversion efficiencies required to meet hydrogen production cost goals.

Other barriers to reactor development and capital costs include cycle phase separation and purification, including the extraction of sufficiently pure hydrogen product. Ideally, the product stream will be composed of only hydrogen and water. However, there may be small amounts of other contaminants similar to those in hydrogen produced via water electrolysis. In hybrid cycles, efficiency of the electrolysis step needs to be optimized in terms of low voltage, high efficiency, long lifetime and efficient reactant/product management to reduce overall system losses.

**Solar Receiver Development**
STCH reactors can be broadly classified as directly heated by the sun or indirectly heated (e.g., a thermal transfer medium absorbs the thermal energy and transfers the energy to the reactor). The solar receiver is the focal point of the solar concentrator (e.g., heliostat field or dish concentrators) and directs the thermal power to the reactor and/or thermal storage. Efficient heat transfer at the interface with the heliostat remains a barrier as the cycles move toward commercialization. The interface with the chemical reactor is an important consideration in selecting a solar receiver. For directly heated reactors (e.g., rotating disk, fluid wall, and centrifugal), the receiver and reactor are integrated, enabling solar flux to heat the reactor. Ideally, the solar thermal input rate would match the heat of reaction at constant temperature. However, the chemistry and dynamics of each system establish the equilibrium temperature required.

The solid particle and volumetric receivers are heated indirectly by the sun. For these reactors, the heat is absorbed by solid particles (e.g., sand) or molten salts, which then heat the reactors. Heat addition is, therefore, not isothermal. In addition, the amount of energy transferred to the thermochemical reaction from the intermediate heat transfer media depends on the range of temperature absorbed by the chemical reaction. The non-isothermal nature of these receivers may be suitable for cycles with steps requiring different temperatures. In addition to interfacing with the receiver, the reactor must also interface with thermal storage, if used.

**Ongoing Research Needs**
Table lists critical technology needs for STCH. R&D activities within these categories address the critical technology barriers associated with the ultimate commercialization and successful development of the STCH production pathway.
### Table 4: Solar Thermochemical Hydrogen | Critical Technology Needs in Promising Cycles.

| Reactant Materials Challenges | → Engineer known chemical cycle materials to optimize heat transfer, kinetics and durability; and to minimize cost  
| | → Discover and develop new materials/materials classes, guided by theory and experimentation, with the potential for high efficiency, long cycle lifetime and low cost  
| | → Validate cycle efficiency and cycle life associated with all cycle reactant materials/phases  
| Innovative Thermochemical Reactor Designs | → Develop receiver materials and designs to minimize re-radiation losses and optimize lifetime  
| | → Develop receiver/reactor interface materials and designs for maximum thermal coupling, minimum loss and long lifetime  
| | → Develop thermal management and heat recuperation in receiver/reactor designs  
| | → Develop system to manage cycle reactants and products, including phase separations and purification  
| | → Develop system to manage variable demand and solar power, including thermal/chemical storage and required interfaces  
| Improved Electrolysis (Hybrid Cycles) | → Improved membrane materials with optimal conductivity, minimal chemical cross-over, and high durability  
| | → Improved end plate and catalyst materials  
| | → Optimize electrolyzer for low voltage, high efficiency and long lifetime  
| Need for Practical Storage | → Develop thermal storage materials/strategies  
| | → Develop chemical storage materials/strategies  
| High Solar Concentrator Costs | → Reduce heliostat system cost (leveraging CSP R&D)  
| | → Reduce dish concentrator systems (leveraging CSP R&D)  
| BOP and O&M Costs | → All system components must be considered in reducing BOP and O&M costs, including feed pre-conditioning, solar concentrators, solar receivers, reactor, hydrogen purification, controls, utilities, QA/QC (e.g., sensors), compression, storage, and safety  
| Technoeconomic Analysis | → Develop detailed technoeconomic models of prospective STCH reactors (including concentrator/receiver/reactor capital and O&M projected costs) to guide R&D efforts toward meeting H2 cost threshold goals |
INTERNATIONAL RESEARCH INITIATIVES

Overview

Task 35 researchers have been supported under a number of different international research programs and initiatives. This section provides information on the scope and objectives of a few examples of these programs organized by the regions below. These are by no means the only research programs and efforts involved in high-impact R&D for renewable hydrogen production, but represent important examples with significant Task 35 participation.

- **EUROPEAN REGION**
  - The Fuel Cell and Hydrogen Joint Undertaking
  - The Hydrogen Europe Research Association

- **ASIAN REGION**
  - International Institute for Carbon-Neutral Energy Research (I2CNER)
  - The Korean Center for Artificial Photosynthesis (KCAP)

- **NORTH AMERICAN REGION**
  - The Joint Center for Artificial Photosynthesis (JCAP)
  - The HydroGEN Consortium on Advanced Water Splitting Materials
European Initiatives and Opportunities

Fuel Cells and Hydrogen Joint Undertaking (FCHJU)\textsuperscript{12}

The FCHJU is a public-private partnership with three members: the European Union, represented by the European Commission, the Industry Grouping "Hydrogen Europe" and the Research Grouping "Hydrogen Europe Research". The Joint Undertaking is the legal entity, in which the partners come together to support R&D activities in hydrogen and fuel cell technologies.

Mission and Overview

The main objectives of the FCHJU are to support research and development to reduce cost and production and increase efficiency and durability of fuel cells, increase energy efficiency of hydrogen production, demonstrate large scale used and feasibility of hydrogen, reduce use of EU defined “critical raw materials” such as rare earth elements. As part of these objectives, the FCHJU has developed a vision for the near-term future: "To develop by 2020 to the point of market readiness a portfolio of clean, efficient and affordable solutions that fully demonstrate the potential of \textit{H}_2 as an energy carrier and fuel cell as energy converter, as part of an energy system that integrates sustainable solutions and energy supplies with low carbon stationary and transport technologies." Additional information on the FCHJU vision and objectives can be found at: \url{http://www.fch.europa.eu/page/vision-objectives}.

Examples of FCHJU research and development projects relevant to renewable hydrogen production are shown in the following section. For a more comprehensive list of research activities supported by the FCHJU since its inception, explore the project site at: \url{http://www.fch.europa.eu/fchju-projects}. Task 35 researchers have coordinated closely with such research efforts being supported under the FCHJU.

Example FCHJU Projects Relevant to Renewable Hydrogen Production\textsuperscript{13}

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<tr>
<th>ADEL</th>
<th>256755</th>
<th>ADVanced Electrolyser for Hydrogen Production with Renewable Energy Sources</th>
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<td>ARTIPHYCTION</td>
<td>303435</td>
<td>Fully artificial photo–electrochemical device for low temperature hydrogen production</td>
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<td>BIG HIT</td>
<td>700092</td>
<td>Building Innovative Green Hydrogen systems in an Isolated Territory: a pilot for Europe</td>
<td>2015</td>
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\textsuperscript{12} \url{http://www.fch.europa.eu/page/governance}

\textsuperscript{13} \url{http://www.fch.europa.eu/fchju-projects}
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<th>Project</th>
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<th>Description</th>
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<td>BIOROBURplus</td>
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<td>Advanced direct biogas fuel processor for robust and cost-effective decentralised hydrogen production</td>
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<td>BOR4STORE</td>
<td>303428</td>
<td>Fast, reliable and cost effective boron hydride based high capacity solid state hydrogen storage materials</td>
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<td>CERTIFHY</td>
<td>633107</td>
<td>Developing a European Framework for the generation of guarantees of origin for green hydrogen</td>
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<td>CHIC</td>
<td>256848</td>
<td>Clean Hydrogen In European Cities</td>
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<td>Don Quichote</td>
<td>303411</td>
<td>Demonstration of new qualitative innovative concept of hydrogen out of wind turbine electricity</td>
<td>2011</td>
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<td>FLHYSAFE</td>
<td>779576</td>
<td>Fuel cell hydrogen system for aircraft emergency operation</td>
<td>2017</td>
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<td>GAMER</td>
<td>779486</td>
<td>Game changer in high temperature steam electrolyser with novel tubular cells and stacks geometry for pressurized hydrogen production</td>
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<td>GRASSHOPPER</td>
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<td>Grid assisting modular hydrogen PEM power plant</td>
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<td>GrInHy</td>
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<td>Green Industrial Hydrogen via Reversible High-Temperature Electrolysis</td>
<td>2015</td>
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<td>Haeolus</td>
<td>779469</td>
<td>Hydrogen–aerobic energy with optimised electrolyser upstream of substation</td>
<td>2017</td>
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<td>HPEM2GAS</td>
<td>700008</td>
<td>High Performance PEM Electrolyzer for Cost–effective Grid Balancing Applications</td>
<td>2015</td>
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<td>Hy2Seps-2</td>
<td>278538</td>
<td>Hybrid Membrane – Pressure Swing Adsorption (PSA)</td>
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<td>HY4ALL</td>
<td>671457</td>
<td>Hydrogen Purification Systems</td>
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<td>HYDROSOL-3D</td>
<td>245224</td>
<td>SCALE UP OF THERMOCHEMICAL HYDROGEN PRODUCTION IN A SOLAR MONOLITHIC REACTOR: A 3RD GENERATION DESIGN STUDY</td>
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<td>HYDROSOL-PLANT</td>
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<td>Thermochemical HYDROgen production in SOLar monolithic reactor: construction and operation of a 750kWth PLANT</td>
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<td>HYGUIDE</td>
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<td>GUIDANCE DOCUMENT FOR PERFORMING LCAs ON HYDROGEN AND FUEL CELL TECHNOLOGIES</td>
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<td>Hyprofessionals</td>
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<td>Development of educational programmes and training initiatives related to hydrogen technologies and fuel cells in Europe</td>
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<td>Project</td>
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<td>HyTIME</td>
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<td>KNOWHY</td>
<td>621222</td>
<td>Improving the Knowledge in Hydrogen and Fuel Cell Technology for Technicians and Workers</td>
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<td>NEMESIS2+</td>
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<td>New Method for Superior Integrated Hydrogen Generation System 2+</td>
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<td>245262</td>
<td>Next-Generation PEM Electrolyser for Sustainable Hydrogen Production</td>
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<td>PECDEMO</td>
<td>621252</td>
<td>Photoelectrochemical Demonstrator Device for Solar Hydrogen Generation</td>
<td>2013</td>
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<td>PECSYS</td>
<td>735218</td>
<td>Technology demonstration of large-scale photo-electrochemical system for solar hydrogen production</td>
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<td>REMOTE</td>
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<td>Remote area Energy supply with Multiple Options for integrated hydrogen-based Technologies</td>
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<td>RESElyser</td>
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<td>Hydrogen from RES: pressurised alkaline electrolyser with high efficiency and wide operating range</td>
<td>2010</td>
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<td>SHEL</td>
<td>256837</td>
<td>Sustainable Hydrogen Evaluation in Logistics</td>
<td>2009</td>
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</tbody>
</table>

**Project Example**

In 2015, FCHJU-supported work published a *Study on Hydrogen From Renewable Resources in the EU.* In this report, “FCH JU has been supporting research and development of electrolyser technology and application projects, aiming to increase the energy efficiency of electrolytic hydrogen production from renewable sources and to reduce costs. This study complements these activities by focusing on renewable hydrogen generation other than electrolysis. In this report, these alternative hydrogen generation technologies are described, characterized by their technical capabilities, maturity, and economic performance, and assessed for their future potential.” Interestingly, eleven proposed pathways use solar thermal energy, sunlight or biomass as major energy input. Details of additional FCHJU projects are included below.

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FCHJU: PEC Demonstrator Device for Solar Hydrogen Generation

The main goal of PhotoElectroChemical DEMOnstrator (PECDEMO)\(^\text{15}\), a collaborative project coordinated by the Helmholtz-Zentrum Berlin (HZB) Institute for Solar Fuels that is co-funded by FCH JU, was to develop a photoelectrochemical water splitting device based on low-cost and abundant materials that shows a solar-to-hydrogen (STH) efficiency of 10\%, a stability of 1000 hours, and an active area of at least 50 cm\(^2\). PECDEMO has addressed these challenges by focusing its efforts on three metal oxide photoelectrode materials (Fe\(_2\)O\(_3\), BiVO\(_4\), and Cu\(_2\)O) and by combining them with a silicon- or perovskite-based photovoltaic (PV) cell in a tandem configuration. PECDEMO targets have been individually achieved, but meeting them simultaneously with a single system remains a major challenge to be addressed.

To achieve the project goals, five science and technology objectives\(^\text{16}\) were defined:

1. Demonstrate a chemically stable and highly efficient stand-alone hybrid water splitting cell based on a metal oxide photoelectrode in tandem with a photovoltaic solar cell
2. Develop deposition technologies that are suited for fabricating components for large-area hybrid PEC-PV devices
3. Design, construct, and test complete large-area hybrid PEC-PV devices for water splitting
4. Carry out extensive techno-economic and life-cycle analyses based on the devices’ demonstrated performance characteristics, and evaluate the potential for large-scale commercialization
5. Build a prototype module consisting of an array of large area devices and to test this prototype in the field

The first work package focuses on the development of an efficient and chemically stable small-area hybrid PEC-PV water splitting device, by utilizing metal oxides as the PEC materials. Three metal oxides were chosen: Fe\(_2\)O\(_3\), BiVO\(_4\), and Cu\(_2\)O. Activities in the last three years include the development of:

- (1) small-area metal oxide photoelectrodes
- (2) optically-transparent counter electrodes
- (3) PEC-PV without photon management (1st generation device)
- (4) effective light management strategies
- (5) PEC-PV including photon management (2nd generation)

**Fe\(_2\)O\(_3\)** Photoanode

To avoid problems of Ag oxidation during high-temp deposition of hematite, the films were prepared by reverse deposition (heteroepitaxial). Optimizing the heteroepitaxial films for photoelectrochemical performance is still ongoing, and have achieved photocurrents of 1.8 mA/cm\(^2\). Noteworthy, the flat-band potential of heteroepitaxial Ti-doped hematite films was found to be ~0.2 VRHE, considerably lower than reported values for polycrystalline hematite photoanodes that typical range between 0.4 and 0.6 VRHE. Fe\(_2\)O\(_3\) photoanode is known to be highly stable, and stability data of up to 1000 hours, achieving our deliverable 1.4 target (less than 10\% performance decrease after 100 hours of operation). No noticeable degradation was observed.

\(^{15}\) [pecdemo.epfl.ch/home](https://pecdemo.epfl.ch/home)

\(^{16}\) [pecdemo.epfl.ch/page-113311-en.html](https://pecdemo.epfl.ch/page-113311-en.html)
**BiVO₄ Photoanode**

BiVO₄ deposition techniques were explored with an anneal BiVO₄ in a mild hydrogen atmosphere (2.4% H₂ in Ar) at relatively low temperature of 300 °C. The onset potential and plateau photocurrent were both improved by hydrogen treatment. An AM1.5 photocurrent of 4 mA/cm² was achieved at 1.23 V vs RHE for a hydrogen treated W-doped BiVO₄. A dual photoelectrode approach was implemented, where an additional BiVO₄ photoelectrode was placed behind the same BiVO₄. This resulted in further photocurrent improvement to 4.8 mA/cm² at 1.23 V vs RHE and > 5.4 mA/cm² at 1.7 V vs RHE. This satisfied the deliverable 1.1 20% photocurrent improvement (i.e., from 4 to 4.8 mA/cm²). BiVO₄ photoanode displayed a photocurrent decrease within the 100-hour measurement period however, decrease is due to bubbles in the device.

**Cu₂O Photocathode**

Focused on developing a transparent Cu₂O photocathode toward the ultimate goal of designing an efficient PEC-PV stacked tandem configuration. Remarkably, photocurrent densities up to 8 mA/cm² at 0 V vs RHE were reached in pH 5 electrolyte under 1 sun condition, with photocurrents exceeding 10 mA/cm² at more negative potentials. Cu₂O photocathodes’ stability is shown to be enhanced with the protection layer strategy. Although 10% performance decrease is observed within ~55-60 hours, the improvement in stability is unprecedented for Cu₂O photocathodes.

For the PV, perovskite solar cell shows increasing efficiency within the first 500 hours of measurement, without noticeable change of efficiency afterwards, up to more than 2000 hours of operation. HIT silicon solar cell shows stable short-circuit current and open-circuit potential within 100 hours, and a slight decrease of fill factor is observed.

**PEC-PV Devices**

Fabricated a solar water splitting device consisting of the dual BiVO₄ photoelectrode and a device combining a BiVO₄ and a Fe₂O₃ photoanode (Figure 8). As a result, STH efficiency of 9.2%, which fulfils the deliverable 1.2 target, was obtained.

![Figure 8: Schematic illustration of a dual (a) BiVO₄-BiVO₄ and (b) BiVO₄-Fe₂O₃ photoelectrode used in tandem configuration with a silicon solar cell. STH efficiencies of 7.5% and 9.2% have been achieved with these configurations, respectively.](image-url)
The second work package aims to guide the optimization efforts of PEC-PV tandem cells by identifying material degradation processes and efficiency losses. In order to identify the root cause for Cu$_2$O and BiVO$_4$ photoelectrode degradation, different techniques were used such as: electrochemical measurements, SEM, TEM, XPS and more.

**Modeling the optical and electrical coupling of the PEC and PV cells in PEC-PV tandem cells**

**Large-scale Cu$_2$O photocathode**

Large-area, transparent photocathode consisting of electrodeposited Cu$_2$O thin film atomic-layer deposited AZO/TiO$_2$ over-layers and photo-deposited RuO$_x$ catalysts were deposited on up to 5 x 10 cm$^2$ area. A photocurrent density of 3.7 mA/cm$^2$ at 0V vs RHE, corresponding to a STH efficiency of 4.6\% using Cu grids and Ag contacts in pH 5 electrolyte under 1 sun Illumination was obtained.

**Large-scale W:BiVO$_4$ Photo-anodes**

Large-scale photo-anodes consisting of TEC 15$^{\text{TM}}$ FTO substrate with a electrodeposited Ni grid, a spray pyrolysis deposited thick 1\% Tungsten doped BiVO$_4$ (W:BiVO$_4$) absorber (~ 200 nm), and photo-deposited CoP$_2$ catalyst were fabricated on up to 7 x 12 cm$^2$ area, with an active area of 5 x 10 cm$^2$. A photocurrent density of of 1.5 mA/cm$^2$ at 1.23 V vs RHE corresponding to a STH efficiency of 1.85\%, with Cu contacts in a pH 7, 2.0 M KPi electrolyte, with a 3 electrode setup, under 1 sun illumination.

**Final Design**

![Image of PEC cell prototype](image)

**Figure 9:** Single PEC cell identical to the 4 units of the sub-module prototype used in the field tests. 1 – Photoelectrode (back window); 2 – Stainless steel frame with an in-built screw for electrical contact; 3 – platinized-Ti meshes (CE) fixed against the ionic exchange membrane; 4 – Screws for electrical contact with the CE; 5 – Electrolyte inlets; 6 – Electrolyte outlets.

A demonstration module comprising four identical PEC cells of 50 cm$^2$, tandem PEC/PV arrangement was tested. The experiments under concentrated sunlight were conducted employing DLR’s test facility SoCRatus in Cologne$^{17}$. 

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IEA-HTCP Task 35 Final Report
17 https://pecdemo.epfl.ch/page-113308-en.html
-With hematite a total experimental time of about 15 h was reached, thereof more than 8.5 h without additional bias and close to 6.5 h with 325 mV additional bias. A total irradiance of 12.4 kW/m² on average and of 14.0 kW/m² in peak time was applied. Current densities of about 0.2 mA/cm² and 0.5 mA/cm² as well as maximum hydrogen flows of 924 μmol/h and 2.078 μmol/h were achieved without and with the additional bias respectively. The daily STH was 0.059% based on the higher heating value of hydrogen reached with additional bias.

- With BiVO₄ photoelectrodes covered about 48 h. An applied total irradiance of 7.85 kW/m² on average and of 16.5 kW/m² in peak time was estimated. The mean current density was calculated to 0.87 mA/cm² while a maximum value of 1.88 mA/cm² was obtained on Day 2 at about 13 kW/m². Hydrogen was produced at rates up to 6,741 μmol/h. The daily STH reached 0.42% on Day 5.

To assess the stability of the optimized hybrid PEC-PV device under non-concentrated sunlight an experimental setup was assembled at UPorto applying the Sulphur plasma lamp system AS 1300 V 2.0 (Plasma International GmbH) which provides 1,000 W/m².

i) with bare hematite photoelectrodes. At the initial instant a photocurrent density of 0.62 mA/cm² was produced by the hematite photoelectrode at 1.6 V in a 2-electrode configuration. Accordingly, to supply the hematite photoelectrode with the necessary bias potential of ca. 1.6 V, two 50 cm² PV modules were connected in series and an Autolab potentiostat was used for continuous monitoring the photocurrent produced by the semiconductor over 1,000 h

ii) with BiVO₄ photoelectrodes. A constant electrolyte feeding of ca. 200 ml min⁻¹ was promoted. During a 24h period an average photocurrent density of 0.41 mA/cm² was recorded at 1.28 V, corresponding to a STH efficiency of 0.61%. Over this time the BiVO₄ continuously decreased with a current density loss rate of 2 nA cm⁻² s⁻¹.

**Design of process, pilot plant and infrastructure**

Three hydrogen production and application scenarios were considered. Using H2A Hydrogen Production model levelized costs of hydrogen production were estimated using 1 m² PEC-PV cells.

- single home application (SHA, 1 kg/d @ 6 bar), 9 €/kg (10.21 $/kg)
- hydrogen refuelling station (HRS, 400 kg/d @ 810 bar), 19-23 €/kg (21.55-26.09 $/kg)
- industrial process (IP, 4,000 kg/d @ 20 bar). 16-20 €/kg (18.15 – 22.69 $/kg)

Comparison of H₂ production costs showed that the hydrogen production costs for all three considered scenarios (9-23 €/kg H₂) are higher than estimated costs for steam reforming of methane (0.8-3.0 €/kg H₂), coal (0.9-2.1 €/kg H₂) and biomass gasification (1.0-4.3 €/kg H₂), as well as wind electrolysis (4.2-6.4 €/kg H₂). In the case of PV electrolysis, which shows most similarity to PEC-PV water splitting since it uses the same feedstocks, a rather broad range of 5.3-22.4 €/kg H₂ of costs has been estimated.
FCHJU: HYDROSOL Project\(^\text{18}\)

On 28 November 2017, the German Aerospace Center (Deutsches Zentrum für Luft- und Raumfahrt; DLR), together with international project partners, presented what is currently the largest solar-chemical installation for the production of hydrogen. In the HYDROSOL Plant project\(^\text{19}\), scientists and companies have jointly further developed the process of direct hydrogen production using solar radiation. By redeveloping both the materials used and the structure of the reactor, the facility can now provide a power of 750 kilowatts. This is a significant improvement over the previous development stage of this facility, which had a power output of approximately 100 kilowatts. At Plataforma Solar de Almería (PSA) of the Spanish research centre CIEMAT (Centro de Investigaciones Energéticas Medioambientales y Tecnológicas), scientists will in the coming months produce hydrogen in test operations and demonstrations in southern Spain, and investigate the suitability of materials.

![Image of HYDROSOL Plant](image_url)

**Figure 10:** HYDROSOL Plant: Hydrogen from sunlight, showing heliostats, tower and innovative solar receiver design.

*Hydrogen – an important energy source for the power and transport sector*

Hydrogen has the potential to increase the proportion of renewable energies used, particularly in the transport and heating sectors. This energy source can, for example, be used directly in vehicles with fuel-cell drives. In addition, it is a component in the production of synthetic fuels such as methane, methanol, petrol and kerosene. Hydrogen generated using renewable energies can thus significantly reduce carbon dioxide emissions in the transport and heating sectors. Karsten Lemmer, DLR Executive Board Member responsible for Energy and Transport emphasised: “In the transport sector, hydrogen drives can make a significant contribution towards climate protection. The HYDROSOL Plant research project is thus a significant step on the road to efficient production of hydrogen using solar energy.”

This international project, coordinated by the Greek Aerosol and Particle Technology Laboratory (CERTH-CPERI-APTL), is a collaboration between DLR, the Spanish Centro de Investigaciones Energéticas Medioambientales y Tecnológicas (CIEMAT), the Dutch company HyGear and the Greek energy supply company Hellenic Petroleum. The DLR Institute of Solar Research is predominantly responsible for the development of the solar reactor, the layout of the facility and the measuring and control technology. The project is funded by the European Technology Initiative on Fuel Cells and Hydrogen Joint Undertaking (Fuel Cells and Hydrogen Joint Undertaking, FCH JU).

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\(^\text{19}\) Additional information on HYDROSOL can be found at [https://www.fch.europa.eu/sites/default/files/S3_PS_Pres6_LORENTZOU_HYDROSO-PLANT%20%28ID%202909496%29%20%28ID%202910364%29.pdf](https://www.fch.europa.eu/sites/default/files/S3_PS_Pres6_LORENTZOU_HYDROSO-PLANT%20%28ID%202909496%29%20%28ID%202910364%29.pdf) and [https://join.ises.org/sites/default/files/webinars/2015_04_17%20ISES%20Webinar%20HYDROSOL%20Experiences.pdf](https://join.ises.org/sites/default/files/webinars/2015_04_17%20ISES%20Webinar%20HYDROSOL%20Experiences.pdf).
**Efficient water splitting using sunlight**

Hydrogen is produced directly via a thermo-chemical redox reaction using the thermal energy of the Sun. A set of mirrors focuses the sunlight onto a single point that is heated up to very high temperatures. With this heat, water can be split into hydrogen and oxygen. In the first part of the procedure, the Sun heats redox materials, such as nickel ferrite or cerium oxide, in the interior of the reactor to 1400 degrees Celsius. At these temperatures, the metal oxide is chemically reduced, that is oxygen is released and transported out of the reactor. The actual water splitting occurs in the second step, which takes place at 800 to 1000 degrees Celsius. Here, the researchers let water vapour flow through the reactor. The previously reduced material is reoxidised. As the oxygen is now bound into a metal oxide, it remains in the reactor, whilst the hydrogen is free to be transported out of the reactor. Once the material is completely reoxidised, it is regenerated through the first step of the procedure and the cycle starts again.

**Higher efficiency, greater durability**

Building on earlier research projects, the scientists have significantly advanced both the structure of the reaction chamber as well as the materials. The solar radiation is secondarily focused using a cone with a coating of reflecting material, which increases the efficiency of the process as less heat can escape. Newly-developed ceramic foams hold promise for a higher hydrogen yield and greater durability. The researchers expect that these will produce around three kilograms of hydrogen per week in test mode. Martin Roeb, Project Manager at the DLR Institute of Solar Research explains: “With the HYDROSOL_Plant, we have for the first time designed a plant that reproduces the entire process, from generation, through the separation of high-purity hydrogen, to its storage. Although our work is still in the research phase, we can already generate one kilogram of hydrogen per week, which is a significant amount. An efficient fuel-cell vehicle can travel well over 100 kilometres on one kilogram of hydrogen.”


**Hydrogen Europe Research Association**

The *Hydrogen Europe Research Association* was formerly known as N.ERGHY. It is a public private partnership supporting research, development and demonstration (RD&D) activities in fuel cell and hydrogen energy technologies in Europe, representing European universities and research institutes in the Fuel Cell and Hydrogen Joint Undertaking (FCH JU). Comprising more than 60 research institutions (e.g., the universities and research institutions indicated in Figure 11), it creates a framework for cooperation framework for science and industry in Europe. It is an association that helps, along with the *Industry Grouping Hydrogen Europe* and the *European Commission* to formulate the FCHJU’s program plans, represented in its Multi-Annual Working Plan 2014-2020.\(^{21}\)

In 2014, the Council of the European Union formally agreed to continue the Fuel Cells and Hydrogen Joint Technology Initiative under the EU Horizon 2020 Framework Program. The programme (2014-20) has a total budget of €1.33 billion provided on a matched basis between the EU represented by the European Commission, the European Industry and Research.

![Figure 11: Map of universities and research institutes participating in the Hydrogen Europe Research Association.](https://www.nergy.eu/map/)

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20 [https://www.hydrogeneurope.eu/research](https://www.hydrogeneurope.eu/research)
22 [https://www.nergy.eu/map/](https://www.nergy.eu/map/)
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The mission of Hydrogen Europe Research is to promote, support and accelerate the deployment of hydrogen and fuel cell technologies by aligning the European RD&D community and industrial stakeholders. According to its website\(^{23}\), the Association pursues its objectives by conducting the following activities in the field:

- Providing expertise and advice to the stakeholders, e.g. industrial companies, the European Community and its Member States, including the European Hydrogen and Fuel Cell Stakeholder Forum, about the results and needs of European research, and how this research can contribute to the acceleration of the deployment of hydrogen and fuel cell technology;

- Actively participating as a member in the decision process of the Joint Undertaking, in particular through Governing Board, its highest decision making organ, or any other committees by electing from among its members representatives for such purpose and defining positions of the research community;

- Reaching a better gathering of the above-mentioned research community by mapping existing research competences, facilities and expertise and maintaining a respective knowledge base for its Members and third parties;

- Formulating joint views on existing and future needs on research infrastructures and programmes; special attention is drawn to the interrelation and cooperation along upstream, basic and applied research, with the support of national and European programmes;

- Issuing any other coordinated positions of the research community and representation of the interests of its Members as research organisations and the research community in general towards third parties.

In the Europe Hydrogen Research Association, the Working Group on Energy Innovation: Pillar Energy to Hydrogen deals with the following topics\(^{24}\):

- Hydrogen production from renewable electricity for energy storage and grid balancing
- Hydrogen production with low carbon footprint from other resources and
- Waste hydrogen recovery
- Hydrogen storage, handling and distribution

\(^{23}\) [https://www.nerghy.eu/about-us/](https://www.nerghy.eu/about-us/)

\(^{24}\) [https://www.hydrogeneurope.eu/energy-hydrogen](https://www.hydrogeneurope.eu/energy-hydrogen)
Asian Initiatives and Opportunities

**International Institute for Carbon-Neutral Energy Research (I²CNER)**

**Background**

I²CNER is a good example of international collaboration that includes a major focus on renewable hydrogen. In 2007, the Japanese Ministry of Education, Culture, Sports, Science, and Technology (MEXT) launched the World Premier International Research Center Initiative (WPI) to build world-class research centers in Japan. Five research centers were established throughout Japan including the Advanced Institute of Materials research (AIMR), the Kavil Institute for the Physics and Mathematics for the Universe (IPMU), Institute for Integrated Cell-material Sciences (iCeMS), the Immunology Frontier Research Center (IRFeC), and the International Center for Materials Nanoarchitectonics (MANA). In 2010, I²CNER was inaugurated as the sixth WPI research center at Kyushu University (KU). Two years later, three more research centers were added the WPI programs: the International Institute for Integrative Sleep Medicine (IIIS), the Earth-Life Science Institute (ELSI), and the Institute of Transformative Bio-Molecules (ITbM). In 2017, the WPI founded the International Research Center for Neurointelligence (IRCN) and the Nano-Science Life Institute (NanoLSI).

**Objective**

I²CNER's overall focus is aimed at obtaining a sustainable and environmentally friendly society by contributing in the study of alternatives to fossil fuel based energy and to the reduction carbon dioxide emissions. An ultimate objective is to foster a carbon neutral society. Its scientific approach centers on the development of technological advancements and breaking down of scientific barriers to achieve a hydrogen-based society as well as introducing carbon dioxide capture and sequestration. Some of the areas under researched for a feasible hydrogen based energy system include hydrogen production and storage, hydrogen compatible materials, fuel cells, and photosynthetic chemical reactions and catalysts.

**Organization Structure**

I²CNER was set up as an international collaboration (as seen in Figure 12), and has a unique organizational structure compared to the other WPI centers. Its main facility is located at KU in Japan and its Satellite facility is located at the University of Illinois at Urbana-Champaign (UIUC) in the United States. Both centers have a symbiotic relationship with each other such as that the research projects at UIUC are complementary to and integrated with those at KU. In 2014, both KU and UIUC signed an agreement on academic cooperation and student exchange to further develop the ties between both centers. Chiharu Kubo, the president of KU, promotes collaboration with industry as well as improve IP management and technology transfer, by reinforcing the cooperation between KU’s Academic Research and Industrial Collaboration Management office and UIUC’s Office of Technology Management. I²CNER is subjected to annual reviews conducted by the External Advisory Committee.

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25 Information here on I²CNER can be found at the following sites:
http://i2cner.kyushu-u.ac.jp/en/
http://i2cner.illinois.edu/wpi/
Figure 12: International extent of the I2CNER collaborative nexus.26

Research
I2CNER is divided into several research divisions, each of which led by a designated WPI Principal Investigator of the facility. The following are the categories studied at the institute:

- Molecular Photoconversion Devices
- Hydrogen Materials Compatibility
- Electrochemical Energy Conversion
- Thermal Science and Engineering
- Hydrogen Storage
- Catalytic Materials Transformations
- CO₂ Capture and Utilization
- CO₂ Storage
- Energy Analysis
- Industrial Research Unit
- Applied Math for Energy

The areas being researched include developments for smart power grids by utilizing applied mathematics and renewable energy pathways to achieve a carbon-neutral energy society. Task 35 researchers have coordinated closely with research efforts being supported under the I2CNER specifically related to fields of renewable hydrogen production.

Recent Publications
Yearly publications for each research division in I2CNER are being curated through the center’s website.27 Some recent publications in the Electrochemical Energy Conversion and Molecular Photoconversion Devices research divisions are shown below.

26 http://i2cner.kyushu-u.ac.jp/en/about/structure.php
27 A full listing of publications can be found at: http://i2cner.kyushu-u.ac.jp/en/results/thesis.php
Recent publications from 12CNER Electrochemical Energy Conversion Division include:


Recent publications from I2CNER Molecular Photoconversion Division include:

- Bryka, K., Morgiel, J., Faryna, M., Edalati, K. and Horita, Z. (2017) Effect of high-pressure torsion on grain refinement, strength enhancement and uniform ductility of EZ magnesium alloy, Materials Letters, 212, 323-326. DOI: 10.1016/j.matlet.2017.10.113

Korea Center for Artificial Photosynthesis (KCAP)\textsuperscript{30}

Background

The Korea Center for Artificial Photosynthesis (KCAP) is a centralized research center with students and postdoctoral researchers working together under the guidance of professors. KCAP was institutionalized in 2009 at Sogang University, resulting from a research collaboration the Helios-Solar Energy Research Center at Lawrence Berkeley National Lab aiming to formulate artificial photosynthesis as a technology that is environmental friendly, affordable, and suitable as an alternative of crude oil. KCAP won a grant from the Ministry of Education, Science, and Technology constituting 50 billion Korean Won (45 million USD) through the use of the National Research Foundation of Korea. KCAP is also supported by the Pohang Iron and Steel Company (POSCO). In August, 2010, Sogang University signed a MOU with POSCO for a joint research to commercialize artificial photosynthesis. Due to this relationship, In January 2013, a special research building for KCAP was constructed.

Objective

KCAP’s goal is to research and develop materials and manufacturing methods to build devices that produce liquid fuel, carbon monoxide, formic acid, formaldehyde, methanol, and oxygen from water and carbon dioxide by taking advantage of solar energy. KCAP searches to integrate original technology with readily available elements on Earth to produce a commercial device with an energy efficiency of at least 3\%. Similar to the Joint Center for Artificial Photosynthesis in the United States, a critical focus is on the hydrogen production needed in the synthesis of fuels and chemicals.

Challenges

KyungByung Yoon, a professor of Chemistry at Sogang University and a president of KCAP mentioned that some of the challenges present for attainable and commercialized artificial photosynthesis are “the high price of device installation and related materials, and the low production efficiency.” To combat these inadequacies, KCAP is working to combine already commercialized technologies such as solar cell technology and water electrolysis technology to produce hydrogen to mix with carbon dioxide and produce fuel. According to Yoon, “the key to improving economic feasibility lies in water electrolysis technologies.” KCAP is currently searching for more efficient hydrogen production as well as cheaper substitutes for platinum, a material used for water electrolysis.

Other Establishments Researching Artificial Photosynthesis

While the KCAP is the main innovator for artificial photosynthesis in Korea, the Korean Government has also funded other institutions and universities that have also made strides in artificial photosynthetic research. Some of these prominent establishments are the Korea Institute of Science and Technology, the Korea research institute of Chemical Technology, Seoul National University, the Korea Advance Institute of Science and Technology, and Kyungpook National University.

Sample Projects:

\textsuperscript{30}Information here for KCAP can be found at the sites: http://www.k-cap.or.kr/eng/info/index.html?sidx=2 and http://www.k-cap.or.kr/eng/info/index.html?sidx=1
Examples of KCAP research and development publications are shown below\(^\text{31}\). A complete list of KCAP publications and patents is also available.\(^\text{32}\) Task 35 researchers have coordinated with KCAP in specific areas related to renewable hydrogen production.

<table>
<thead>
<tr>
<th>Main Author</th>
<th>Publication</th>
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<tbody>
<tr>
<td></td>
<td>Growth of Uniformly Oriented Silica MFI and BEA Zeolite Films on Substrates Tung Cao Thanh Pham, Hyun Sung Kim, Kyung Byung Yoon <em>Science</em>, 2011, 334, 1533–1538</td>
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<td></td>
<td>Highly porous gallium oxide with a high CO2 affinity for the photocatalytic conversion of carbon dioxide into methane Hang-ah Park, Jung Hoon Choi, Kyung Min Choi, Dong Ki Lee and Jeung Ku Kang <em>J. Mater. Chem.</em>, 2012, 22, 5304–5307</td>
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\(^\text{31}\) [http://www.k-cap.or.kr/bbs/zboard.php?id=emember](http://www.k-cap.or.kr/bbs/zboard.php?id=emember)

\(^\text{32}\) KCAP publications can be found at: [http://www.k-cap.or.kr/bbs/zboard.php?id=thesis&page=1&sn1=&divpage=1&category=1&sn=off&ss=on&sc=on&select_arrange=headnum&desc=asc&no=22](http://www.k-cap.or.kr/bbs/zboard.php?id=thesis&page=1&sn1=&divpage=1&category=1&sn=off&ss=on&sc=on&select_arrange=headnum&desc=asc&no=22)
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<td>Photoelectrochemical water splitting over ordered honeycomb hematite electrodes stabilized by alumina shielding Hwwichan Jun, Badro Im, Jae Young Kim, Yong-O Im, Ji-Wook Jang, Eun Sun Kim, Jae Yul Kim, Hyeon Joon Kang, Suk Joon Hong and Jae Sung Lee Energy Environ. Sci., 2012, 5, 6375–6382</td>
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<td></td>
<td>Enhancing the photoelectrochemical performance of hematite (--Fe2O3) electrodes by cadmium incorporation Ayoung Bak, Wonyong Choi, Hyunwong Park Applied Catalysis B, 2011 207–215</td>
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<tr>
<td>Yong Soo Kang</td>
<td>Axis–Oriented, Anatase TiO₂ Single Crystals with Dominant {001} and {100} Facets Cuong Ky Nguyen, Hyun Gil Cha, and Yong Soo Kang Cryst. Growth Des. 2011, 11, 3947–3953</td>
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<td>Name</td>
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<tr>
<td>Hee Woo Rhee</td>
<td>Nafion®/Silane Nanocomposite Membranes for High Temperature Polymer Electrolyte Membrane Fuel Cell</td>
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<td>Wan In Lee</td>
<td>Formation of highly crystallized TiO2(8) and its photocatalytic behavior</td>
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<td>Double–heterojunction structure of SbxSn1–xO2/TiO2/CdSe for efficient decomposition of gaseous 2-propanol under visible–light irradiation</td>
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<td>Jong Hak Kim</td>
<td>Enhanced Performance of I 2 –Free Solid–State Dye–Sensitized Solar Cells with Conductive Polymer up to 6.8%</td>
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<td></td>
<td>Highly Efficient, Iodine–Free Dye–Sensitized Solar Cells with Solid–State Synthesis of Conducting Polymers</td>
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<td>Woonsup Shin</td>
<td>A Miniature, Nonpumping Electroosmotic Pump Operating at 0.5 V</td>
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<td>Microbes as Electrochemical CO2 Conversion Catalysts</td>
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<td>Reduction of CO2 to CO at Low Overpotential in Neutral Aqueous Solution by a Ni (cyclam)Complex Attached to Poly(allylamine)</td>
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<td>Nam Hwi Hur</td>
<td>Confined Pt and CoFe2O4 Nanoparticles in a Mesoporous Core/Shell Silica Microsphere and Their Catalytic Activity</td>
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North American Initiatives and Opportunities

**The U.S. Department of Energy’s Solar Fuels Innovation Hub: Joint Center for Artificial Photosynthesis**

The Joint Center for Artificial Photosynthesis (JCAP), founded in 2010, is a (DOE) Energy Innovation Hub whose primary mission is to find a cost-effective method to produce fuels (including hydrogen and other hydrocarbon fuels) using only sunlight, water, and carbon-dioxide. JCAP’s main centers are located at the California Institute of Technology and the Lawrence Berkeley National Laboratory. In addition, JCAP has partners from Stanford University, the University of California at Berkeley, University of California at Santa Barbara, University of California at Irvine, the University of California at San Diego, and Stanford Linear Accelerator. In addition, JCAP also serves as a hub for other solar fuels research teams across the United States, including several DOE Energy Frontier Research Center.

![Photosynthesis](image1)  ![Artificial Photosynthesis](image2)

**Figure 13:** Researchers from across disciplines are working together to create energy and fuels directly from sunlight, and create a process that's economically viable.

**The Solar Energy-to-Fuels Conversion Challenge**

Designing highly efficient, non-biological, energy conversion “machines” that generate fuels directly from sunlight, water, and carbon dioxide is both a formidable challenge and an opportunity. Such a process could revolutionize our ability to tap new energy sources that are both renewable and environmentally-friendly while improving energy security.

Basic research has already provided enormous advances in our understanding of the subtle and complex mechanisms behind the natural photosynthetic system as well as in the use of photochemical methods that mimic key steps in the process -- splitting water and reducing carbon dioxide. While we have come far, we still lack sufficient knowledge to design solar energy-to-fuel conversion systems with the required efficiency, scalability, and sustainability to be economically viable.

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33 The information on JCAP included here is directly from the site: [https://www.energy.gov/articles/fuels-sunlight-hub](https://www.energy.gov/articles/fuels-sunlight-hub)

34 [https://en.wikipedia.org/wiki/Joint_Center_for_Artificial_Photosynthesis](https://en.wikipedia.org/wiki/Joint_Center_for_Artificial_Photosynthesis)
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While the task is no doubt a challenge, it holds great promise. By tapping into new energy sources through innovative projects that are both renewable and environmentally friendly, we have the potential to transform America’s energy future.

The Joint Center for Artificial Photosynthesis (JCAP)

The Fuels from Sunlight Energy Innovation Hub was specifically designed as a highly structured organization with three main objectives:

1. Discovering earth-abundant, robust light absorbers with optimal band gaps to harvest sunlight most effectively and efficiently.
2. Accelerating the rate of catalyst discovery for solar energy-to-fuel conversion reactions.
3. Providing system integration and scale-up so that laboratory experiments can be transitioned into prototypes for commercial development.

The progress of the Hub is measured against research and development milestones that are monitored and adjusted based on progress or new directions dictated by new scientific discovery. Research is focused on creating a prototype device that can produce fuel from the sun 10 times more efficiently than plants. On July 22, 2010, the Department of Energy announced the selection of JCAP, a team led by the California Institute of Technology (Caltech), to run the Fuels from Sunlight Energy Innovation Hub. This group directly partners with the Lawrence Berkeley National Lab (LBNL), SLAC National Accelerator Laboratory (SLAC), and the Universities of California at Irvine and San Diego and will collaborate with the DOE Energy Frontier Research Centers (EFRCs), the DOE core programs, and other national and international organizations.

Recent JCAP High-Impact Publications Relevant to Water Splitting35

Task 35 researchers have coordinated closely with JCAP and the high-impact research relevant to renewable hydrogen production supported by the center. A few examples of the many publications generated by the JCAP research are included below:


35 From https://solarfuelshub.org/publications Year 2016; See this site for a full listing of JCAP publications organized by publication year.


• Cooper, J. K. et al. Role of Hydrogen in Defining the n-Type Character of BiVO4 Photoanodes. Chemistry of Materials, DOI: 10.1021/acs.chemmater.6b01994 (2016).


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• Ping, Y., Nielsen, R. J., and Goddard, W. A. The Reaction Mechanism with Free Energy Barriers at Constant Potentials for the Oxygen Evolution Reaction at the IrO2 (110) Surface. Journal of the American Chemical Society, DOI: 10.1021/jacs.6b07537 (2016).


• Shinde, A. et al. Discovery of Fe–Ce Oxide/BiVO4 Photoanodes through Combinatorial Exploration of Ni–Fe–Co–Ce Oxide Coatings. ACS Applied Materials and Interfaces, DOI: 10.1021/acsmat.6b06714 (2016).


• Tolstova, Y., Omelchenko, S. T., Shing, A. M. & Atwater, H. A. Heteroepitaxial growth of Pt and Au thin films on MgO single crystals by bias-assisted sputtering. Scientific Reports, 6, 23232, DOI: 10.1038/srep23232 (2016).


• Wan, Y. et al. Magnesium Fluoride Electron-Selective Contacts for Crystalline Silicon Solar Cells. ACS Applied Materials and Interfaces, 8(23), 14671-14677, DOI: 10.1021/acsami.6b03599 (2016).
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- Xu, X. et al. Chemical Bath Deposition of p-Type Transparent, Highly Conducting (CuS)x−(ZnS)1−x Nanocomposite Thin Films and Fabrication of Si Heterojunction Solar Cells. Nano Letters, 16(3), 1925-1932, DOI: 10.1021/acs.nanolett.5b05124 (2016).
The HydroGEN Advanced Water Splitting Materials consortium aims to accelerate the research, development, and demonstration of advanced water splitting technologies for clean, sustainable hydrogen production.

HydroGEN is a consortium of six U.S. Department of Energy (DOE) national laboratories that addresses advanced water splitting materials challenges by making unique, world-class national lab capabilities in photoelectrochemical, solar thermochemical, and low- and high-temperature electrolytic water splitting more accessible to academia, industry, and other national labs.

Led by the National Renewable Energy Laboratory, the HydroGEN consortium includes Lawrence Berkeley National Laboratory, Sandia National Laboratories, Idaho National Laboratory, Lawrence Livermore National Laboratory, and Savannah River National Laboratory. HydroGEN is funded by DOE’s Fuel Cell Technologies Office in the Office of Energy Efficiency and Renewable Energy.

HydroGEN aims to facilitate collaborations between federal laboratories, academia, and industry. The consortium is guided by a steering committee with representatives from each member lab and DOE. The steering committee is available to clarify the capabilities offered by the consortium and to help interested users identify capabilities relevant to a given research project.

HydroGEN leverages national lab consortia launched under DOE’s Energy Materials Network (EMN) supports the Materials Genome Initiative (MGI) and advanced manufacturing priorities. The EMN consortia have been launched to make unique, world-class capabilities at the national laboratories more accessible to industry and academia, facilitating collaborations that will expedite the development of advanced materials.

Task 35 experts have coordinated closely with HydroGEN research, which is broadly addressing key materials challenges in all the major renewable hydrogen production pathways, including low- and high-temperature electrolysis as well as photoelectrochemical and solar thermochemical water splitting.

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36 The information here on the DOE HydroGEN Consortium can be found at the site: https://www.energy.gov/eere/fuelcells/hydrogen-advanced-water-splitting-materials-consortium
### HydroGEN Advanced Water Splitting Materials Consortium: Current Research Projects

#### List of Initial HydroGEN ‘Seedling’ Projects by Category

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<th>Prime Institution</th>
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<td><strong>High-Temperature Electrolysis</strong></td>
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<tr>
<td>Proton-Conducting Solid Oxide Electrolysis Cells for Large-scale Hydrogen</td>
<td>University of Connecticut</td>
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<tr>
<td>Production at Intermediate Temperatures</td>
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<tr>
<td>Degradation Characterization and Modeling of a New Solid Oxide Electrolysis</td>
<td>Northwestern University</td>
</tr>
<tr>
<td>Cell Utilizing Accelerated Life Testing</td>
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<tr>
<td>Thin-Film, Metal-Supported High-Performance and Durable Proton–Solid Oxide</td>
<td>United Technologies Research Center</td>
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<tr>
<td>Electrolyzer Cell</td>
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<tr>
<td><strong>Low-Temperature Electrolysis</strong></td>
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<td>High Efficiency PEM Water Electrolysis Enabled by Advanced Catalysts,</td>
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<td>Membranes and Processes</td>
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<td>Developing Novel Platinum Group Metal–Free Catalysts for Alkaline Hydrogen</td>
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<td>and Oxygen Evolution Reactions</td>
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<td>PGM–free OER Catalysts for PEM Electrolyzer</td>
<td>Argonne National Laboratory</td>
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<tr>
<td>High–Performance Ultralow–Cost Non–Precious Metal Catalyst System for AEM</td>
<td>Los Alamos National Laboratory</td>
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<tr>
<td>Electrolyzer</td>
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<td>Scalable Elastomeric Membranes for Alkaline Water Electrolysis</td>
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<td><strong>Photoelectrochemical Water Splitting</strong></td>
<td></td>
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<tr>
<td>Best–in–class Platinum Group Metal–free Catalyst Integrated Tandem Junction</td>
<td>Rutgers University</td>
</tr>
<tr>
<td>PEC Water Splitting Devices</td>
<td></td>
</tr>
<tr>
<td>Protective Catalyst Systems on III–V and Si–based Semiconductors for Efficient,</td>
<td>Stanford University</td>
</tr>
<tr>
<td>Durable PEC Water Splitting Devices</td>
<td></td>
</tr>
<tr>
<td>Novel Chalcophorites for Advanced Photoelectrochemical Water–Splitting</td>
<td>University of Hawaii</td>
</tr>
<tr>
<td>Monolithically Integrated Thin–Film/Silicon Tandem Photoelectrodes for High</td>
<td>University of Michigan, Ann Arbor</td>
</tr>
<tr>
<td>Efficiency and Stable PEC Water Splitting</td>
<td></td>
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<tr>
<td>Efficient Solar Water Splitting with 5,000 Hours Stability Using Earth–abundant</td>
<td>Los Alamos National Laboratory</td>
</tr>
<tr>
<td>Catalysts and Durable Layered 2D Perovskites</td>
<td></td>
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<tr>
<td><strong>Solar Thermochemical Water Splitting</strong></td>
<td></td>
</tr>
<tr>
<td>Computationally Accelerated Discovery and Experimental Demonstration of</td>
<td>University of Colorado, Boulder</td>
</tr>
<tr>
<td>High–Performance Materials for Advanced STCH Hydrogen Production</td>
<td></td>
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<tr>
<td>Transformative Materials for High–Efficiency Thermochemical Production of</td>
<td>Northwestern University</td>
</tr>
<tr>
<td>Solar Fuels</td>
<td></td>
</tr>
<tr>
<td>Mixed Ionic Electronic Conducting Quaternary Perovskites: Materials by Design</td>
<td>Arizona State University</td>
</tr>
<tr>
<td>for STCH H2</td>
<td></td>
</tr>
<tr>
<td>Accelerated Discovery of STCH Hydrogen Production Materials via High–</td>
<td>Colorado School of Mines</td>
</tr>
<tr>
<td>Throughput Computational and Experimental Methods</td>
<td></td>
</tr>
<tr>
<td>High Temperature Reactor Catalyst Material Development for Low Cost and</td>
<td>Greenway Energy</td>
</tr>
<tr>
<td>Efficient Solar Driven Sulfur–Based Processes</td>
<td></td>
</tr>
</tbody>
</table>
IEA-HTCP Task 35 Final Report

Project Summaries
Summaries of the above-listed projects which address a broad spectrum of fundamental, early-stage R&D challenges relevant to all the major water-splitting pathways for renewable hydrogen production are provided below in the following sections.

HydroGEN
Advanced Water Splitting Materials

High- and Low-Temperature Electrolysis Projects
Proton-Conducting Solid Oxide Electrolysis Cells for Large-scale Hydrogen Production at Intermediate Temperatures

**Project Motivation**
- Extensive background in HT/IT electrochemical systems
- Experience with functional ceramics, electrolytes, electrochemical testing, performance degradation and data analysis
- Well established laboratory capabilities in materials processing and characterization
- On going research in SOFC, SOEC and H-SOEC

| Key Impact |
|---|---|---|---|
| Metric | State of the Art | Proposed | Actual |
| Conductivity (S/cm) | $\sim 10^2$ | $10^2$ | $4 \times 10^2$ |
| Sintering temp. (°C) | $> 1450$ | $\leq 1350$ | 1350 |
| Thickness (µm) | $> 25$ | $\sim 15-20$ | 20 |

**Project Relevance and Impact**
- Identify novel materials and processing techniques to develop cost effective and efficient proton-conducting solid oxide electrolysis cells (H-SOECs) for large-scale hydrogen production at intermediate temperatures (600–800°C) to meet DOE cost and performance targets to meet hydrogen production cost target of < $2/gge hydrogen
- Innovation in materials chemistry - electrolyte and electrode formulations
- Use of non–noble and non–strategic cell and stack component materials
- Bulk, interface, and surface optimizations to achieve low ASR
- High proton–conductivity with a low sintering temperature (< 1450°C)
- Operating current density (> 1 A/cm²) with the performance degradation rate not to exceed the DOE performance metric (< 4 mV/1000 h)

**Innovative Approach**
- Use of proton conducting electrolyte < 700 °C; produces pure hydrogen without the need of separation
- Electrolyte densification temperature reduced to ~1350–1400°C for > 97% density; improved conductivity (> 0.01 S/cm) obtained at lower temperatures 550–750°C

**Accomplishments and Future Work**
- Proton conducting- electrolyte and electrode materials have been selected and synthesized
- BZY and BZCY–Yb electrolyte discs have been prepared using reactive / fugitive sintering aids (nanosized ZnO)
- H–SOEC full cells with low area specific resistance have been fabricated using thin dense electrolyte (15–40 µm) and porous electrodes using INL node
- Button cell testing of steam electrolysis in the temperature range of 600–800°C has been initiated

**HydroGEN Engagement**
- INL–UConn collaboration spanned over the topics for the development of dense electrolyte and performance improvement of the anode
- National Lab Capabilities and Collaboration
  - Developing and testing H–SOEC (PNNL)
  - Optimization of electrolyte chemistry (NREL, INL, LBNL)

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37 [https://www.h2awsm.org/sites/default/files/kickoff-project-hte-uconn.pdf](https://www.h2awsm.org/sites/default/files/kickoff-project-hte-uconn.pdf)
Degradation Characterization and Modeling of a New Solid Oxide Electrolysis Cell Utilizing Accelerated Life Testing\textsuperscript{38}—Northwestern University

### Project Motivation
Barnett has been using accelerated testing combined with 3D tomography to develop quantitative Solid Oxide Fuel Cell degradation models for several years, and has worked with Voorhees in this area. It was natural to extend these ideas and methods to electrolysis cells.

<table>
<thead>
<tr>
<th>Metric</th>
<th>State of the Art</th>
<th>Expected Advance</th>
</tr>
</thead>
<tbody>
<tr>
<td>Current Density</td>
<td>0.5 A/cm\textsuperscript{2}</td>
<td>&gt; 1.0 A/cm\textsuperscript{2}</td>
</tr>
<tr>
<td>Degradation Rate</td>
<td>&gt; 10 mV/kh</td>
<td>&lt; 4 mV/kh</td>
</tr>
<tr>
<td>Electrode Overpotential</td>
<td>&gt; 0.2 V</td>
<td>&lt; 0.2 V</td>
</tr>
</tbody>
</table>

### Key Impact

#### Project Relevance and Impact
- Solid oxide electrolysis cells (SOECs) have the potential to achieve the highest electricity–to–hydrogen conversion efficiency amongst electrolysis technologies
  - This project addresses the long-term stability of these cells at high current density, widely regarded as being a critical barrier for their commercial development
- Developing accelerated testing protocols and a basic understanding of degradation mechanisms will have a broad impact on the field
  - A key outcome will be improved SOECs that allow long lifetime at higher current density
- Baseline SOECs are fabricated and accelerated electrochemical life testing carried out along with microstructural/chemical characterization

#### Innovative Approach
- A model has been developed that predicts the oxygen potential across the electrolyte in a solid oxide electrolysis cell
  - Can predict materials and operating conditions causing degradation
  - Applicable to wide range of materials and conditions
- SOECs fabricated using tape casting and screen printing
- First-ever results on metal–supported solid oxide electrolysis cells
- Electrolyte degradation model predicts the experimentally–observed electrolyte resistance degradation caused by over potential

#### HydroGEN Engagement
- Metal–Supported Solid Oxide Electrolysis Cells Analysis and Stability (LBNL)
- Facilitate the R&D by Carrying out Cell Testing beyond that done at Northwestern, and Assisting in Data Interpretation and Analysis, and Possible Personnel Exchange (INL)
- Test and Develop their Novel Metal–Supported Fuel Cells for the Electrolysis Application, Providing Cells for Electrolysis Testing at both Berkeley and NWU (LBNL)

\textsuperscript{38} \url{https://www.h2awsm.org/sites/default/files/kickoff-project-hiie-northwestern.pdf}
Thin-Film, Metal-Supported High-Performance and Durable Proton-Solid Oxide Electrolyzer Cell — United Technologies Research Center

**Project Relevance and Impact**
- Develop a highly efficient and cost competitive high temperature electrolysis for $\text{H}_2$ generation
- Using thin-film, high efficiency and durable metal-supported solid oxide electrolysis cell based on proton-conducting electrolyte at targeted operating temperatures of 550–650°C
- Aim to accelerate the commercialization of high-temperature electrolysis, and advance reversible-SOFC technology for renewable-energy applications
- Successful demonstration of the concept should result in a path to low cost and durable p-SOEC for $\text{H}_2$ production at <$\text{S2/kWe}$

**Innovative Approach**
- Low cost, scalable fabrication of metal-supported cell
- Further material optimization for an efficient & durable p-SOEC
  - Phase 1: focus on demonstrating the feasibility of the proposed concept via electrolysis performance demonstration of a Gen 1 metal-supported single cells
- Half Cell Fabrication
  - Hydrogen electrode deposition on porous metal support is complete
  - Electrolyte deposition by RSDT and SPS in progress, focus on process optimization
  - OCV results of the electrolyte indicate density of electrolyte needs further improvement (OCV=0.8–0.9 on cells with either RSDT or SPS electrolyte)
- Alternative Cell Fabrication: LBNL Co–sintering
  - Doped BYZ compatible with Stainless Steel Support Material and Processing Conditions
  - Processing conditions dictated by stainless steel: 2% Hydrogen, 1450°C

**HydroGEN Engagement**
- Metal alloy candidates, oxidation testing conditions, electrolyte powder and process for co–sintering (LBNL)
- Testing on UTRC metal-supported button cell (INL)
- Modeling of SOEC (NREL)
- Sintering and powder process (UTRC/INL/LBNL)

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39 [https://www.h2awsm.org/sites/default/files/kickoff-project-hse-utrc.pdf](https://www.h2awsm.org/sites/default/files/kickoff-project-hse-utrc.pdf)
High Efficiency PEM Water Electrolysis Enabled by Advanced Catalysts, Membranes and Processes Project Onsite

Project Summary

High Efficiency PEM Water Electrolysis
Kathy Ayers, Proton OnSite
Ivinya Zenyuk, Tufts University
Karin Morel, ORNL

Project Vision
We are solving the cost barriers for PEM electrolysis by integrating advanced cell designs, materials and fundamental characterizations of performance.

Project Impact
The anticipated impact of Phase I is to define a reliable MEA configuration with high efficiency (through new catalysts) and optimized membrane processing.

Approach Summary

Project History
Thinner catalysts and alternate catalysts have shown promise for stable operation of PEM electrolyzers at improved efficiency. This project advances material performance and integrates components together, while leveraging fundamental characterization to understand the push design limits.

Barriers
- Long-term durability: understand electrode materials and their interaction through accelerated tests and fundamental characterization
- Higher bifunctionality with anodic and cathodic reactions
- Refinement of electrode fabrication process
- Integration of these characteristics into a full MEA

Proposed Targets
- Achieved through material characterization, in-operando analysis, and advanced modeling of membrane and PTL interactions
- Final deliverable of the project will be an advanced electrolysis stack producing H2 at 43 kWh/kg and at costs of $2/kg H2

Innovative Approach

- PEM electrolysis has the potential for significant efficiency improvement - challenge is integrating and extending what we know, where complex interactions exist
- Project combines and advances promising directions in multiple areas
  - Catalyst composition
  - Stable 3-D structures
  - Thinner membranes
  - Robust manufacturing
  - Optimized interfacial layers

HydroGEN Engagement

- NREL
- ORNL
- LBNL

40 https://www.h2awsm.org/sites/default/files/kickoff-project-lte-proton.pdf
Developing Novel Platinum Group Metal-Free Catalysts for Alkaline Hydrogen and Oxygen Evolution Reactions\(^{41}\) — *Northeastern University*

### Project Motivation

The focus of this project is on durable, high-performance materials advanced water splitting, enabling a pathway for achieving <6$\$/kg\(_{\text{H}_2}\) with efficiency of 43 kWh/kg H\(_2\) via anion exchange membrane (AEM)-based electrolysis. We aim to advance these goals via an understanding of both hydrogen and oxygen evolution reactions leading to novel platinum group metal (PGM)-free catalyst materials in conjunction with improvements in membrane and ionomers and gas evolution electrodes with corresponding characterization and testing.

### Project Relevance and Impact

- Develop thermally sustainable anionic membranes for cost–efficient transition metal catalysts
- Materials with potential for cost advantages of Anion Exchange Membrane (AEM) electrolyzers
  - <6$\$/kg\(_{\text{H}_2}\) (on scale) with efficiency of 43 kWh/kg H\(_2\)
- Stable, high strength, and high conductive AEMs
- Stable and active Platinum Group Metal (PGM)–free catalysts for hydrogen and oxygen evolution reaction (HER/OER)
- High–performance electrode architectures

### Innovative Approach

- Novel HER/OER catalysts:
  - Metal–Metal Oxides/Functionalized mono–metallic/Embedded Metal–N–C Systems (OER)
  - Double layer metal oxides on Raney Ni (HER)
- Half and Single Cell Tests (NEU)
- Experimental Analysis by using of Raman and Synchrotron X–ray Spectroscopy
- Novel Membranes and Ionomers (University of Delaware)
  - Multi–cation Poly(aryl–piperidinium) Tri–quaternary–ammonium membranes and ionomers for high temperature operation (90 °C)
- New Electrodes designed for gas evolution with and without liquid flow (Advent North America)

### HydroGEN Engagement

- Membrane Electrode Assembly Preparation and Testing (*NREL*)
- Interfacial Modeling about the Response of the Ionomer Active Site to Charge (*SNL*)
- Small Angle X–ray Scattering Studies for Morphology of the Anion Exchange Membrane in Different States of Hydration (*LBNL*)
- Modeled the Interaction of Carbonate Ions at Catalyst Interface Layer and AEM (*LBNL*)

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\(^{41}\) [https://www.h2awsm.org/publications/project-kick-off-meeting](https://www.h2awsm.org/publications/project-kick-off-meeting)
PGM-free OER Catalysts for PEM Electrolyzer — ANL

**Project Motivation**
Both ANL and UB teams are the pioneers in the MOF derived PGM-free catalysts for oxygen redox reactions (ORR). PGM-free catalyst for oxygen evolution reaction (OER) calls for different approach. Promising results are shown recently at both institutes. Giner is an industrial leader in PEMWE technology responsible for MEA/electrolyzer development.

**Key Impact**

<table>
<thead>
<tr>
<th>Metric</th>
<th>State of the Art</th>
<th>Proposed</th>
</tr>
</thead>
<tbody>
<tr>
<td>Difference in overpotential against Ir black by RDE</td>
<td>Overpotential of ~330 mV @ 10 mA/cm² for PGM-free catalyst in acid</td>
<td>Overpotential &lt;350 mV or 15 mV higher than Ir black @ 10 mA/cm² in 1 M KOH electrolyte</td>
</tr>
<tr>
<td>Current density in operating PEM</td>
<td>Non-exiting for PGM-free catalyst in PEME</td>
<td>PEME/MEA with target performance of &gt; 250 mA/cm² @ 1.80 V</td>
</tr>
</tbody>
</table>

**Project Relevance and Impact**
- Next-generation, low-cost PGM-free OER catalysts
- Goal - produce one or more PGM-free OER catalysts with the performance approaching to the Ir catalyst but at < 1/20 of the cost, demonstrated through the operating PEM electrolyzer
- Impact - reduce the electrolyzer capital cost and facilitate broad implementation of PEME for low-cost hydrogen production (<$2/kg) coupled with renewable energy sources

**Innovative Approach**
- Metal–Organic Framework (MOF) Derived PGM-free OER Catalysts
  - MOF derived catalysts can significantly reduce the cost by using inexpensive ligand and earthy abundant transition metal
- Porous Nano–Network Electrode (PNNE) via Electrospin
  - MOF embedded PNNE can improve OER mass/charge transfers via direct macro–to–micropore connection
- Zeolitic Imidazolate Framework (ZIF–8) based OER catalyst (high performance)

**Accomplishments and Future Work**
- New MOF–derived PGM-free OER catalysts (ANL) showed excellent activity and durability in acidic electrolyte compared to PGM–free benchmark catalysts in literature, with performance approaching to Ir black
- PNNE OER catalysts (ANL) also demonstrated very promising activity and excellent durability when measured against Ir black in strong acidic electrolytes
- Excellent progresses in activity and durability improvements for FeMx–ZIF–8 and FeMx–ZIF–8/Oxide based catalysts
- Initial studies have validated our project approaches demonstrated by very promising catalytic activity and durability

**HydroGEN Engagement**
- Computational chemistry and predictive modeling (LLNL and LBNL)
- Advanced electron microscopic imaging (SNL)
- High throughput electrode optimization support / catalyst surface characterization (NREL)

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High-Performance Ultralow-Cost Non-Precious Metal Catalyst System for AEM Electrolyzer

Project Motivation
The need for low-cost, active and durable PGM-free OER and HER catalysts for AEM electrolyzer. Perovskite oxides were chosen as OER catalysts and porous Ni-La alloys as HER catalysts.

Key Impact

<table>
<thead>
<tr>
<th>Metric</th>
<th>State of the Art</th>
<th>Proposed</th>
</tr>
</thead>
<tbody>
<tr>
<td>OER activity</td>
<td>5.0 mA/cm² at 1.65 V with carbon addition</td>
<td>5.1 mA/cm² at 1.65 V without carbon addition</td>
</tr>
<tr>
<td>HER activity</td>
<td>20 mA/cm² at 0.20 V overpotential</td>
<td>34 mA/cm² at 0.20 V overpotential</td>
</tr>
<tr>
<td>Durability</td>
<td>Performance durability of IrO₂</td>
<td>The same degradation rate compared with IrO₂</td>
</tr>
</tbody>
</table>

Project Relevance and Impact
In PEM water electrolyzer, titanium flow fields/separators, PGM IrO₂ and Pt catalysts, and Nafion® perfluorinated membrane account for more than 70% of the stack cost. If PGM-free catalyst development for AEM water electrolysis is successful, in addition to PGM catalyst replacement by PGM-free catalysts, titanium flow fields/separators and Nafion® perfluorinated membrane can be replaced by stainless steel and cheaper hydrocarbon membrane. This is expected to reduce the stack cost by more than 50% and facilitate reaching the DOE Hydrogen and Fuel Cells Program cost target of sustainably produced hydrogen of < $2/kg.

Innovative Approach
- The barrier, the need of alkaline solution feeding to achieve high performance in AEM technology, is demonstrated. With alkaline solution feeding, this technology can be considered a kind of alkaline water electrolysis, not the AEM water electrolysis technology by definition. Screen >1000 perovskites for suitability and stability under two-step STCH cycling conditions
- Catalyst/organic cation interface study
  - Development of PGM-free catalysts
  - Electrochemical cell measurement and selection of catalysts for AEM electrolyzer test
  - MEA fabrication and AEM electrolyzer test
  - Validation of the project’s innovative approach

HydroGEN Engagement
- Hydrogen in site testing capabilities for H₂ generation
- Surface analysis cluster tool
- DFT and Ab initio calculations
- Separators for hydrogen production

Accomplishments
- Establishment of catalyst synthesis equipment, including spray pyrolysis, with La–doped Ni HER and LSC OER catalysts successfully fabricated as verified by XRD
- Alkaline electrolyzer system set-up at LANL with first experiments with PGM–free catalysts complete

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43 [https://www.h2awsm.org/sites/default/files/kickoff-project-lte-lanl.pdf](https://www.h2awsm.org/sites/default/files/kickoff-project-lte-lanl.pdf)
Scalable Elastomeric Membranes for Alkaline Water Electrolysis — LANL

**Key Impacts**

<table>
<thead>
<tr>
<th>Metric</th>
<th>State of the Art</th>
<th>Expected Advance</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hydroxide conductivity (mS/cm)</td>
<td>30-40</td>
<td>40</td>
</tr>
<tr>
<td>% Loss conductivity after 300 h, 1 M NaOH, 80 °C</td>
<td>30</td>
<td>&lt; 5</td>
</tr>
<tr>
<td>Tensile toughness (MPa × cm²)</td>
<td>2000</td>
<td>3000</td>
</tr>
</tbody>
</table>

**Project Relevance and Impact**

- Preparing durable and economically-affordable alkaline hydroxide conducting materials based on SEBS
- Demonstrating the performance and durability in alkaline membrane-based water electrolysis
- This project directly deals with novel membrane fabrication and development of low temperature electrolysis
- Benefits of alkaline membrane water electrolyzer
  - Lowering capital cost by removing the high noble metal loading requirements.
  - Using relatively cheap cell hardware under high pH conditions
  - High pressure operation is possible with less cross-permeation

**Innovative Approach**

- Anion Exchange Membrane (AEM) Synthesis
  - Metal-catalyzed coupling (M–Cat)
    - Good control of IEC (1.5 meq./g)
    - High hydroxide conductivity (40 mS/cm)
    - Excellent chemical stability (1 M NaOH at 80 °C for 4 weeks)
    - Con-Expensive
  - Acid catalyzed
    - IEC, conductivity, and chemical stability are similar M–Cat’s
    - Multi-cation structure is feasible
    - No use of expensive metal catalysts
- Styrene–Ethylene–Butylene–Styrene Block Copolymer
  - Robust polymer backbone / commercially available

**HydroGEN Engagement**

- Provided Membrane Benchmarking/Protocol Suggestions to Proton Onsite Including Conductivity and Membrane Stability Data (LANL, RPI)
- Water Electrolysis Modeling Provides the Insight on AEM Design (BNL)
- Improve Chemical Stability of Benchmark Anion Exchange Membranes (LANL, SNL)

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44 [https://www.h2awsm.org/sites/default/files/kickoff-project-lte-lanl-kim.pdf](https://www.h2awsm.org/sites/default/files/kickoff-project-lte-lanl-kim.pdf)
Photoelectrochemical H₂ Production Projects
IEA-HTTCP Task 35 Final Report

RU-EMN – Best-in-Class Platinum Group Metal-free Catalyst Integrated Tandem Junction PEC Water Splitting Devices\(^4^5\) — Rutgers University

**Project Motivation**

**High-performance Photovoltaics**: State of the art material competing with NREL HP III-V tandems (STH 16.7%) vs. Multi-junction Silicon (STH 3.9%).

**High-value (HV)** – emerging photoabsorbers (level 3 readiness). NREL-developed ZnSnN\(_2\) coupled with SrHbCl\(_2\)N are potential efficient and low-cost with high potential impact on global energy economy. Early development hurdles.

**TIN vs TiO\(_2\)** - Rutgers developed thin-film passivation and protection layer.

**LiCoO\(_2\)**, OER catalyst – Rutgers developed alkaline cat. w. performance on par with PGM-catalysts.

**NiP\(_3\)**, HER catalyst - Rutgers developed acid & alkaline cat. w. performance on par with Pt.

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**Key Impact – year 1**

<table>
<thead>
<tr>
<th>Metric</th>
<th>State of the Art</th>
<th>Expected Advance</th>
</tr>
</thead>
<tbody>
<tr>
<td>HP - STH</td>
<td>Non-PMG STH 10%</td>
<td>Match or beat using non-PMG RU-eCats</td>
</tr>
<tr>
<td>HV - Parameter 1</td>
<td></td>
<td></td>
</tr>
<tr>
<td>BiVO(_4)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(J_{ph} \approx 1.12)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(10^{-1} \text{A/cm}^2)</td>
<td>Stable (\geq 90%) for 1h, material cost</td>
<td>Improve two or more metrics</td>
</tr>
</tbody>
</table>

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**Project Relevance and Impact**

- Identify the best technical approaches to fabricate both High Performance (HP) & High Value (HV) PGM–free PECs using:
  - HP PEC NREL–proprietary tandem III–V photovoltaic
  - HV PEC NREL nitrides & Rutgers oxynitrides in tandem
  - Rutgers–proprietary electro-catalysts for O\(_2\) – and H\(_2\) – evolution
- Reveal performance limits of two limiting PV configurations (HP vs HV) using best PGM–free Cats; identify and solve interfacing problems
- Supports the development of non–PGM and scalable electrocatalysts for PEC water splitting
- Aim to lower H\(_2\) costs by increasing STH efficiency, decreasing production costs using lower cost materials, and increase lifetime; critical to achieving the DOE target of hydrogen for \(<\$2/\text{kg}\)

**Innovative Approach**

- Design of catalyst/photoabsorber interfaces using PGM–free RU–eCats with state–of–the–art performance to NREL proprietary photoabsorbers
  - Proprietary OER catalyst (Rutgers)
  - Proprietary HER catalyst (Rutgers)
- Design, fabricate, characterize, and test first example of Rutgers protection (TIN) and eCats (Ni\(_3\)P\(_4\), and LiCoO\(_2\)) layers on NREL HP (np–GaInP/n+–GaAs) and NREL HV (ZnSnN\(_2\))

**Accomplishments and Future Work**

- Electrochemical (dark) anode, successful integration and benchmarking of Ni\(_3\)P\(_4\)/TiN on p–type GaInP; fabrication of GaIn/GaAs high–efficiency PV and of thin–film ZnSnN\(_2\)
- Future work; high performance and value PEC

**HydroGEN Engagement**

- MOCVD GaInP/GaAs growth & engineering capabilities (NREL)
- Solar testing and benchmarking capabilities (NREL)
- Multi–source and reactive sputtering capabilities (NREL)

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\(^{45}\) [https://www.h2awsm.org/sites/default/files/kickoff-project-pec-rutgers.pdf](https://www.h2awsm.org/sites/default/files/kickoff-project-pec-rutgers.pdf)
Protective Catalyst Systems on III-V and Si-based Semiconductors for Efficient, Durable PEC Water Splitting Devices

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**Project Relevance and Impact**

- In order to meet < $2/kg H₂ via STCH pathway need:

**Innovative Approach**

- **Barrier: Stabilization of III–V surfaces in acid**
  - Innovation: Use MoS₂ and other non-precious protective catalysts that are stable in acid, conductive, and active for HER. Developing an understanding of fundamental degradation mechanisms through in situ studies and leverage those insights into better protective catalysts

- **Barrier: Fabrication scheme for high-quality InGaN growth on Si**
  - Innovation: First demonstration of direct nucleation and growth of high-crystalline-quality InGaN on Si by MOCVD in this field

- **Barrier: Stabilization of III–V surfaces in acid**
  - Barrier: Collecting on-sun data at the weeks time-scale
  - Innovation: By stabilizing III–V unassisted water splitting devices for 100’s of hours, we can test them outside for weeks

**HydroGEN Engagement**

- NREL: Characterization of Semiconductor Bulk and Interfacial Properties, Todd Deutsch
  - Characterization of fundamental semiconductor properties and growth defects before and after testing
- NREL: Corrosion Analysis of Materials, Todd Deutsch
  - Pre- and post- failure analysis and improved understanding of catalyst corrosion and interfaces
- NREL: III–V Semiconductor Epi-structure and Device Design and Fabrication, Daniel Friedman
  - Fabrication of III–V materials & improved understanding of growth defects
- NREL: On-Sun Solar-to-Hydrogen Benchmarking, Todd Deutsch
  - Testing station for collection of on-sun data for unassisted water splitting devices

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46 [https://www.h2awsm.org/sites/default/files/kickoff-project-pecstanford.pdf](https://www.h2awsm.org/sites/default/files/kickoff-project-pecstanford.pdf)
Novel Chalcopryites for Advanced Photoelectrochemical Water-Splitting — University of Hawaii

**Project motivation**
- UH/UNLV/Stanford/NREL/LLNL funded by EERE (2014) to identify promising chalcopryites for PEC H₂.
- New absorbers, interfaces and surface protection schemes were evaluated.
- Key barriers identified with these systems will be addressed in this new project.

**Key Impact**

<table>
<thead>
<tr>
<th>Metric</th>
<th>State of the Art</th>
<th>Proposed</th>
</tr>
</thead>
<tbody>
<tr>
<td>STH Efficiency</td>
<td>4%</td>
<td>&gt;10%</td>
</tr>
<tr>
<td>Durability</td>
<td>350 hrs</td>
<td>&gt;1,000 hrs</td>
</tr>
</tbody>
</table>

**Project Relevance and Impact**
- Strengthen theory, synthesis and advanced characterization “loop” to accelerate development of efficient materials for PEC H₂ production.
- Synthesize and integrate existing or exploratory chalcopryites into low-cost PEC devices.
- Chalcopryites are excellent candidates for PEC water splitting
  - Meet efficiency requirements for PEC Hydrogen production at < $2/kg H₂
  - High photocurrent density generation potential
  - Low-cost processes available
  - Demonstrated water splitting with co-planar devices
  - Bandgap tunable and compatible with tandem architecture

**Innovative Approach**
- Novel chalcopryites alloying using printing techniques
  - Replace evaporation with "printing" technique to synthesize Cu(In,Al,B)Se₂ using molecular inks
  - Lower material cost
- Innovative tandem device integration schemes
  - Exfoliation of finished PEC cells and bonding onto fully processed PV drivers to create a semi-monolithic tandem device
  - Concept could be extended to other low-temp. PV classes

**HydroGEN Engagement**
- Leveraging the EMN model for computational material diagnostics, optimization, and synthesis of PEC devices
- National Lab Capabilities:
  - Computational Materials Diagnostics and Optimization (LLNL)
  - I–III–VI Compound Semiconductors for Water-Splitting (NREL)
  - High-Throughput Thin Film Combinatorial Capabilities (NREL)
  - Corrosion Analysis of Materials (NREL)

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47 [https://www.h2awsm.org/sites/default/files/kickoff-project-pec-uhawaii.pdf](https://www.h2awsm.org/sites/default/files/kickoff-project-pec-uhawaii.pdf)
Monolithically Integrated Thin-Film/Silicon Tandem Photoelectrodes for High Efficiency and Stable PEC Water Splitting — U. Michigan, Ann Arbor

**Project motivation**
We aim to tackle the challenges of achieving efficient, cost-effective PEC water splitting devices by developing tandem photoelectrodes, which consist of a bottom Si light absorber and a 1.7-2 eV top light absorber (Ta$_3$N$_5$, BCTSSe, or InGaN). We have previously developed:

- Ta$_3$N$_5$, BCTSSe, or InGaN top photoelectrodes.
- Low resistivity nanowire tunnel junction, which will be used to fabricate top photoelectrode.
- N-terminated GaN, which can protect against photocorrosion and oxidation.

**Key Impact**

<table>
<thead>
<tr>
<th>Metric</th>
<th>State of the Art</th>
<th>Expected Advance</th>
</tr>
</thead>
<tbody>
<tr>
<td>Stability/ Efficiency</td>
<td>~1 hr @ 16%</td>
<td>&gt;1,000 hrs @15%</td>
</tr>
<tr>
<td>Cost/ scalability</td>
<td>~$150 for 4” GaAs wafers</td>
<td>~$100 for 12” Si wafers, i.e. ~10 times reduction in wafer cost</td>
</tr>
</tbody>
</table>

**Project Relevance and Impact**

- Tackle the challenges of achieving efficient, cost-effective PEC water splitting devices by developing tandem photoelectrodes
- Establish a Si-based low cost and scalable platform for high efficiency and highly stable PEC water splitting devices and systems
- Develop monolithically integrated Si-based tandem photoelectrodes, with the objective to achieve high efficiency (up to 20%) and long-term stability (>1,000 hours) solar–to–H$_2$ conversion through PEC water splitting
- Success of this project will help meet the DOE technical target for H$_2$ production from PEC water splitting

**Innovative Approach**

- Si as the bottom light absorber to reduce the cost of tandem water splitting devices
  - 1.7–2 eV top light absorber (Ta$_3$N$_5$, BCTSSe, or InGaN)
- Low cost Ta$_3$N$_5$, BCTSSe, and In0.5Ga0.5N photoelectrodes as the top light absorber
- Wide bandgap GaN nanowire tunnel junction to fabricate top photoelectrodes on Si
- Surface protection by N-terminated GaN surfaces
  - Stable in water splitting; efficient hole extraction since polarization field is aligned along the growth direction.

**Accomplishments and Future Work**

- Demonstrated 1.7 – 2 eV top photoelectrodes with improved performance
- Achieved functional nanowire tunnel junction on Si wafer
- Studied the mechanism for the stability of N-rich GaN photoelectrodes

**HydroGEN Engagement**

- Surface analysis cluster tool, surface measurements (NREL)
- Photoelectrochemical AFM and STM (LBNL)
- Ab initio modeling of electrochemical interfaces (LLNL)
- Surface modifications and protection (NREL)

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[48](https://www.h2awsm.org/sites/default/files/kickoff-project-pec-umichigan.pdf)
Efficient Solar Water Splitting with 5,000 Hours Stability Using Earth-abundant Catalysts and Durable Layered 2D Perovskites \(^{49}\) LANL

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**Project Relevance and Impact**

- Long term goal
  - Demonstrate a disruptive PEC technology with >5000 hours of operation by interfacing stable hybrid perovskites with HER and OER catalysts with 12% STH efficiency to produce hydrogen for <$2/kg

- 1 year goal
  - Demonstrate band-gap tunability from 1.5 to 2.0 eV with the appropriate band alignments
  - Demonstrate photocathode and photoanodes using hybrid perovskites with standard catalysts (with EMN Node LBNL)
  - Demonstrate first of its kind photocathode and photoanode with 1000 hours of stability

**Innovative Approach**

- Innovative PEC device design for optimal collection of sunlight using tandem perovskite solar cells in series.
- Design of tunnel barriers for >20% perovskite solar cells with 1000 hrs stability in operation (<10% \(V_{OC}\) degradation).
- Synthesis of perovskite materials with optimal optical and electronic properties for water splitting: bandgap tunability, energy level alignment, work functions, transport properties
- HER and OER catalysts made from earth abundant materials (precious metal free).
- Discovery of a new mechanism to stabilize perovskite thin films (Science 2018) \(>1500\) hrs perovskite solar cells with >20% efficiency
- Perovskite with tunable bandgap (1.5 – 2 eV) and optimized band alignment

**HydroGEN Engagement**

- LBNL: PEC measurements and benchmarking
  - Established device design and interface layers for photocathode & anode
  - Design of complete PEC cell and validated design by loading perovskite/Pt photocathodes
  - Three batches of perovskite solar cells exchanged with different barrier layers
- NREL: Techno economic analysis of perovskite based PEC system – Dr. Genevieve Saur
  - Working to develop a rough techno-economic evaluation of the perovskite–based PEC
- Benchmarking PECs: Participating in ECS working group for standardizing PECs
- Data Hub: Uploaded data on perovskite solar cells with >20% efficiency and stability

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49 https://www.h2awsm.org/sites/default/files/kickoff-project-pec-lanl.pdf
Solar Thermochemical H₂ Production Projects
Computationally Accelerated Discovery and Experimental Demonstration of High-Performance Materials for Advanced STCH Hydrogen Production

Project motivation and Key Impacts
This project builds on prior collaborative computational and experimental work at CU Boulder which demonstrated the viability of new spinels for STCH. This project combines efforts at CU, NREL, and SNL involving machine learning, ab initio calculations, and experiment to develop new perovskites and spinels for more efficient STCH production.

<table>
<thead>
<tr>
<th>Metric</th>
<th>State of the Art</th>
<th>Proposed</th>
</tr>
</thead>
<tbody>
<tr>
<td>Computational Validation</td>
<td>N/A</td>
<td>Matching expt and comp. thermo. and kinetic properties</td>
</tr>
<tr>
<td>H₂ productivity</td>
<td>Ceria: 130 μmol/g (1500°C/1000°C)</td>
<td>200 μmol H₂/g</td>
</tr>
<tr>
<td>Temperature</td>
<td>TREQ≥1500°C</td>
<td>Treq≤1450°C</td>
</tr>
<tr>
<td></td>
<td>ΔT≥700°C</td>
<td>ΔT≤400°C</td>
</tr>
</tbody>
</table>

Project Relevance and Impact
- Utilize machine-learned models coupled with *ab initio* thermodynamic and kinetic screening calculations to accelerate the RD&D of new STCH materials
- Demonstrate the accuracy of thermodynamic and kinetic models predicting the properties of STCH materials which will allow for rapid screening and discovery of new materials
- To reach goal of <$2/kg H₂
  - Improved redox material efficiency and stability

Innovative Approach
- Develop machine learning models to predict material stability of materials at STCH conditions for rapid screening
- Thermodynamic screening of active materials
  - Computationally evaluate candidate materials for thermodynamic viability
  - Utilize ML models to filter materials; provide candidate materials for computational kinetic screening
- Kinetic screening of active materials
  - Identify kinetically active materials through computational screening
  - Rapid TS Search for Kinetic Screening
  - Study of charged O vacancies
- Experimental demonstration of active materials
  - Utilize SFR and TGA to evaluate thermodynamic and kinetic properties of new materials

HydroGEN Engagement
- Leveraging the EMN model to provide critical information/feedback to all aspects of the project National Lab Capabilities:
  - Machine Learning the Gibbs Energy of Compounds (NREL)
  - Thermodynamic Evaluation of Charged vs. Neutral Defects in Spinels (NREL)
  - Kinetic Screening (SNL)
  - Experimental Testing of Materials Stagnation Flow Reactor Provides Measurement of H₂ Produced by New Materials (SNL)

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50 https://www.h2awsm.org/sites/default/files/kickoff-project-stch-cu.pdf
Transformative Materials for High-Efficiency Thermochemical Production of Solar Fuels\textsuperscript{51} — Northwestern University

### Project Motivation

Project builds on background of PIs in STCH materials, attempt to combine high-throughput computational and experimental exploration of oxygen off-stoichiometric oxides and phase change materials for enhancing the efficiency of STC production of solar fuels

### Key Impact

Identify promising compounds which show:
- a) ground state stability/synthesizeability of compound
- b) thermodynamics favorable for $<1400^\circ\text{C}$ reduction and c) thermodynamics favorable for facile water splitting. State-of-the-art currently CeO$_2$ and SLMA perovskite.

### Project Relevance and Impact

- Combine high-throughput computation and experiment to study the properties of novel, predicted STCH materials and explore enormous combinatorial space of materials, to “tune in” desired STCH enthalpy and entropy of reduction; combination will greatly accelerate this materials discovery effort
- Design materials with reduced temperatures of reduction but sufficient gas-splitting rates
- Identify promising compounds which show:
  - Ground state stability/synthesizeability of compound
  - Thermodynamics favorable for $<1400^\circ\text{C}$ reduction and facile water splitting

### Innovative Approach

- Break false dichotomy of off-stoichiometric material exhibiting better connects and phase transforming materials exhibiting large degree of reduction by designing a set of new materials and reactions:
  - Phase transformation—with specifically tuned off-stoichiometric composition in both phases
- The Open Quantum Materials Database (OQMD)
  - High-Throughput of $\sim$11,000 ABO3 perovskites screened for stability and reduction enthalpy

### Accomplishments and Future Work

- Thermodynamics Measurements
- YMnO$_3$: synthesis and characterization, reference state nonstoichiometry, TG measurements and redox thermodynamics in oxidizing conditions
- Engineering the reduction enthalpy of RMnO$_3$ perovskites
- High-throughput discovery of double perovskites

### HydroGEN Engagement

- Computational materials science (NREL)
- Mesoscale modeling capabilities (SNL)
- In-situ XRD and materials synthesis (NREL)

\textsuperscript{51} https://www.h2awsm.org/sites/default/files/kickoff-project-stch-northwestern.pdf
Mixed Ionic Electronic Conducting Quaternary Perovskites: Materials by Design for STCH H₂ — Arizona State University

Project Relevance and Impact

- Efficiency of the hydrogen production pathway is of critical importance to achieving :: $2/kg.
  - This project makes a direct connection between computational thermodynamics, the efficiency, and management of the uncertainties.

Innovative Approach

- $\mu_0$ of gas phase components (H₂O, H₂, and O₂) can be obtained from experimental data
  - Available at the National Institute of Standards and Technology (NIST)
- $\mu_0$ of the solid phase requires calculating the Gibbs energy as a function of temperature
  - Density functional theory (DFT+U) based approaches can yield good estimates for enthalpy, but estimating entropy is non-trivial
  - Aim to construct ‘simple’ thermodynamic models to estimate Gibbs energies.
- Validate models with available data
  - Systems of interest: CeO₂, (Ce,Zr)O₂, La₁₋₅Sr₅MnO₃, other perovskites (up to doubly substituted) and possibly fluorites

HydroGEN Engagement

- Uncertainty Quantification (SNL) in Computational Models of Phys. Sys.
  - Facilitate answering the question how accurate in measurements or computation is accurate enough to meaningfully inform materials discovery
  - Controlled Materials Synthesis and Defect Engineering (NREL)
  - Facilitate validation of DFT+U predictions and further testing of candidates
- HT-XRD and Complementary Thermal Analysis (SNL)
  - Facilitate experimental determination of the oxygen chemical potential, $\Theta_{0}\to\Theta
- Laser Heated Stagnation Flow Reactor (SNL)
  - Facilitate a potentially faster but less accurate determination of $\Theta_{0}\to\Theta

Accomplishments

- Predictive power demonstrated
- Two candidates with thermodynamic response maps completed and submitted to the consortium; synthesized in collaboration with NREL Node
- X-ray diffraction (SNL) measures structure, phase purity, and lattice constants HT-XRD and Complementary Thermal Analysis (SNL)

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High Temperature Reactor Catalyst Material Development for Low Cost and Efficient Solar Driven Sulfur-Based Processes\textsuperscript{53}—Greenway Energy

### Project History and Key Impacts
- GWE, USC and SRNL have been working together on H\textsubscript{2} and renewable energy based systems
- INL and SRNL were involved in the NHI for sulfur based thermochemical cycles development
- NREL and GWE have common experiences in solar applications

<table>
<thead>
<tr>
<th>Metric - Milestones</th>
<th>State of the Art</th>
<th>Proposed</th>
</tr>
</thead>
<tbody>
<tr>
<td>Catalyst</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Activity (molSO\textsubscript{2}/h/gcat)</td>
<td>0.23</td>
</tr>
<tr>
<td></td>
<td>Degradation (%)/hour</td>
<td>0.030</td>
</tr>
<tr>
<td>Efficiency - Sun to H\textsubscript{2} (%)</td>
<td>16 % (LHV)</td>
<td>&gt; 20 % (LHV)</td>
</tr>
<tr>
<td>Cost - H\textsubscript{2} cost ($/kg)</td>
<td>3.6 – 7.6</td>
<td>&lt; 2</td>
</tr>
</tbody>
</table>

### Project Relevance and Impact
- Objective – efficient and low cost solar thermochemical process
  - Improved catalyst development and test (100 hours) showing reduced deactivation
  - Design of improved reactor allowing for increased efficiencies and cost reduction
  - Techno-economic analysis of the overall solar HyS plant
- Desirables
  - Increase of the energetic and exergetic efficiency (solar to H\textsubscript{2} energy efficiency > 20%)
  - Cost reduction of H\textsubscript{2} to < $2/kg

### Innovative Approach
- Catalyst fundamentals understanding, development, and tests
  - Novel Electroless Deposition approach for bi–metallic catalyst formulations based on the Surface Free Energy of the metals
  - New catalyst material using our demonstrated surface free energy (SFE) and electro–less deposition technique
- Engineering Design in reactor baseline configuration, numerical modeling, fabrication, and tests
  - Novel direct solar cavity receiver–reactor, based on NREL concept (cavity solar reactor)
- System Analysis on overall solar plant design and economic–financial analysis
  - Novel HyS flowsheet with chemical storage and direct solar receiver
  - New effective solar–thermochemical plant process integration

### HydroGEN Engagement
- Identified Baseline Monometallic Configuration and Initial Bimetallic Formulations through Testing (INL)
- Scaled up Receiver Reactor Design with Integrated Solar Received–Reactor Configuration (NREL)
- HyS Process Flowsheet (SRNL)
- Solar Plant System Design and Analysis (NREL)

\textsuperscript{53} \text{https://www.h2awsm.org/sites/default/files/kickoff-project-stch-greenway.pdf}
Accelerated Discovery of STCH Hydrogen Production Materials via High-Throughput Computational and Experimental Methods — Colorado School of Mines

Project Relevance and Impact

- In order to meet < $2/kg H₂ via STCH pathway need:
  - Large improvements in hydrogen production capacity (mmol H₂/g oxide cycle)
  - Lower reduction temperatures
  - High conversion capability
  - Fast redox reaction kinetic
- Merging combinatorial synthesis methods with combinatorial theoretical calculations to rapidly discover new potential materials for use in two–step metal oxide cycles for STCH—greatly increasing the number of viable STCH material candidates
- Promising new STCH materials candidates as well as the broader structure–property–performance relationships discovered in this project will be shared

Innovative Approach

- DFT Screening
  - Screen > 1000 perovskites for suitability and stability under two–step STCH cycling conditions
  - Directly calculate the effect on vacancy formation energy by adding cerium to the perovskite families that meet the stability screening
  - Expand search to more complex multi–cation permutations to identify potential trends
- Experimental Screening
  - Combinatorial thin–film deposition allows for the synthesis of compositional libraries enabling screening of large compositional spaces and also provides validation data to inform the next round of computations
  - Many transition metal containing oxides change color depending on O₂ content allowing for potential of a single screening experiment to evaluate multiple compositions simultaneously

HydroGEN Engagement

- Leveraging the EMN model of merging high–throughput computational and experimental techniques to accelerate new materials discovery

National Lab Capabilities:

- First Principles Materials Theory for Advanced Water Splitting Pathways
- (NREL) High–Throughput Experimental (HTE) Thin Film Combinatorial Capabilities (NREL)
- Virtually Accessible Laser Heated Stagnation Flow Reactor for Characterizing Redox Chemistry of Materials under Extreme Conditions (SNL)

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54 https://www.h2awsm.org/sites/default/files/kickoff-project-stch-csm.pdf
Water-Splitting Benchmarking/Protocols Project\textsuperscript{55}
IEA-HTCP Task 35 Final Report

Benchmarking Advanced Water Splitting Technologies

Presenter: Kathy Ayers
November 15, 2017
HydroGEN Kick-Off Meeting, NREL

HydroGEN Kick-Off Meeting

Benchmarking Advanced Water Splitting Technologies

PI: Kathy Ayers, Proton OnSite
Co-PIs: Ellen B. Stachel, ASU; Olga Marina, PNNL; CK Xiang, Caltech
Consultant: Karl Gross

Project Vision
A cohesive R&D community working together, interacting with the EMN to define targets, best practices, gaps, and priorities, aggregating and disseminating knowledge, leading to accelerated innovation and deployment of advanced water splitting technologies.

Project Impact
Development of a community-based living roadmap across technologies to assist in maintaining a balanced DOE portfolio.

Innovation and Objectives

Project history
Team of subject matter experts assembled for each sub-area to engage with each sub-community.
Consultant from a similar effort in hydrogen storage added to convey lessons learned.

Proposed targets

<table>
<thead>
<tr>
<th>Metric</th>
<th>State of the art</th>
<th>Protocol</th>
</tr>
</thead>
<tbody>
<tr>
<td>Surveys for priorities</td>
<td>High N-response and opportunity for dialogues</td>
<td></td>
</tr>
<tr>
<td>Metrics</td>
<td>CA/Ni</td>
<td>Component-level parameters; system considerations</td>
</tr>
<tr>
<td>Node assessment</td>
<td>NA</td>
<td>Identification of gaps and strategies</td>
</tr>
</tbody>
</table>

Barriers
Lack of consensus regarding testing protocols/standards
Large diversity of information to sample and develop recommendations from different TEIs for different technologies.

Partnerships
- LTE (TRL/FSM): Proton
- HTE (SOEC): PNNL
- STCH: ASU
- PEC: Caltech
- Consultant: Karl Gross

Specific Project Objectives

- Develop a database for protocols/standards and performance of materials, components, devices, and systems
- Facilitate acceptance of community-wide technology
- Establish an annual workshop to share learnings and develop recommendations within and across technology areas
- Assess capabilities and identify gaps for development
- Promote acceptance of protocols and methodologies including cost and performance assessments
- Assemble roadmaps to further development of each technology pathway

Effective Leveraging of the EMN Resource Nodes

- Overarching effort for HydroGEN consortium
  - LTE, HTE, STCH, and PEC technologies
- Goal: develop a roadmap across technologies to assist in maintaining balanced DOE portfolio
  - Protocol and benchmarking development
  - Specific needs for each technology
  - Coordination effort across technologies
- Approach: engage subject matter experts, Steering Committee, FCTO staff, and community in dialogue for each pathway
  - Gather through surveys and questionnaires
  - Assess capabilities and gaps, including EMN lab nodes
  - Recommend standards, protocols, and priorities
  - Assemble themes into cohesive strategy

Project Tasks

Task 1: Framework Set-up
Task 2: Capabilities Assessment
Task 3: Protocol Definition
Task 4: Protocol Verification and Revision
Task 5: Program Management

73
IEA-HTCP Task 35 Final Report

**Task 1: Framework Set Up**
- **Goal:** Develop a searchable library of screening tools, materials, and state of the art technology (with HydroGEN)
  1. Survey Development (Sept-Nov): Develop initial questions to guide standardization
  2. Data Collection (Dec-Feb): Solicit input from the water splitting community via questionnaires, conference symposia, and network interaction
  3. Data Analysis and Workshop Planning (March-Aug): Work with the HydroGEN Steering Committee and DOE to plan the Year 1 workshop

**Task 2: Capabilities Assessment**
- **Goal:** Assess existing capabilities within the EMN across all water splitting pathways
  1. Assessment of EMN Nodes (Nov-Feb): Summarize Node capabilities based on website, interviews, and expert knowledge
  2. Gap Assessment (Mar-Jul): Define technology subcomponents and potential metrics of importance. Assess additional needs and recommend capabilities.

**Task 3: Protocol Definition**
- **Goal:** Develop bench scale protocols for each water splitting pathway as output of Year 1 workshop
  1. Data Collection and Parameter Definition (Jun-Aug): Comparison and evaluation of test configurations for each technology area; assessment of benefits and disadvantages to determine what works best
  2. Bench Scale Protocols (Aug-Feb): Solicit feedback from Year 1 workshop on testing standards and conditions. Synthesize into recommended protocols.

**Task 4: Protocol Verification / Refinement**
- **Goal:** Verify procedures and configurations have been sufficiently defined for reproducible results
  - Nov ‘18- Feb ‘19:
    1. Compile and publish workshop outcome results.
    2. Initiate round robin testing at project team and EMN locations, and by additional experts in the specific technology area.

**Task 6: Program Management**
- **Goal:** Ensure protocols and Best Practices are developed in accordance with broader EMN guidelines
  - Sept ‘17 - Feb ‘19
    1. Work closely with DOE FCTO Managers and technical and data experts in the HydroGEN EMN Consortium
    2. Apply lessons learned from similar effort in storage
    3. Participate in HydroGEN collaboration meetings as requested by DOE (including up to annual presentations to HydroGEN Production Tech Team)
    4. Re-examine status and outcomes of Tasks 1-2 annually and provide up to date capability and gap assessments.

**Groundwork for 2B Efforts**
- Electrolysis workshop at NREL, 2014
- ECS Cross-cutting symposium
- Water splitting workshop at Stanford, 2016
- IEA task on electrolysis (fuel cell annex)
  - Initial discussions of protocols
  - Round robin testing
  - International workshop on STCH, 2017
  - Knowledge of community for each of the leads
  - Hydrogen storage perspective
Risks and Mitigation

• Differing TRLs and pace of progress:
  - Maintain strong core team and HydroDEN Steering Committee engagement
  - Okay to have different timelines for different technologies; focus on vision

• Engagement of the broader (non-EMN) community:
  - Consider different access levels and means for participation/feedback from broader group

• Managing wide diversity of information:
  - Leverage data experts at NREL for organization
  - Lessons learned from storage effort and PEC working group on getting to consensus and identifying key directions

• Lack of controls and baselines/standard conditions:
  - Potential round robin testing for certain tools

Specific Challenges: LTWE

• Degradation of membranes over time (chemical or mechanical) resulting in lack of strength/robustness

• Lack of accelerated stress tests with relevant mechanisms for long term durability assessment

• Interfacial contact between catalyst layer, membrane, and gas diffusion layer

• Lack of stable materials with required conductivity and mechanical strength at 2V potentials

• Lack of long term data for more aggressive operating conditions (temperature, pressure, current density)

Specific Challenges: HTWE

• Only lab scale single cell or short stack test data is available.

• There are no reliable methods or diagnostic techniques to predict lifetime of SOEC systems

• With dynamic load and temperature transients, it is difficult to accurately collect and validate the long-term performance data.

• High temperatures affect material stability, long term durability; slow start-up required to avoid component cracking and oxidation. Cycling operation is challenging.

• Effects of operating conditions on SOEC performance and lifetime are not well understood.

Specific Challenges: PEC

• Scale-up challenge: from current laboratory scale (typically <0.00001 kg/day) to bench scale (0.1 kg/day) and sub-scale (2 kg/day).

• Lack of performance data and test protocols for photoelectrodes under real-world operating conditions (diurnal cycle or/and elevated temperature).

• Lack of fundamental understanding of photocathode corrosion mechanisms and accelerated test protocols.

• Integration challenges at component level for catalysts, light absorbers and protective coatings.

Specific Challenges: STCH

• Identifying suitable materials with required redox capacity and/or fast enough kinetics

• Measuring thermodynamic and kinetics over wide operating conditions for a range of materials

• Developing accelerated durability testing protocols

• Understanding and/or minimizing degradation of redox active materials over time (chemical or mechanical)

• Acquiring long term data for aggressive operating conditions (temperature and oxygen partial pressure swings)

• Performance and degradation results will depend on the material form factors, which will depend on the reactor designs (still in development in parallel and outside the consortium)

Support: H2 Technology Consulting

• Dr. Karl Gross: consultant to the Benchmarking Advanced Water Splitting Technologies Project; led similar project on development of best practices for the DOE Hydrogen Storage subprogram.
  - Goal: establish uniform practices and standards in measurement and evaluation of crucial material performance data.
  - Involved wide-ranging community involvement (15 co-authors and 34 international contributors).
  - Resulting public document can be found at: https://nrel.gov/acs/wealth/downloads/recommended-best-practices-characterization-storage-properties-hydrogen.pdf

• Goal of H2Tech in this EMN project is to provide clear support based on experience and knowledge gained from the H2 storage work.
Major challenges in creating a unified framework

Across the advanced water splitting technologies:
1. Large discrepancy in TRU/MRLs
2. Large discrepancy in definition of targets amongst and between widely differing technologies,
3. IP issues with cell designs for more mature technologies,
4. Component interactions and relative scale between components
5. Differing perspectives as to the most important performance characteristics.

For all four technologies, electrode integration, reactor design, and system design can be as important as ex-situ, in-situ, and in operando material testing in influencing performance and cost.

2B Breakout Sessions

Goals:
- Lay early groundwork for Year 1 workshop
- Input on status and needs for each community
  - What level of background exists
  - What analysis and modeling techniques can be applied
- Understand important operating considerations
  - Degradation understanding
  - For comparison of materials across different cell/system set ups
- Initial feedback from 2A teams on desired outcomes

Working with the EMN Teams

- We are relying on input from all technology areas
  - Key information resources, roadblocks, needs, etc.
  - Open discussion on different pathways within and between technologies
- We need your feedback on the approach!
  - Ideas on how to do things differently
  - How you want to work with us as a team
INTERNATIONAL COLLABORATIVE ACTIVITIES

SUBTASK 1: Renewable Electrolysis

- Meeting Participation:
  - 2014 Fall ECS Meeting Electrolysis Section: held in conjunction with the 2014 Fall ECS Joint International Meeting on October 5-9 2014 in Cancun, Mexico.
  - 215 IEA-AFCIA Annex 30 Workshop: A workshop was held at the Herten Hydrogen Centre of Excellence on April 20-21, 2015 in Herten, Germany. This workshop allowed electrolysis experts to share knowledge and develop standards and protocols in stress testing. The standardization of definitions, terminology and electrolyzer classification was also discussed.
  - 2016 The CertifHy Public Launch Meeting was held on April 23, 2015 in Brussels, Belgium.
  - 2016 The IEA Annex 30 Workshop was held on February 29 – March 1, 2016 in Tokyo Japan.
  - 2016 The International Hydrogen & Fuel Cell Expo was held on March 2 – 4, 2016 in Tokyo, Japan.
  - 2016 The IEA Annex 30 & Task 33 Meeting was held on October 20– 21, 2016 in Oslo, Norway (Summary Below).
  - 2016 The Next Generation Power Electronics Workshop held by the US DOE Fuel Cell Technologies Office, National Institute of Standards and Technology, and the PowerAmerica Institute on wide bandgap semiconductors will be held on December 5, in Gaithersburg, Maryland.

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56 From https://orise.orau.gov/iccpt/
• **Special Projects:**
  o 2015 Book chapter “Hydrogen Production from Renewable Energies – Electrolyzer Technologies” edited by electrolysis experts Tom Smolinka, Emile Tabu Ojong, and Jürgen Garche was published by Elsevier.
  o 2015 The Electrolysis Metric Standardization Project was initiated.

**SUBTASK 2: Photoelectrochemical Water Splitting**

• **Meeting Participation:**
  o 2014 Hu’a Iki SF: April 21st, 2014 Co-located IEA-HIA Renewable Hydrogen PEC subtask meeting and the DOE PEC WG Meeting, held at Stanford University, in conjunction with PEC session organizers at the 2014 Spring MRS Meeting in San Francisco.
  o 2014 Hu’a Iki Berlin: held in conjunction with the 20th International Conference on Photochemical Conversion and Storage of Solar Energy (IPS-20), 27 July – 1 August 2014 in Berlin.
  o 2015 Spring MRS: The Materials Research Society Conference was held in San Francisco on April 6-10, 2015. PEC Subtask members met to discuss whitepapers other priority actions.
  o 2015 The Electrochemical Society 2015 Fall meeting was held on October 11 – 16, 2015 in Phoenix, Arizona.
  o 2016 The Gordon Research Conference: Renewable Energy: Solar Fuels conference was held on February 28 – March 4, 2016 in Tuscany, Italy.
  o 2016 The Electrochemical Society 2016 Spring meeting was held on May 20 – June 2, 2016 in San Diego, California.
  o 2016 The Materials Research Society International Materials Research Congress meeting was held on August 13 - 19, 2016 in Cancun, Mexico (Summary Below).
  o 2016 The Electrochemical Society PRiME Conference was held on October 2-7, 2016 in Honolulu, Hawaii.

• **Special Projects:**
  o 2014 Ten existing PEC White Papers were updated and four new PEC White Papers were initiated
  o 2015 A special PEC issue written by experts in the international PEC community is being published in *Energy & Environmental Science*.

**SUBTASK 3: Solar-Thermochemical Water Splitting**

• **Meeting Participation:**
  o International Workshop on Reaction Kinetics of Solar Thermochemical Redox Cycles for Splitting H2O and CO2 held on 11 September 2014 in Zurich, Switzerland.
  o 2015 CMCEE-11: The American Ceramics Society co-hosted the 11th conference on Ceramic Materials and Components for Energy and Environmental applications held in Vancouver, B.C., Canada on June 15-19, 2015. STCH working group members met to discuss various aspects of STCH R&D including redox active materials, reactor designs, and opportunities for collaboration.
o 2015 Sandia National Labs and DOE hosted technical experts and working group members from the German Aerospace Center (DLR) at the National Solar Thermal Test Facility (NSTTF) located in Albuquerque, NM on June 24-26, 2015. Dr. Christian Sattler gave an overview presentation of ongoing STCH projects funded by the European Union.


o 2016 A workshop in Melbourne and Canberra, Australia at the annual review of the Australian Solar Thermal Research Institute (ASTRI) was held in mid-May of 2016.

o 2016 The International Energy Agency – SolarPACES: 22nd Annual Meeting was held in Abu Dhabi, United Arab Emirates on October 11-14, 2016 (Summary Below).

o 2016 The Capacity Building Workshop – Soiling Mitigation for Solar Energy and innovations in Concentrating Solar Power was held by the University of Florida. on December 7-8 in Gainesville, Florida.

• Special Projects:
  o 2014 Initial discussions on the development of STCH White Papers were held.
  o 2015 The STCH Cycles Reevaluation Project was initiated.

Cross-Cutting Activities:

• Meeting Participation:
  o 2015 AMR All-Hands Renewable Hydrogen Meeting: The US Department of Energy’s Hydrogen and Fuel Cells Program Annual Merit Review (AMR) Meeting, one of the premier world meetings dedicated to the research and development of hydrogen and fuel cell technologies, was held in June 2015 and included an “All-Hands Renewable Hydrogen” side meeting that brought together leading experts in electrolysis, PEC, STCH and biological hydrogen production, (including numerous IEA-Task 35 experts) to discuss technology status and to define high priority technology-specific projects which would provide the best benefit to the entire renewable hydrogen research and development community.

  o 2016 The Solar Fuels Generation: PV and Electrolysis Workshop sponsored by the Institute of Energy Conversion (IEC) and the University of Delaware Energy Institute (UDEI) was held on March 7-8, 2016 at the University of Delaware.

  o 2016 The Advanced Water Splitting Materials Consortium Meeting was held on April 14-15, 2016 in Stanford, California.


• Special Projects:
  o 2015 Projects initiated at the All-Hands Meeting included the previously-listed Electrolysis Metrics Standardization Project; the PEC International Roadmap Project; and the STCH Cycles Reevaluation Project.
Sample Detailed Summaries

SUBTASK 1: Renewable Electrolysis

- **2014 ECS Meeting Electrolysis Session:** HyET led off the session with discussion of electrochemical compression. Operating efficiency was compared for different mechanical compressors vs. the electrochemical cell. HyEt has demonstrated 150 bar compression with less than 10 mA/cm2 hydrogen crossover current. DLR (the German Aerospace Center) presented a talk on sintering titanium on stainless steel bipolar plates. The plates are still plated with platinum but estimated cost for large scale plates was significantly lower than current plates. KIST gave a presentation on electrodeposited IrO2 (from Ir(CO)2(OH)4) and claimed they could reduce loading from 0.5 mg/cm2 to 0.05 without initial performance degradation. Giner presented work on OER supports, including TiC, ITO, TiN, W-doped TiO2, TiO2 nanowires, graphitic carbon nitride, and borocarbon nitride. TiO2 based materials showed the best stability. DTU discussed high temperature KOH electrolysis. Catalysts evaluated for the cathode side were Raney Ni, Mo, or Pt; anode catalysts were Co3O4, perovskites, Ni-oxides, and Ir/Ru oxides. Maximum operating temperature was 300°C; maximum pressure was 95 bar. At 250°C they were able to demonstrate 2.3 A/cm2 at 1.75V. Another interesting talk which was not part of the electrolysis session was by the Naval Research Lab, on 3D printing of bipolar plates, with Treadstone coatings (protective oxide layer with conductive islands). Some of the issues encountered included dimensional tolerances from plate to plate and resulting issues in stack up/compression, and post machining which added cost. The Treadstone layer did very well even on the fairly rough parts – the coating was required because the print media was a Ti-6Al-4V alloy, which was not stable by itself.

- **2015 IEA-AFCIA Annex 30 Workshop in Herten:** A workshop was held at the Herten Hydrogen Centre of Excellence on April 20-21, 2015 in Herten, Germany. This workshop brought together leaders in electrolysis and fuel cells from around the world including Proton, Hydrogenics, H2Gen, Siemens, Giner and more. This workshop allowed experts to learn from other experts by discussing what the fuel cell industry and market will look like in the future. In support of the industry as a whole, discussions were held on how to move the entire industry forward through the implementation of stress testing protocols and standards for components including catalysts, membranes and separator plates. In addition, progress was made by identifying and initiating efforts to establish standard definitions, terminology and classifications of electrolyzers. Other discussion topics included cost targets and cost reduction for electrolysis, and recent developments in the electrolysis industry. There was also a laboratory tour of a wind powered electrolysis system which allowed participants to view an example of renewable electrolysis.

- **2015 International Book Chapter:** The international community, including experts from IEA-HIA and IEA-AFCIA, has written a book chapter titled “Hydrogen Production from Renewable Energies – Electrolyzer Technologies” that was published in the Elsevier book *Electrochemical Energy Storage for Renewable Sources and Grid Balancing* in early 2015. This chapter, written by Tom Smolina, Emile Tabu Ojong, and Jürgen Garche, gives an introduction and overview on modern electrolyzer technologies. Specific topics covered in the chapter include the fundamentals of water electrolysis, alkaline water electrolysis, proton exchange membrane (PEM) electrolysis, high-temperature water electrolysis and a discussion on cost.
**2015 CertifHy Public Launch Meeting in Brussels:** The goal of the CertifHy Project Consortium is to develop the first EU-wide framework for the generation of guarantees of origin (GoO) for green hydrogen. The project, brings together the Energy Research Centre of the Netherlands (ECN), Ludwig Bölkow Systemtechnik (DE) and TÜV SÜD, and is supported by a wide range of key European industry leaders including gas companies, energy utilities, green hydrogen technology developers and automobile manufacturers. The CertifHy project public launch conference took place on April 23th, in Brussels. The goals, activities and first results of the project were presented. Over 50 participants from over 8 countries had the opportunity to provide their experiences and input on existing schemes. All participants were invited to provide their views on how to best set an effective system that can gain acceptance and support among policy makers. Electrolysis was well represented, including Task 35 Experts.

**2015 International Hydrogen & Fuel Cell Expo in Tokyo:** The 12th International Hydrogen & Fuel Cell Expo was held in Tokyo, Japan. This exposition had over 21,000 attendees from 65 different countries. This expo, the largest of its kind, highlighted Fuel Cell Electric Vehicles, hydrogen infrastructure, hydrogen stations, storage tanks, sensing devices, dispensers and component technologies. Keynote presentations were given by Chihiro Tobe of the Ministry of Economy, Trade and Industry’s Hydrogen and Fuel cell Promotion office, Sunita Satyapal of the U.S. Department of Energy’s Fuel Cell Technologies Office, Toshihiro Mibe of Honda Motor, Eiichi Harada of Kawasaki Heavy Industries, Toshimitsu Fujiki of the Ministry of Economy, Trade and Industry’s Energy Conservation and Renewable Energy Department, and David Friedman, the Deputy Assistant Secretary of the U.S. Department of Energy’s Energy Efficiency and Renewable Energy Office.

**2015 IEA-AFCIA Annex 30 & Task 33 Meeting in Norway- Detailed Report:**

Dr. Guido Bender is the lead scientist for NREL’s fuel cell and electrolysis development and testing laboratory. Dr. Bender was asked to participate International Energy Agencies (IEA) combined Task33 and Annex 30 meeting which was held at the Institute for Energy Technology (IFe) in Kjeller near Oslo, Norway. Here, he presented an overview of water electrolysis activities at NREL and in the United States. Below is a summary of his activities at the Meeting involving renewable hydrogen production through electrolysis.

Dr. Bender attended the International Energy Agencies (IEA) combined Task33 and Annex 30 meeting which was held at the Institute for Energy Technology (IFe) in Kjeller near Oslo, Norway. Introduction and overviews of both activities were given by the respective operating agents Øystein Ulleberg and Jürgen Mergel. The main purpose of Task 33, Local H2 Supply for Energy Applications, is to contribute to the development, evaluation, and harmonization of on-site hydrogen production technologies and systems in order to facilitate optimal use of local feedstock and removal of barriers for introduction into energy markets. The task force envisions achieving this by continuing and strengthening an existing IEA network of reformer and electrolyzer technology providers and hydrogen end-users, including gas and car companies. The Annex 30 focuses on electrolysis, particularly alkaline electrolysis with liquid alkaline electrolyte, acidic PEM electrolysis with a proton conducting polymeric solid electrolyte, and high temperature electrolysis with a solid oxide based electrolyte.

Day 1 started out with a Water Electrolysis Seminar in the morning followed by a joint meeting of Task 33 and Annex 30. There were about 60 attendees, mostly from Europe, with some attendees from Asia and two from the US. Attendees from industry slightly outnumbered attendees from research institution, but it was almost a 1:1 ratio. The main events in the morning were a key note lecture by Marcelo Carmo from FZ Jülich followed by company
presentations from NEL Hydrogen, Siemens, Hydrogenics, and Proton OnSite. Marcelo listed the main challenges that need to be overcome to make water electrolysis cost effective and successful on a large scale to be: the scale up towards MW systems, the decrease of investments cost, the improvement of stack performance via membrane (PEM WE) / diaphragm (alkaline WE) and catalyst development for oxygen evolution reaction (PEM WE) and hydrogen evolution reaction (alkaline WE), dynamic/more flexible operation including start-up, and pressure operation. He pointed out that it is important to have targets for these development areas and presented the plans from the Fuel Cells and Hydrogen Joint Undertaking (FCH JU), which is a partnership between the European Commission, fuel cell and hydrogen industries presented by Hydrogen Europe and the research community represented y the research grouping N.ERCHY as follows:

Table 1: Development targets formulated by FCH JU.

<table>
<thead>
<tr>
<th></th>
<th>SOA</th>
<th>2017</th>
<th>2020</th>
<th>2023</th>
</tr>
</thead>
<tbody>
<tr>
<td>Efficiency [kWh/Nm³]</td>
<td>5.40</td>
<td>4.95</td>
<td>4.68</td>
<td>4.5</td>
</tr>
<tr>
<td>Investment Costs [€/kW]</td>
<td>3.200</td>
<td>1620</td>
<td>920</td>
<td>720</td>
</tr>
<tr>
<td>Long-term Stability [%/year]</td>
<td>2-4</td>
<td>2</td>
<td>1.5</td>
<td>&lt;1.0</td>
</tr>
<tr>
<td>Flexibility, Dynamics with degradation of &lt;2% a year [% nominal power]</td>
<td>5-100</td>
<td>5-150</td>
<td>0-200</td>
<td>0-300</td>
</tr>
<tr>
<td>Reactivity: hot start from min to max power [seconds]</td>
<td>60</td>
<td>10</td>
<td>2</td>
<td>&lt; 1</td>
</tr>
<tr>
<td>Reactivity: cold start [seconds]</td>
<td>300</td>
<td>120</td>
<td>30</td>
<td>10</td>
</tr>
</tbody>
</table>

Marcelo further indicated that water electrolysis is a well established industrial technology for hydrogen production. Commercial systems are based on alkaline and PEM electrolyte technologies. Recently PEM electrolysis has been demonstrated in the MW class. The main challenges are related to decreasing investment costs, longevity and efficiency.

NEL Hydrogen’s Bjørn Halvorsen presented on an alkaline specific rotolyzer solution. This technology includes a rotating chamber has the potential to increases the current density of the alkaline system while reducing the footprint. The system operates at 15 bar and it seemed at first glance to have a significantly increased complexity compared to conventional system.

Manfred Waidhas reported on Siemens’ effort to demonstrate PEM electrolyzer technology in the MW range. They have offered containerized solutions in the 100-300kW in the past and are now demonstrating in the MW range with a 3x 2MW system. Design studies go up to 10-100 MW and their 2020 cost targets are ~600-1000 €/kW. He specifically pointed out that titanium and membranes are cost drivers for the cost of the stack and that electricity prices pay a role in the operating strategy of the system.

Denis Thomas from Hydrogenics gave an overview on two alkaline and two PEM water electrolysis systems. They have projects inside and outside of Europe. He stated that the alkaline technology is a proven technology with little room for improvements. The mass market
will bring most of the benefits. He showed slides on a wind to gas project with a 2MW system that had most challenges associated with the compressors, and a 1MW BioCat system that targeted biogas to biomethane upgrading by adding the electrolyzer system and a reactor. The PEM activities were a 1.5MW wind to gas project that delivers H₂ at 40 bar without an additional compressor. The system had ~73% overall efficiency.

Everett Anderson from Proton OnSite also reported on PEM WE technology. The company offers commercial products from table top units to MW units and he introduced a number of different systems that are operating across the US and Europe, including an electrolyzer for a self sufficient boat that is an activity CEA Liten is involved in. Proton OnSite system operate at ambient pressures on O₂ side and at pressure on the H₂ side. To date they have stacks operating at 165 and 350 bar and to their knowledge the largest stack operating at these pressure drops. He pointed out that for lowering the cost, thinner membranes will need to be developed, and operation will require higher temperatures, higher currents and lower the catalyst loadings. Furthermore, it was discussed that material coatings in the stack are also important. Lower coating thicknesses and higher durability will be required. Everett stated that the development of accelerated stress tests is important and that the scaling between RDE and in-situ experiments has to be improved significantly.

Øystein Ulleberg from IFE discussed the Mobility Zero Emission Energy System in Norway. Norway has a unique situation as it’s power needs are covered by large amounts of hydropower. They would like to use the power for Zero Emission Vehicles including automotive and maritime vehicles. They are interested in battery / hydrogen use combinations because they don’t consider it useful to convert electrical hydropower to H₂ and then back to electrical energy. It is recognized, however, that larger vehicle applications like trucks or buses need H₂ for their weight and range and are interested in uniting battery and hydrogen technology for the transportation sector. He was further interested and motivated the audience to consider if the hybridization of batteries and electrolyzers would be a solution for certain applications in the future.

In the afternoon sessions Jürgen Mergel and Øystein Ulleberg gave overview presentations of the Annex 30 and Task 33, respectively. The objectives of the Annex 30 presentation and discussions were to provide a platform for information exchange, give a market overview and introduce new members. Further motivation was the standardization of definitions and the harmonization of test protocols for membranes, CCMs, stacks, i.e. materials testing, and accelerated stress tests and long term testing, i.e. life time testing. I personally believe that this is a very important aspect and recommend to DOE to continue to support contributing to these activities. The Annex 30 meets twice a year at changing locations. Task 33 is aiming at the unbiased evaluation of various pathways for local H₂ supply. The group is tasked to assess local H₂ systems, monitor, review and evaluate them and study the barriers and challenges encountered. They also recommend harmonization of monitoring, assessing and review procedures.

Guido Bender gave a talk about the water electrolysis related activities at NREL. NREL has capabilities ranging from synthesis of catalyst and ex-situ characterization over device fabrication to small scale and large scale testing. He gave examples of the work in these areas including some of the electrolyzer grid connection studies and wind to hydrogen studies that have been performed in the past.

Stefan Neis from Waterstofnet an NGO from the Netherlands reported on a project running hydrogen refueling stations with local water electrolysis. A 350 bar station with over 4000
fueling events was operated as part of a small grid with windmill, 1 MW solar and a 120 kW fuel cell system. The system provides fueling to 25 forklifts which will be expanded to 200 forklifts in the near future. Other refueling stations included a 350 / 700 bar station with more than 650 fueling events and 3kg/hr capacity and a maritime fueling station. Reported challenges were the high maintenance cost at currently low station utilization, long lead times for highly specialized parts and compressor utilization and complexity.

Activities in Japan and Europe were covered by Yoshiki Sakaguchi from NEDO, Japan and Tom Smolinka from ISE Fraunhofer, Germany. Japan has a strategic road map on hydrogen and fuel cells. They follow three phases: Phase 1 - Expanding Fuel Cell use has started, Phase 2 - H₂ Power Plant / Mass Supply Chain will be intensified by the mid 2020s and Phase 3 - CO₂-free hydrogen is envisioned to be kicked off around 2040. They currently focus on Micro-CHP for households , FCV (40.000 by 2020) and Hydrogen Refueling Stations (160 by 2020). All of these efforts are currently expanding and aim at a hydrogen society using renewable energy by around 2040. Europe activities reported on the Fuel cells and hydrogen 2 Joint Undertaking, which is a funding effort that started in 2008 and will continue to 2020. About 15 projects were funded in the last two calls. The funding effort provided support to all hydrogen production routes such as photoelectrochemical water splitting (PEC), gasification, chemical conversion, thermolysis, and electrolysis. Other funded projects included distribution and storage.

The discussion points for the joint meeting were on the importance of titanium and the membrane as cost drivers for water electrolysis, on the availability of Iridium as a key component for PEM electrolysis, and that the membrane should be considered a key component to increase efficiency.

For Day 2, the Annex 30 group met individually. There were about 30 attendees from the previous day in the group. The morning was devoted to an information exchange. A total of 8 presentations were given on various aspects of analysis.

Jens Jensen from the Technical University of Denmark talked about the different challenges of PEM, PBI, and classic alkaline water electrolysis systems. They are further organizing the first international conference on electrolysis in June 13-16, 2017 in Kopenhagen.

Nadine Menzel and Dominik Härle talked about a recently established Fraunhofer Institute for Microstructure of Materials & Systems (IMWS) located in Halle, Germany. They are developing a center for electrolysis with the objective to increase material efficiencies and cost effectiveness. They are using in-situ and ex-situ diagnostics to optimize individual components and are also building a PEM testing facility for electrolysis systems.

Frank Allebrod from H-Tec systems talked about their research on larger systems. The company has an office in San Mateo, USA. They have a couple of product lines which feature 30cm² and 450 cm² cell sizes. One of their systems is used to combine biogas with water electrolysis. They use cheap electricity to create H₂ as intermittent storage medium.

Fédéric Fouda-Onana gave an overview of the activities at CEA Liten in Grenoble. Their capabilities range from material synthesis to large scale testing, similar than at NREL. They also do stack and integration work as well as the institute is generally positioned at a higher TRL level than US national labs.
Pierre Millet from the Paris Saclay University talked about performance analysis of MW scale electrolyzers. They are interested if PEM or Alkaline MW systems can be used when access to cheap electrical power is available. Fast ramping and startup are required for such a system. Lower temperatures such as 55C significantly increase lifetime. To what extent are constant operating temperatures important for these applications is one questions they’d like to have answered.

Shigenori Mitsushima from Yokohama National University gave an overview of the strategy and path forward in Japan. Japan envisions to import energy carriers such as liquid H2, ammonia, an toluene/methylcyclohexane on a large scale via ship. They road map moves from stationary use of small CHP systems to expansion of FC vehicles and fueling stations to the year 2040.

Shinji Hasegawa from Asahi Kasei talked about alkaline water electrolysis. The company has a large portfolio of products. They used to built chlor-alkali electrolyzing systems and are now also interested in Alkaline electrolysis systems. Key development areas are high productivity / performance, high durability, and fast response to fluctuating input. They have a large demonstration project with 15x 3MW installed wind to power.

Akijoshi Manabe from De Nora Permelec (permanent electrode) have activities in Europe, the US, and Asia. They are based in Italy. They have been working on mesh electrodes. In their system only the anode differs from the chlor alkali system they have experience with. Upscaling of these devices is challenging and optimization is ongoing. They use activated screens as electrodes and improved layer thickness and quality. The materials remain flexible and can provide a better contact. However, challenges include shut downs which may lead to reversed currents and thus impacts on electrode coatings.

In the afternoon there was a presentation and an extended discussion on the harmonization / standardization of protocols. The idea is that all institutions and companies have access to protocols and hardware that enable the direct comparison of results. A significant challenge is that different systems are operated at different conditions and with different intentions and thus cannot be easily compared to specific operating conditions in a meaningful way. NREL has extensive experience in benchmarking fuel cell efforts and participated in the round robin testing. During the summary, example fuel cell results from NREL were presented as an example to what level identical performance results can be achieved by benchmarking efforts. The European Commission (EC) represented by Georgios Tsotridis reported on their harmonization effort for fuel cells that resulted in a couple of very useful documents for the fuel cell R&D community. One addresses the harmonization of the terminology used, the other addresses testing. The EC promotes the undertaking of a similar effort for electrolysis using the fuel cell documents as starting points. The discussion pointed out that this is a useful effort, but much more challenging for water electrolysis, because system type and system use vary significantly.
**SUBTASK 2: Photoelectrochemical Water Splitting**

- **2014 Hu, a lki PEC Meeting in San Francisco:** The Spring MRS meeting week kicked off on Monday April 21, 2014 at Stanford University with the DOE working group on photoelectrochemical (PEC) water splitting. This group has been meeting annually for 8 years, and brings together the leading researchers from around the world on PEC water splitting to discuss the latest advances, and fundamental challenges in the field in an open and collaborative setting. The meeting this year started with short discussions and breakout sessions that focused on 4 different topics concerning PEC water splitting: (1) In-situ characterization techniques, (2) interfacial band edge energetic control, (3) PEC devices and prototype/benchmarking, and (4) surface passivation. These topics were chosen at the previous DOE PEC working group meeting in October as the focuses of the new round of white papers to be discussed. These themes were chosen based on their critical role in understanding and optimizing PEC devices from a fundamental to a practical level, and involved the input from international and national experts in the field. After the breakout sessions concluded, several international researchers were given a chance to present their labs recent progress in PEC water splitting, and lead discussions with the larger group about possible collaborative efforts in benchmarking.

- **2015 Fall ECS Meeting and PEC Working Group Meeting:** The 2015 ECS meeting held in Phoenix, Arizona had over 2080 attendees from 46 different countries. The conference contained a special group of presentations titled the “Electrochemical Energy Summit” which was designed to foster an exchange between leading policy makers and energy experts about society’s needs and technological energy solutions. Dr. Franklin Orr, U.S. Under Secretary for Science and Energy, delivered the keynote address and discussed environmental security, the critical role of energy storage, and how we can move towards a more sustainable future. The summit also included presentations from Dr. Sunita Satyapal of the U.S. Department of Energy’s Fuel Cell Technologies Office, Dr. George Crabtree of the Joint Center for Energy Storage Research (JCESR) and Dr. Harry Atwater of the Joint Center for Artificial Photosynthesis (JCAP). An international PEC working group meeting was held to discuss several things including developing a commercialization roadmap for the PEC technology. This was decided to be an important catalyst which could more efficiently unite PEC researchers toward the common goal of PEC technology development and commercialization. Initial brainstorming was carried out and initial assignments were made. The updated PEC working group SharePoint was also introduced and demonstrated which will further facilitate international collaboration.

- **2015 Energy & Environmental Science Special Issue on PEC**\(^57\): A special PEC issue synthesized by the international community, with primary contribution from IEA-HIA Task 35 experts, is being published in the high-impact journal *Energy & Environmental Science* (EES). The following excerpt from the editorial introduction to this special issue, written by Eric L. Miller, summarizes the motivation, progress and status of PEC technology as discussed in the issue’s articles: *The recent emergence of hydrogen and fuel cell technologies in the transportation and power generation sectors offers the world important and potentially transformative environmental and energy security benefits. The International Energy Agency (IEA) in its recently released Hydrogen and Fuel Cells Technology Roadmap acknowledges that hydrogen is a flexible energy carrier with potential applications across all energy sectors.*

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and is one of the few energy carriers with the potential for near-zero carbon emissions. Consistent with a number of recent respected studies, the IEA Roadmap concludes that the large-scale deployment of hydrogen fuel cell electric vehicles (FCEVs) in the transport sector could account for 14% or more of the annual carbon mitigation necessary to meet 2050 international targets for reduced greenhouse gas (GHG) emissions. The commercial availability of FCEVs today is an exciting first step in this direction. In the near term, low-cost hydrogen from reformed natural gas can meet the demands of initial FCEV rollouts. In the long term, however, realizing the full environmental and security benefits of hydrogen and fuel cells will require low-cost, large-scale hydrogen production from renewable resources using low-carbon methods. Of the varied options for generating clean and renewable hydrogen, the semiconductor-based photo-electrochemical (PEC) methods for direct solar water splitting are among the most promising, yet also the most challenging. While PEC hydrogen production has been demonstrated at the laboratory scale using a variety of materials and reactor schemes, viable systems with sufficient solar-to-hydrogen (STH) conversion efficiency and durability have remained elusive. To address the challenge, the U.S. Department of Energy (DOE) continues to support fundamental and applied research for overcoming the efficiency and durability barriers in PEC materials, processes and systems.... Following the ground-breaking collaborative traditions of the PEC research community, the authors in this collection offer comprehensive and definitive summaries of important topics in photoelectrochemical hydrogen production. Included are expert reviews of the state-of-the-art in particle-based and photoelectrode-based water splitting technologies (Fabian, DOI: 10.1039/C5EE01434D; Ager, DOI: 10.1039/C5EE00457H); of new and advanced methods of PEC characterization and loss-mitigation (Esposito, DOI: 10.1039/C5EE00835B; Smith, DOI: 10.1039/C5EE01822F); and of PEC’s important role in the broader context of solar fuels production (Coridan, DOI: 10.1039/C5EE00777A). [Includes featured works of Task 35 Experts]

- Photoelectrochemical water splitting, E. L. Miller
- Methods for comparing the performance of energy-conversion systems for use in solar fuels and solar electricity generation, Robert H. Coridan ORCID logoa, Adam C. Nielander, Sonja A. Francis ab, Matthew T. McDowell, Victoria Dix, Shawn M. Chatman and Nathan S. Lewis
- Interfacial band-edge energetics for solar fuels production, Wilson A. Smith, Ian D. Sharp, Nicholas C. Strandwitz and Juan Bisquertef
- Particle suspension reactors and materials for solar-driven water splitting, David M. Fabian, Shu Hu, Nirala Singh, Frances A. Houle, Takashi Hisatomi, Kazunari Domen, Frank E. Osterloh and Shane Ardo
- Methods of photoelectrode characterization with high spatial and temporal resolution, Daniel V. Esposito, Jason B. Baxter, Jimmy John, Nathan S. Lewis, Thomas P. Moffat, Tadashi Ogitsu, Glen D. O’Neil, Tuan Anh Pham, A. Alec Talin, Jesus M. Velazquezde and Brandon C. Wood
- Experimental demonstrations of spontaneous, solar-driven photoelectrochemical water splitting, Joel W. Ager, Matthew R. Shaner, Karl A. Walczak, Ian D. Sharp and Shane Ardo
• **2015 MRS Meeting in San Francisco with PEC Session:** The MRS Spring Meeting held in San Francisco, CA was the location for a DOE Photoelectrochemical (PEC) Working Group (WG) Meeting. The meeting began with a general introduction from Dr. Eric Miller (DOE), followed by personal introductions from each attendee. Then Dr. Miller gave a short oral presentation on the purpose and outlook of the Working Group and PEC in general. Notably, Dr. Miller highlighted the recent support of H2 fuel cell vehicles by Secretary of Energy Ernest Moniz as a means to help facilitate introduction of clean H2 technologies, such as PEC H2 production, into the portfolio of large-scale energy technologies and to help transition H2 fuel from one generated by fossil fuels to one supplied by clean, renewable, inexpensive, and efficient technologies.

A PowerPoint slideshow was played continuously during the meeting which presented a history of the PEC WG including an overview and explanation of the white papers, an overview of the previous white papers (9 of them, plus 3 appendices), an overview of the current white papers (7 of them), and plans for future white papers (6 of them, to date). Each ~3 – 5 page executive summary white paper highlights a topic of relevance to PEC H2 production and provides a summary of the state-of-the-art, aims to inform and educate the general scientific community on the topic, identifies key knowledge gaps and areas for advancement in the field, and provides outlooks for continued R&D. At each table were copies of the current white papers that participants read, discussed (or emailed suggestions), and then provided feedback to the authors so they could be incorporated in future versions. In addition, plans to obtain DOI numbers from DOE OSTI for each of the white papers were finalized so that the online white papers could be referenced appropriately.

This meeting also served as an important time to discuss the status and plan for submission of five review papers to the journal Energy & Environmental Science (EES), where each review paper summarized and expanded upon one of the current white papers. This involved reading the current versions of the review papers which were available on the DOE SharePoint website for Renewable H2 as well as paper copies made available at the WG meeting. Informal discussions of these papers in small groups helped clarify and solidify the motivation and usefulness of the reviews (to disseminate the PEG WG efforts quickly to a large and relevant audience). Also discussed were the design and submission of cover artwork for the special EES journal issue, the language of the acknowledgments section for each review paper, cross-referencing other papers in the collection, and not self-plagiarizing between the EES review papers and white papers.

The action items for the next PEC WG meeting included finalizing this round of 7 white papers and peer-reviewed review papers (2 not in EES), planning the next round of white papers (6 proposed topics, to date), brainstorming a cohesive means to disseminate this information to the public, and determining who would be in charge of updating the previous, current, and future white papers and/or tables of important information online. Prof. Tom Jaramillo (Associate Professor at Stanford University, USA) suggested a Wiki site(s) dedicated to the white papers and tables of information that can be updated by the public so that the onus did not fall entirely on the PEC WG. Prof. Roel van de Krol (Head of the Institute for Solar Fuels - Helmholtz-Zentrum Berlin, Germany) suggested that we identify a roadmap for PEC research to streamline the process and minimize duplication of (international) effort or dilution of finite resources. This was met with very warm acceptance and will be an action item moving forward.

• **2015 Fall ECS Meeting in Phoenix with PEC Session:** The 2015 ECS meeting held in Phoenix, Arizona had over 2080 attendees from 46 different countries. The conference contained a special group of presentations titled the “Electrochemical Energy Summit” which
was designed to foster an exchange between leading policy makers and energy experts about society’s needs and technological energy solutions. Dr. Franklin Orr, U.S. Under Secretary for Science and Energy, delivered the keynote address and discussed environmental security, the critical role of energy storage, and how we can move towards a more sustainable future. The summit also included presentations from Dr. Sunita Satyapal of the U.S. Department of Energy’s Fuel Cell Technologies Office, Dr. George Crabtree of the Joint Center for Energy Storage Research (JCESR) and Dr. Harry Atwater of the Joint Center for Artificial Photosynthesis (JCAP).

An international PEC working group meeting was held to discuss several things including developing a commercialization roadmap for the PEC technology. This was decided to be an important catalyst which could more efficiently unite PEC researchers toward the common goal of PEC technology development and commercialization. Initial brainstorming was carried out and initial assignments were made. The updated PEC working group SharePoint was also introduced and demonstrated which will further facilitate international collaboration.

- **Gordon Research Conference on Solar Fuels**: The underlying theme of the meeting focused on integrated systems for artificial photosynthesis. Topics included all aspects of artificial photosynthesis, including light capture and carrier generation, charge transfer/separation at interfaces, and multi-electron catalysis to complete solar-fuel systems (including solar thermal) and scale-up. Insights from advanced and in situ characterization techniques, theory and systems modelling, and biological/bio-inspired/biomimetic systems were also featured. Fully functioning integrated systems were emphasized.

- **2016 MRS International Materials Research Congress in Cancun**: Dr. Todd Deutsch is a Senior Scientist in the Chemistry & Nanoscience Center at the National Renewable Energy Laboratory and is an expert on using III-V tandem semiconductors for high-efficiency solar hydrogen generation. Dr. Deutsch, an active Task 35 Expert, was invited to present his PEC water splitting research at the 2016 Materials Research Society International Materials Research Congress (IMRC) that took place in Cancun Mexico between August 14-19th, 2016. The IMRC is a materials focused conference that normally attracts ~1500 attendees from ~40 countries. The conference had 6 topics which included materials for energy applications. Within this topic, there was a symposium for solar fules and artificial photosynthesis which is relevant to this subtask. Key collaborative outcomes from the meeting are described below.

Toward the goal of strengthening ties with researchers from the Joint Center for Artificial Photosynthesis (JCAP), which is the DOE's Solar Fuels Energy Innovation Hub, Todd met with Adam Weber of Lawrence Berkeley National Lab (LBL) to discuss better integration of complimentary PEC research activities between the two labs. A follow up conference call was planned to explore avenues for forging more personal relationships between researchers at LBL and NREL with the goal of fostering more synergistic collaborative projects that better leverage our individual capabilities.

Todd also met with Sophia Haussener from École polytechnique fédérale de Lausanne (EPFL) in Switzerland. She is a renowned PEC modeling expert her modeling of an integrated PV-Electrolysis reactor was discussed. Certain scenarios showed that it is possible to reach very low hydrogen production costs by using III-V photovoltaics under solar concentration. She shared some manuscript proofs and discussed an online model for cost calculations. A follow up was scheduled to discuss opportunities for international collaboration to develop a photoreactor that uses NREL’s world-record III-V materials.
Todd also met and had technical discussions with Shu Hu from Yale and Josh Spurgeon from the University of Louisville, who were both previously at JCAP South at CalTech. Dr. Hu has been looking at III-V particle systems and Dr. Spurgeon has been interested in electrolysis of water vapor above the ocean surface. Todd met with CX Xiang of JCAP South and discussed the use of bipolar membranes in photoreactors, which is an emerging area of research which allows different anolyte and catholyte pHs.

**SUBTASK 3: Solar-Thermochemical Water Splitting**

- **2014 Zurich STCH Workshop:** A 90 minute panel discussion moderated by Dr. Martin Roeb ensued after presentations concluded. Each of the speakers sat facing the audience and answered questions first posed by the moderator. The group found it difficult to talk about materials outside the context of a specific reactor design because these two concepts are critically linked. For example, Sandia proposes to use perovskites in a moving particle bed, ETH uses a fixed bed of reticulated CeO2 foam, DLR uses a fixed bed of ferrite supported on SiC monolith. The use of various redox chemistries and geometric forms made it difficult to find agreement on any one approach to kinetic modeling, or even the parameters thought most important to material/reactor performance. Dr. Manuel Romero pressed the group to produce or agree upon a “calibration reaction”. For more mature fields of research (e.g. combustion science), there are standardized protocols and specific gas-phase reactions that can be used to: 1) indoctrinate new researchers into the field, and 2) provide a communal reference point for new experimental or numerical methods. This idea is worth further consideration. The discussion moved away from redox kinetics to general properties/behaviors of the reactive materials themselves. Such questions were posed: 1) what properties are required of the materials to ensure high efficiency operation, 2) how to discover materials, 3) how to screen or design materials, etc? Concerns about earth abundance and the amount of material required to produce terawatts of fuel were also expressed. These are all valid questions that come up time and again, and will continue to do so until the community has reached a consensus on a particular base-case material, and feels comfortable with the attributes and requirements of a solar fuel system making use of that material.

- **2015 CMCEE-11 Meeting in Vancouver- Detailed Summary:** The CMCEE-11 conference was attended by several hundred people from 44 countries, including numerous IEA-HIA Task 35 STCH Experts. The Receiver, Absorber, and Solar Fuels track was organized and chaired by M. Schmucker (DLR). Talks ranged from practical aspects of engineering open cavity receivers, to detailed measurements of redox behavior for ceria and perovskite-based compounds. A 90 minute panel discussion moderated by Dr. Martin Roeb (DLR) ensued after the symposium in the form of an informal working group. The discussion focused on three areas: redox active materials, reactor designs, and opportunities for collaboration. Highlights include:

  *Redox Active Materials:* The following two needs were identified; redox active agents for thermochemical heat storage and for gas splitting. Possible materials are simple binary oxides, perovskites, spinels and fluorites. Possible chemistries discussed were fully stoichiometric and non-stoichiometric reactions. It was certainly clear that the needs of the thermal storage community are different than those of the solar fuels community. For example, success in thermal storage is largely predicated on a large reduction enthalpy associated with fully stoichiometric reactions because this application requires high volumetric energy density in order to keep system storage costs low. Key oxides that fall into this category are a small class of inexpensive earth-abundant oxides that will decompose and recompose at temperatures in the range 400-1000°C. Cobalt oxide is the favored compound despite cost because of very favorable fast and reversible kinetics.
For solar fuels (i.e. gas splitting or STCH), the challenges are more difficult and the needs very different. For example, many of the aforementioned oxides will redox in O₂, but will not have sufficiently favorable thermodynamics to split water in the reduced state. It is unclear if reduction capacity (i.e. non-stoichiometry versus stoichiometry) will impose as severe a penalty on system costs because of the higher monetary value assigned to fuel as opposed to heat. An additional concern is that water-splitting oxides may be cycled many more times than thermal storage oxides, on the order of minutes as opposed to hours or days.

The possibility of using First Principles Theory (e.g. DFT) was discussed, focused on leveraging US Materials Genome Initiative (MGI) methodologies and Sandia’s recent demonstration of calculating the energy required to form an oxygen vacancy in the Sr-Ce-Mn-O system (subject of the Vancouver presentation). All agreed that this approach deserved more attention specifically focused on deriving a generalization scheme that would easily point to a maximum expected benefit.

**Reactor Designs:** DLR and ETH both use absorbing cavity receivers with rigid bricks fixed within them. SNL uses particles in a flowing packed bed. Both DLR and ETH reactors shutter the light and use inert sweep gas in order to swing temperature and O₂ pressure; the SNL concept continuously utilizes the solar energy by reducing oxide as it flows through the receiver and uses vacuum to remove O₂. The SNL concept, while attractive because it uses the solar resource more efficiently, is exceedingly more complex than the DLR or ETH systems. Nonetheless, each design has strengths and weaknesses which can be evaluated by comparing degree of complexity and solar conversion efficiency. For example, fixed bed systems can be easily constructed and operated, however, they suffer from poor conversion efficiency due to low material utilization, poor light/thermal penetration, and issues with thermal stresses on cycling. The particle-based concept is vastly more complex and requires moving solids at high temperature through multiple chambers, however, it promises to use the solar resource much more efficiently. Both concepts demand a high level of heat recovery in order to obtain maximum efficiency.

All in attendance expressed the importance of developing scalable design concepts. DLR is moving their monolithic technology to the Hydrosol 3D project, which will demonstrate gas splitting at the 1MW scale. Reactor construction should be completed by January 2016. ETH does not appear to have a formal effort in up-scaling their reticulated foam cavity receiver anytime soon. SNL has demonstrated “scalability” in some of the key reactor components, such as particle elevation via Olds Lift in their SunShot program on thermal storage.

**Collaboration:** The need for more cross-Atlantic collaboration was well recognized; how best to accomplish this remains an open question. DLR and SNL are currently teaming together through a US DOE funded effort for the next two years focused on demonstrating SNL’s moving particle bed with cascade pressure separation concept. Possibilities might also exist through personnel exchange, DFG (the US equivalent to NSF) and NSF have existing agreements that might support visiting research grants. The idea of using IEA to support intellectual exchange was also mentioned. Even expanding current efforts through US DOE funding was discussed. Large uncertainties surrounding movement of personnel and funding were recognized, especially in light of each country’s desire to protect intellectual property. The group briefly discussed conducting collaborative work under the auspices of “pre-competitive” topical areas focused on developing more fundamental understanding of materials. It was also suggested that MGI and large-scale combinatorial screening could fit under such a “pre-competitive” umbrella. Another possible scenario would be that each
country bring its own funds resulting in jointly managed research ventures, as well as expanding the list of potential collaborators to include Australia and Asia. In this regard, SolarPACES could be used to facilitate cross-continental communication.

**Action Items/Next Steps:** Another informal working group meeting will be planned that coincides with SolarPACES in Cape Town, South Africa, October 2015.

- **2015 NSTTF Meeting Summary:** Over the course of two days, working group members from US DOE, DLR, and SNL (including IEA-HIA Task 35 STCH Experts) attended seminars, toured the National Solar Thermal Test Facility, and observed on-sun testing of a falling particle receiver that is a joint research effort between SNL and DLR. Dr. Christian Sattler presented an hour long overview on STCH work carried out by DLR. Here he explained the political drivers behind the EU Sustainable Energy Technology Plan, on-going European programs, and Germany’s strategy and approach to solar fuels (including renewable hydrogen). A key revelation was DLR’s plans to upscale their HYDROSOL demonstration facility to 1 MW of thermal energy in early 2016. Dr. Sattler also mentioned a critical next step for STCH is to build a dedicated solar fuel demonstration tower capable of achieving high concentration ratio (>1000) with heliostats specifically fit to receiver size, and a field control system adapted to the fuel production process.

- **2015 SolarPACES Conference- Detailed Summary:**
  The 2015 SolarPACES Conference had 551 participants from 38 countries. Topics included solar and thermal receivers, thermochemical energy storage, CSP systems, grid integration, solar fuels, manufacturing for CSP and policy and markets. A summary of relevant meeting minutes are included below:

  **Agenda Item 1 – Opening and Report of Operating Agent**
  Operating Agent (OA) welcomed the participants and outlined the proposed agenda, which was approved without modifications. Countries and NCs present: Australia (R. McNaughton), France (G. Flamant), Germany (C. Sattler, representing K.-H. Funken), Israel (R. Sarfati-Sagir), Italy (A. Giaconia), Mexico (H. Romero-Paredes, representing C. Estrada), South Africa (T. Roos, representing J. van Ravenswaay), Spain (A. Vidal), Switzerland (A. Meier), USA (E. Stechel, representing N. Siegel and I. Ermanoski who was not able to enter South Africa due to visa problems). NCs excused: China (Z. Wang), Germany (K.-H. Funken), Israel (M. Epstein; retired), Korea (Y.-H. Kang), Mexico (C. Estrada), South Africa (J. van Ravenswaay), USA (N. Siegel).

  OA presents brief report:
  - Summary of last SolarPACES ExCo Meeting: Rome (Italy, 24-26, 2015).
  - European Energy Research Alliance (EERA) – Joint Program CSP.
  - EU-FP7 integrated research program STAGE-STE:
    - OA Task II is coordinating Work Package „Solar Fuels“ (WP9) with 11 partners.
    - International Cooperation Activities (WP6): among others with SolarPACES.
  - Dissemination: Task II Meeting and Reporting; Conferences and Publications.

  **Agenda Item 2 – Country Status Reports by National Coordinators**
National project updates were presented from Australia (R. McNaughton), France (G. Flament), Germany (C. Sattler), Italy (A. Giaconia), Mexico (H. Romero-Paredes), South Africa (T. Roos), Spain (A. Vidal), Switzerland (A. Meier), and USA (E. Stechel). No presentation from Israel.

**Agenda Item 3 – Special Topics**

Roadmap to Solar Fuels – Task II Special Activity funded by SolarPACES ExCo:
- As an introduction, the OA presented a brief summary on “Roadmap to Solar Fuels – Strategy for Industry Involvement and Market Penetration”. He mentioned that the final report on Phase 1 (2012-2013) and Phase 2 (2013-2015) for the two selected countries Australia and South Africa has been submitted to the ExCo. After approval, it will be posted on the SolarPACES website. The OA also reported the status of Phase 3 on “Solar Fuels Roadmap for China” (2015-2016).
- A very engaged discussion followed the oral country reports on the outcome of the solar fuels roadmaps for Australia (R. McNaughton) and South Africa (T. Roos).

International Collaboration:
- The EERA Joint Program CSP (in particular, Sub-Program “Solar Thermochemical Fuels”, led by the OA) and the EU-FP7 Integrated Research Program (IRP) STAGE-STE, which started on February 1, 2014, have already been mentioned in the OA report. Of particular interest are WP6 on “International Cooperation Activities” (lead by FISE) and WP9 on “Solar Fuels” (lead by PSI). Due to time restrictions, the presentation was not shown at the meeting, but is included here for completeness.
- Ch. Sattler presented a brief overview on the “Fuel Cells & Hydrogen Joint Undertaking” and “HORIZON 2020”.
- Jim Hinkley briefly summarized the Australian Solar Thermal Research Initiative (ASTRI). L. Vickery (ARENA) emphasized the urgent need for more international collaboration.
- An International Collaborative Initiative was started at the Task II Meeting in Cape Town and established in various meetings during the conference. Partners from Australia, Germany, Japan, South Africa, and USA intend to collaborate to avoid duplication of research. ARENA (Australia) will take the lead for this coordination activity. Proposed initial tasks:
  - Set up a database on knowledge and experience of partners and their industrial contacts.
  - Identify one or two projects that have the potential for large-scale international demonstration (common funding).
  - Exchange information and pursue high-level project planning on a regular basis (e.g., web conferences).

**2016 Solar Thermal Workshop in Australia:**

The Australian Solar Thermal Research Institute (ASTRI) together with the Australian Renewable Energy Agency (ARENA) sponsored three days of workshops in Melbourne, Australia on the occasion of the annual and mid-term review of ASTRI. ASTRI and ARENA took the opportunity to invite a panel of international experts. The panel included:
- Cedric Philibert, IEA, Paris, France
- Christian Sattler, DLR, Germany
- Ayako Matsumoto, Mitsui, Japan
- Jens Søndergaard, Aalborg CSP, Denmark
- Bill Gould and Daniel Thompson, Solar Reserve, USA
The international team was also invited to Canberra, Australia for two more days of discussions on the opportunities for concentrating solar technologies (CST) in Australia for power, industrial heat, and solar fuels. These conversations were held at ARENA, the Department of Industry, Innovation and Science, and the Australian National University (ANU).

Topics discussed at the event included:

1. **Solar Thermal – Opportunities, Challenges and Commercial Applications for a stable solar future:** Transforming Australia’s energy networks and industrial processes with the following objectives:
   - Provide an overview of the current state of CST research and commercial uptake.
   - Establish understanding of CST End User Applications with a particular focus on Storage for Generation and Industrial Applications including hybridisation.
   - Understand the CST market position in the bigger context – what benefit CST can provide, to whom, for what energy outcomes over what timeframes.
   - Engage with end users to create the important market pull.
   - Establish the role of research in meeting industry / market needs.
   - Establishing for future research focus and research/industry collaboration clusters.

2. **CST research landscape - ASTRI and beyond:** CST research and development powering Australian industry creation: The purpose being:
   - Provide CST research information to end users and technology providers.
   - Research to understand industry needs for future research focus and establish research/industry collaboration clusters.
   - Use ASTRI’s Energy System approach to map domestic and international CST research activities – to highlight what is being done where by whom to deliver what outcomes, and to then establish areas of mutual interest, duplication, gaps and opportunity areas.

3. **International Collaboration Opportunities.**

- **2016 SolarPACES Conference- Detailed Summary:** Dr. Ivan Ermanoski is a senior Member of the Technical Staff in the Materials, Devices & Energy Technologies Department at Sandia National Laboratories (SNL). He is an expert in solar-thermochemical fuel production and a member of the IEA HIA task 35, subtask 3 experts group. Dr. Ermanoski presented the scientific results from SNL at the IEA SolarPACES conference (Concentrated Solar Power and Chemical Energy systems). He also provided an update on solar fuels research in the US, and participated in a discussion at the 30th Annual SolarPACES Task II Meeting (Solar Chemistry Research). He also attended a technical tour of the Shams 1 Concentrating Solar Power Plant, and Masdar Institute, and its beam down solar platform. The visit also included a tour of the Jülich Solar Tower, and the world’s largest solar simulator, Synlight, currently under construction. Below is a summary of the events.

  **Summary from Task II meeting:** The task II meeting (held on Oct.10) gathered a small subset of the overall conference attendees—mostly national coordinators, who gave 10 minute updates
on the state of solar chemistry research. The meeting was led by Dr. Anton Meier, Deputy Head of the Solar Technology Laboratory at the Paul Scherrer Institute in Switzerland, who retired as the Task II operating agent this year, and Philipp Furler, Chair in Renewable Energy Carriers at ETH Zurich, who took over the position.

A relatively small subset of the research presented in the task meeting is in the area of solar fuels and hydrogen specifically. The most important impression permeating the task meeting was that there is a serious and long term commitment to solar chemistry research in Australia, throughout the EU, Japan, and Switzerland. The vision and programmatic commitment appears to be on the 5-10 year timescale. Most notably, Japan appears to be fully committed to decarbonizing its economy, and gradually converting to domestic and imported hydrogen over the next 25 years.

In addition to funding a wide spectrum of research areas (solar gasification, solar metallurgy, solar fuels, solar thermochemical storage), there appeared to be a substantial emphasis on international collaboration, with teams routinely consisting of researchers from multiple countries (often funded by multiple agencies), as well as cross border use of specialized facilities and capabilities. The level of international collaborations prompted a discussion of the future format of the Task II meeting, specifically whether national presentations are still as relevant as they have been in the past.

In the area of solar thermochemical fuel production, most of the research came from Europe and Japan, with multiple ongoing programs and tests at the 1MW and 100kW scale that are under way or planned, with many prototype devices already tested. While Sandia STCH reactor design and modeling results, are recognized by the solar fuels community as outstanding and cutting edge, there is no doubt that groups in Japan and the EU are far ahead in terms of facilities and resources dedicated to building and evaluating test articles. Three facilities described in the Task II meeting especially stand out. First, the now completed beam down solar platform at Nigata University (prof. Tatsuya Kodama). Second, DLR’s (nearly complete) Synlight—the world’s largest solar simulator. This truly outstanding facility will be able to deliver an incredible 280 kW into test articles, at an equally incredible 11 MW/m2 maximum flux density. Finally, DLR is moving toward adding a second tower at their Jülich test facility, owing to a very high demand for experimental time.

*SolarPACES highlights:* At just under 600 participants, SolarPACES 2016 was somewhat smaller than recent conferences. From a STCH perspective, most important is the continuing interest in approaches to increasing receiver temperatures, beyond the existing molten salt at ~600°C. Generally, this change is driven by three factors: (1) the understanding that significant efficiency benefits in concentrated solar electricity generation can be realized if receiver and storage temperatures can be taken to 800-1200°C; (2) an increased interest in thermochemical storage for electricity generation; (3) increased interest in solar coal gasification, natural gas augmentation, solar metallurgy, solar cement manufacture, etc. This added interest also translates into considerations regarding solar collection for higher temperatures. As higher temperatures gradually make their way into the concentrated solar power mainstream, solar fuel production (especially hydrogen) is likely to be seen as technology substantially closer to application than even just a couple of years ago. Nonetheless, much skepticism remains in the CSP community regarding the feasibility of solar fuel applications.

One of the outcomes of the increased interest in high temperature particle receivers, is the formation of a SolarPACES sponsored Particle Technology Working Group, led by Cliff Ho from Sandia National Laboratories. This group is very international, with participants from
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Australia, China, France, Germany, Italy, Japan, Saudi Arabia, Spain, Turkey, UAE, and the U.S. The group includes researchers as well as industry participants from the particle and CSP areas.

Ivan Ermanoski presented a talk titled “Pressure Separation and Gas Flows in a Prototype Vacuum-Pumped Solar Thermochemical Reactor” which attracted considerable attention from groups from Japan, Germany, Australia, and Switzerland. Many researchers are excited to hear about the operation and performance of the Cascading Pressure Reactor, currently under construction at Sandia.

Papers presented at the conference were dominated by the storage topic, likely because of the increasingly evident need for it in the renewable energy mix.

**Technical Tour to the Shams 1 Concentrating Solar Power Plant, and Masdar Institute:** The Shams 1 power plant visit was most interesting from the aspect of operation of such a plant in the environment at UAE. Specifically, operators have learned a lot about operation of the 100 MW plant in high ambient temperatures, which put a strain on the cooling system, as well as in high winds, combined with the surrounding desert landscape. The latter has required the erection of a 3.5 m concrete wall around the solar field, to prevent the encroachment of sand dunes. Situated on top of the wall are 3.5 m tall permeable wind breakers, which decrease wind speed and minimize the formation of high speed vortices inside the field. These measures have significantly improved the plant capacity factor, decreased the need for trough cleaning and removal of sand from the solar field, and erosion of mirrors by sand abrasion.

The visit to Masdar was brief, but informative. Masdar Institute of Science and Technology is the world’s first graduate-level university dedicated to providing real-world solutions to issues of sustainability. The Institute’s goal is to become a world-class research-driven graduate-level university, focusing on advanced energy and sustainable technologies. Located in the Masdar City in Abu Dhabi, Masdar Institute appears to be making slow but steady progress toward attracting researchers from around the world, by offering an increasing array of high tech facilities. The Institute’s campus is an evolving landscape of sustainability technologies, integrated at every level of building, urban, and transportation design.
Cross Cutting Activities

- **Solar Fuels Generation: PV and Electrolysis Workshop Summary:** The “Solar Fuels Generation: PV and Electrolysis Workshop” was held at the University of Delaware to identify R&D needs to develop systems for the generation of fuels and industrial chemicals based on renewable resources with a focus on photovoltaic (PV) driven electrolysis for the production of H₂. The following research areas were identified as important opportunities that should be addressed to help accelerate a transition towards a renewable hydrogen future: 1) Advanced electrolyzer designs, catalysts, and membranes; 2) Design and control of microgrid systems consisting of multiple generators including fuel cells, storage and controllers; 3) Leveraging ‘free’ electricity from PV and wind facilities experiencing curtailment due to grid-capacity to generate H₂; and 4) potential use of CO₂ as feed stock for fuels generation.

- **Advanced Water Splitting Materials Consortium Summary:** On April 14-15, 2016 the U.S. Department of Energy’s (DOE’s) Fuel Cell Technologies Office (FCTO) conducted a workshop on Advanced Water Splitting Materials for Hydrogen production from renewable energy sources. The Workshop brought together more than 120 experts in the fields of Water Electrolysis, PEC and STCH to discuss common cross-cutting needs in research and development of new materials needed to allow wide scale hydrogen production from renewable energy sources and guide DOE in establishing an EMN consortium on Advanced Water Splitting Materials development.

Introductory plenary presentations on the needs for accelerating renewable hydrogen technologies and for a comprehensive technoeconomic and lifecycle analysis of renewable hydrogen production were given by Eric Miller, Sunita Satyapal, Arun Majumdar, Reuben Sarkar, Brian James, Amgad Elgowainy and Neha Rustagi. The plenary presentations were followed by four breakout sessions where experts in Low-Temperature Electrolysis; High-Temperature Electrolysis; PEC and STCH. Each group discussed the status and research needs for their respective technology. Cross-cutting opportunities and challenges were discussed at report-out sessions between interdisciplinary panels. Issues that were discussed in the breakout sessions included:

- Critical gaps and needs in system and component TEA and LCA analysis and metrics
- Performance, parameters and metrics for critical functional and Balance-of-Plant materials
- Requirements and design for benchmarking / demonstration platforms
- Resource availability and needs for effective EMN consortium.

The cross-cutting benefits and lessons learned at this workshop can be implemented in the international subtasks of Task 35.

April 14th - 15th, 2016: Stanford
• **21st World Hydrogen Energy Conference**: WHEC 2016 was attended by more than 900 international participants from all over the world and offered high quality plenary sessions, 600 scientific and technological presentations from 50 different countries, a Trade Fair, a Test&Drive zone, several parallel events and multiple networking areas and activities. The conference went over the past, present and future of the hydrogen energy sector worldwide, covering all the aspects related to hydrogen energy such as the progress in hydrogen production, storage, distribution and applications, the latest hydrogen technologies for mobility ivor the hydrogen strategies developed by the sector leading regions of the globe, among other issues of interest.

• **International Solar Hydrogen Pathways Workshop**\(^{58}\): On June 13–17, 2016, fifty-two participants from 10 countries and 32 different organizations with expertise in multiple areas of solar hydrogen gathered at the Lorentz Center in Leiden, The Netherlands (http://www.lorentzcenter.nl/), with representation from leading research institutions, the industrial sector, social scientists evaluating the societal impact and perception of solar-hydrogen technologies, and delegates from several governments. Attendees with this breadth in expertise and experience in solar hydrogen, including several Task 35 Experts, made this workshop unique. Over the five days of the workshop multiple topics were discussed and debated, including the state-of-the-art and limitations of materials, device architectures, early-stage market opportunities, and a roadmap for the implementation of solar-hydrogen technologies into large-scale energy markets. Several coupled considerations were examined for successful implementation of solar-hydrogen devices: (1) technical constraints for the robust and stable long-term operation of the system, (2) economic viability and environmental sustainability, and (3) societal impacts and political drivers. The most important outcome from the workshop was a specific technology roadmap for solar hydrogen devices, which had not previously existed.

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\(^{58}\) Shane Ardo, David Fernandez Rivas, Miguel Modestino, et. al, Pathways to Electrochemical Solar-Hydrogen Technologies, Energy and Environmental Science, 2018 in publication.
### APPENDIX –
**Task 35 experts listed in 2015 IEA Hydrogen Annual Report**

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