Identifying cost-effective, low-carbon H₂ production could accelerate the energy transition through decarbonization of end-use applications where direct electricity use remains challenged. Mallapragada et al. investigate the techno-economic outlook of industrial-scale H₂ supply produced from integrating commercially available PV, electrolyzer, and storage technologies across the continental United States.
Can Industrial-Scale Solar Hydrogen Supplied from Commodity Technologies Be Cost Competitive by 2030?

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SUMMARY

Expanding decarbonization efforts beyond the power sector are contingent on cost-effective production of energy carriers, like H2, with near-zero life-cycle carbon emissions. Here, we assess the levelized cost of continuous H2 supply (95% availability) at industrial-scale quantities (~100 tonnes/day) in 2030 from integrating commodity technologies for solar photovoltaics, electrolysis, and energy storage. Our approach relies on modeling the least-cost plant design and operation that optimize component sizes while adhering to hourly solar availability, production requirements, and component inter-temporal operating constraints. We apply the model to study H2 production costs spanning the continental United States and, through extensive sensitivity analysis, explore system configurations that can achieve $2.5/kg levelized costs or less for a range of plausible 2030 technology projections at high-irradiance locations. Notably, we identify potential sites and system configurations where PV-electrolytic H2 could substitute natural gas-derived H2 at avoided CO2 costs (~$120/ton), similar to the cost of deploying carbon capture and sequestration.

INTRODUCTION

Can solar-powered electrolytic hydrogen (H2) supply industrial-scale quantities at sufficiently low cost by 2030 to allow large-scale, low-carbon production of energy-intensive products such as ammonia, carbon-neutral hydrocarbons, chemicals, or steel? This question is relevant for broader decarbonization efforts and in particular for industrial sectors, where progress regarding emissions reduction has been relatively modest (CO2 emissions from the United States industrial sector decreased by 9% from 2008–2018 versus 26% for the power sector1), and direct use of low-carbon electricity may be difficult.2–5 Although low-carbon H2 production has historically attracted interest for decarbonizing transportation,6 it might be more important in displacing fossil fuel use in industrial processes or as an intermediate in producing energy carriers such as ammonia or hydrocarbons. This observation is supported by recently announced pilot projects for use of electrolytic H2 in steel production and petroleum refining.7 Such large-scale demands for low-carbon H2 will only be relevant under policies that drive rapid decarbonization with stringent carbon emission constraints. Assuming such policies, we examine the cost effectiveness of solar-powered electrolysis for industrial-scale (~100 tonnes/day) H2 supply with high (95%) annual availability and its competitiveness with natural gas (NG) with carbon capture and sequestration (CCS).

Compared with distributed end uses, centralized end uses may provide a more appealing near-term opportunity for deploying emerging H2 production routes,
like electrolysis, for a few reasons. First, existing H$_2$ demand is centralized, originating from petroleum refineries and chemical production facilities, whose typical H$_2$ consumption is supported by one or more production facilities producing H$_2$ on the order of 100 tons per day.\textsuperscript{6} Second, centralized energy uses can potentially be served with on-site H$_2$ production that avoids the need for significant additional infrastructure for H$_2$ transport.\textsuperscript{6} Third, targeting centralized end uses provides an opportunity to rapidly scale up commercially available but nascent technologies, like polymer electrolyte (PEM) electrolyzers, and, in the process, lower costs that could make them cost-effective for serving distributed end uses of H$_2$, like residential heating or transportation, in the future. Fourth, compared with direct electrification of distributed energy demands, like transportation, there is limited potential for direct electrification of many industrial operations, especially those relying on high-temperature heat inputs or direct use of fossil fuels as a feedstock (e.g., steel and ammonia), which makes H$_2$ use for these applications more appealing.

Here we focus on the techno-economic outlook in 2030 for round-the-clock electrolytic H$_2$ supply using dedicated solar photovoltaics (PV) installations and other commodity hardware (Figure 1)—battery energy storage, PEM electrolyzer systems, and gaseous H$_2$ energy storage—in pressure vessels or in geological formations, with the caveat that the latter may be geographically limited in its availability. We focus on 2030 for two reasons: industrial sector decarbonization will need to start by then to meet mid-century climate stabilization goals,\textsuperscript{6} and it is far enough away that significant cost declines in electrolysis can possibly be realized but close enough that forecasts are meaningful. The rapid ongoing development of large-scale electrolysis\textsuperscript{7,9–11} and the continued cost declines of utility-scale PV\textsuperscript{12,13} make it more likely that solar H$_2$ systems developed by combining commodity hardware will be cheaper
than advanced first-of-kind integrated H₂ production systems within this time frame.¹⁴ With respect to H₂ storage, currently available pressure vessel bulk H₂ storage is based on storing H₂ in pressurized tubes (~100 bar) that can be bundled together according to required storage volumes.¹⁵,¹⁶ Unlike NG, storage of H₂ in pressure vessels requires specialized construction materials that are resistant to H₂ embrittlement and fatigue.¹⁵ With growing interest in developing H₂ supply chains for refueling stations, pressure vessel bulk H₂ storage in pipe bundles is offered by several vendors (see Air Products and Chemicals Inc.¹⁶ as an example) for commercial deployment. In contrast, large-scale H₂ storage in geological formations is practiced at scale, with five currently operating facilities across the world that use salt caverns and other hard rock formations to store thousands of tonnes of H₂ at pressures of around 100–200 bar.¹⁷–¹⁹ Available literature regarding potential geological H₂ storage sites in the United States has focused on salt caverns, depleted oil and gas reservoirs, and aquifers distributed across the country, many of which are currently used for NG storage.²⁰

For convenience, we model a strictly isolated PV-H₂ system (Figure 1) that does not account for possible interactions with the grid to sell excess PV electricity or import electricity during times of low PV output. Of course, any real-world system may choose to be grid connected, but our analysis provides a limiting case. In a world with policy sufficiently strong to justify industrial-scale low-carbon H₂ production, it may be reasonable to assume relative oversupply of electricity from variable renewable energy (VRE) at certain times of the day and strong economic incentives for low-carbon dispatchable electricity sources.²¹ Policy supporting low-carbon fuel production would therefore also entail much larger growth of solar electricity generation, which is likely to intensify diurnal electricity price structures like the “Duck” curve currently observed in California,²² where prices are depressed during hours of peak PV output and increase sharply at sundown. In this context, standalone systems, like that shown in Figure 1, may be advantageous because they can potentially mitigate the facility’s exposure to intra-day and intra-year electricity price volatility.

Additionally, the process shown in Figure 1 can also maximize the credits earned from low-carbon policies, such as the Low Carbon Fuel Standard (LCFS) in California, by relying exclusively on carbon-free electricity. The credit value for zero-carbon H₂ has been estimated at $2/kg.²³ Finally, we analyze PV rather than wind-based H₂ production because the former resource is more widely available and has a nearly an order of magnitude higher areal density and lower land use impact compared with wind generation (28 MW/km² versus 5 MW/km²).²⁴

Although techno-economic analysis of electrolytic H₂ production has been studied extensively in the literature, few studies have accounted for the temporal variability in the attributes of electricity supply (availability, emission intensity, and costs) and its effect on system metrics like levelized costs and emission intensity.²,¹⁴,²⁶–²⁹ A key finding across these studies is that grid-based or grid-supported electrolytic H₂ production tends to be more cost effective than systems using VRE generation exclusively because they allow increased electrolyzer utilization and do not need additional investment in electricity generation equipment. For example, one study estimates the levelized cost for PV electricity-based electrolytic H₂ to be $6.1/kg when supplemented by grid electricity (priced at $0.07/kWh) and $12.1/kg when electricity is sourced entirely from PV.¹⁴ However, electrolysis using on-site VRE generation and no storage versus using on-site VRE generation and grid-based electricity not only results in different H₂ production patterns over time but also potentially different greenhouse gas (GHG) emissions per kilogram of H₂ produced. Another study evaluated the cost of electrolytic H₂ across a variety of electricity
tariffs and with dynamic electrolyzer operation to be in the range of $2.6–$12.3/kg\(^{30}\) but did not consider optimizing relative sizing of system components. Similarly, other studies that account for the effect of hourly operational variability on levelized costs of electrolytic \(\text{H}_2\) did not optimize the relative sizing of system components (e.g., electrolyzer, PV, or wind capacity)\(^{31–33}\) or consider the effect of onsite \(\text{H}_2\) storage (G. Saur, 2011, Fuel Cell and Hydrogen Energy, conference).\(^{35}\) Other analyses have focused on potential interactions of electrolyzers with the electric grid by flexibly scheduling power consumption and provision of energy and ancillary services.\(^{29,36,37}\)

Our analysis of the cost-effectiveness of electrolytic \(\text{H}_2\) production focuses on a facility (Figure 1), which relies exclusively on PV-sourced electricity to provide a continuous supply of \(\text{H}_2\) for an industrial customer using on-site energy storage. A novel methodological contribution of this study involves the co-optimization of capacity of PV, electrolysis, energy storage, and other balance-of-plant components (e.g., inverter, \(\text{H}_2\) compressor) to ensure continuous production while accounting for hourly variations in PV resource throughout the entire year and inter-temporal constraints governing equipment operation. This is accomplished by solving an integrated design and operations optimization model that models plant operations throughout the entire year at an hourly resolution (Experimental Procedures). Using this framework, we are also able to evaluate the trade-offs between energy storage as electricity or \(\text{H}_2\) and the resulting effect on levelized cost under current and possible future technology cost and performance projections. Optimal sizing of system components is particularly important for VRE-dominant processes and systems where capital cost tends to dominate total costs.\(^{29}\) For example, we find that the least-cost system design for the process shown in Figure 1 consistently sizes electrolyzer capacity smaller than the PV capacity across range of locations and cost scenarios. Additionally, we perform a spatial analysis of levelized \(\text{H}_2\) production costs across the continental United States that, when considered with spatial distribution of existing \(\text{H}_2\) demand, reveals regions with near-term deployment potential. For these candidate locations, we perform extensive sensitivity analysis to identify the impact of component cost and performance parameters and system factors, like plant annual availability, on achieving costs of $2.5/kg or less. The threshold value of $2.5/kg is near the higher end of the range of estimated levelized costs for \(\text{H}_2\) production from NG with CCS ("blue \(\text{H}_2\"), either via steam methane reforming (SMR) or autothermal reforming (ATR) approaches. There is a wide range of cost estimates for blue \(\text{H}_2\) produced in central facilities in the literature, from $1.2/kg to nearly $3/kg, primarily because of varying assumptions about NG prices, cost of capital, and cost of \(\text{CO}_2\) transportation and storage.\(^{6,38–42}\) Incidentally, another assessment of the long-term cost competitiveness of \(\text{H}_2\) to serve various end-use sectors also highlights $2.5/kg as a key cost benchmark.\(^{32}\) Finally, we compare our results against the costs of NG-based \(\text{H}_2\) production and conclude by noting the main implications and areas of future work.

RESULTS

Design and Cost Outcomes for a Plausible 2030 Cost Scenario

Figure 2 highlights the cost-optimal system design trends to produce \(\text{H}_2\) round-the-clock at 4.17 tonnes/h (or 100 tonnes/day) across nearly 1,500 locations in the United States for the 2030 cost scenario defined in Table 1. These results are based on modeling a full year of plant operations at an hourly resolution, with PV resource characterized using typical meteorological year (TMY) data (Experimental Procedures; Note S2). Here we define “round-the-clock” to correspond to an annual plant
availability of 95% (defined in Table 1) while allowing hourly H₂ supply rates to vary within 10%. The 2030 cost scenario was developed based on component cost projections in the literature and includes (1) PV capital cost of $500/kW (based on direct current [DC] capacity), which is plausible according to available projections;\(^{12,43,44}\) (2) a 62% decline in capital costs for electrolyzer systems from their current levels of $800/kW (for multi-MW-scale systems\(^{10,11,45}\)), which is the lower end of projections available in the literature\(^{10,11,46,47}\) (see Note S2 for further details); (3) an increase in electrolyzer efficiency from current estimates of 58% to 70% on a lower heating value (LHV) basis\(^{37}\); (4) a 33% reduction in capital cost of pressure vessel H₂ storage compared with current (2020) cost estimates.\(^{48}\) (the 2030 capital cost estimate is based on adjusting costs for pipe storage of NG [maximum pressure of 100 bar]\(^{15}\) to account for the different volumetric energy density of H₂ and NG); and (5) a lower range of capital costs reported for geological H₂ storage that is consistent with the large storage volumes being considered here\(^{17–19}\) (see Table S5 for a brief
literature summary of bulk H₂ storage capital costs). Although the sensitivity of system outcomes to alternative future component cost and performance assumptions are explored in more detail in the next section, here we present the major system design trends and favorable locations for initial deployment of PV-electrolytic H₂ based on the 2030 cost scenario described above and in Table 1.

Across locations and the two types of H₂ storage, the electrolyzer size is estimated to be less than the PV capacity because peak PV availability, such as with capacity factors greater than 90%, occurs for only less than 100 h of the year across locations (Figure S2). This finding, also observed in the case of the 2020 cost scenario (Figure S1), is in contrast to prior techno-economic assessments of electrolytic H₂ production, which universally assume electrolyzer capacity to be equal to PV capacity irrespective of location or production requirements and, consequently, overlook the cost savings resulting from oversizing PV arrays. Smaller electrolyzer capacity relative to PV array leads to unutilized PV generation at hours of peak output (Figure 2E), but part of the "lost" H₂ production during the peak hours can be offset by increasing electrolyzer utilization during the "shoulder" hours; i.e., hours on either side of the hours with PV peak output. The cost

Table 1. Key Technology Performance and Cost Assumptions for 2020 and 2030 Scenarios and Sources

| Parameters                          | 2020   | 2030   | References/Explanation                                                                 |
|-------------------------------------|--------|--------|----------------------------------------------------------------------------------------|
| **Capital Costs**                   |        |        |                                                                                        |
| PV ($/kW DC)                        | 850    | 500    | single-axis tracking system with 0° tilt from horizontal; 2020 costs based on lower  |
|                                     |        |        | range of values noted in 2018 in the United States (see Figure 8 of Bolinger et al.59); |
|                                     |        |        | 2030 estimate based on projections by Bloomberg New Energy Finance,12 National       |
|                                     |        |        | Renewable Energy Laboratory43, and Mallapragada et al.44                             |
| Electrolyzer, PEM ($/kW)            | 800    | 300    | 2020 costs based on cost estimates reported from multiple sources6–11,45,46 and       |
|                                     |        |        | Figure 4 in Fuel Cells and Hydrogen Joint Undertaking47; 2030 costs based on lower  |
|                                     |        |        | range of reported costs6–11,45,46, consistent with large-scale storage volumes (see  |
|                                     |        |        | Table S5)                                                                              |
| Pressure vessel H₂ storage ($/kg)   | 516    | 345    | pressurized pipes (100 bar); 2020 costs15; 2030 costs based on NG storage while     |
|                                     |        |        | accounting for H₂ volumetric energy density15                                           |
| Geological H₂ storage ($/kg)        | 33     | 3      | salt cavern (100 bar); 2020 costs from Ahluwalia et al.48; 2030 costs based on lower  |
|                                     |        |        | range of reported costs6–11,45,46, consistent with large-scale storage volumes (see   |
|                                     |        |        | Table S5)                                                                              |
| Compressor ($/kW)                   | 1200   | 1200   | Parks et al.51                                                                         |
| Battery storage power ($/kW)        | 589    | 477    | Low-end costs estimates for 2020 and 203013                                             |
| Battery storage energy ($/kWh)      | 206    | 77     | Low-end costs estimates for 2020 and 203013                                             |
| **FOM Costs (% of Capex)**          |        |        |                                                                                        |
| PV                                  | 1%     | 1%     | National Renewable Energy Laboratory43                                                  |
| Electrolyzer                        | 7%     | 5%     | includes annualized stack replacement cost; 2020 values from Eichman et al.37;        |
|                                     |        |        | 2030 values based on International Renewable Energy Agency28                          |
| H₂ storage                          | 1%     | 1%     | Penev and Hunter42                                                                     |
| Compressor                          | 4%     | 4%     | Penev and Hunter42                                                                     |
| **Operational Parameters**          |        |        |                                                                                        |
| Flow rate, minimum hourly utilization factor | 4.17 tonnes/h, 90% | assumption |                                                                                        |
| Annual plant availability           | 95%    |        | Percentage of hours when facility is supplying H₂; similar to NG-based H₂ production  |
| Electrolyzer efficiency, LHV (%)   | 58%    | 70%    | 2020 value based on International Energy Agency6; future values based on Table 2 in   |
|                                     |        |        | Eichman et al.37 and range of values cited in Table 3 of International Energy Agency6   |
| Battery storage round-trip efficiency (%) | 92%   | assumption |                                                                                        |
| H₂ compression electricity input (kWh/kg) | 1.0 | energy input for 30 to 100 bar compression15 |                                                                                        |

Remaining input parameters and their justification are provided in Table S4. Electrolyzer FOM costs reflect the estimated annualized cost of stack replacements based on a current cell stack life time of 5 years47, and a project lifetime of 20 years (Note S2). DC, direct current, LHV, lower heating value. All dollar values are 2016 United States dollars unless noted otherwise.
savings from oversizing the PV array relative to the electrolyzer is reinforced by the finding that the size of the electrolyzer relative to the PV array is positively correlated with the average PV capacity factor, as shown in Figure 2A. Regions with a higher PV capacity factor, synonymous with lower PV installed capacity (Figure 2C) and a greater number of hours of peak PV availability in a day, rely predominantly on these hours to produce the majority of daily H₂ requirements because the ability to produce H₂ during the shoulder hours is limited by PV power output (Figure S3). The opposite is true in the case of regions with a low PV capacity factor that are synonymous with larger installed PV capacity and, consequently, more PV generation during shoulder hours.

The cost of H₂ storage also affects electrolyzer sizing, with higher relative electrolyzer capacity (58%–76% of PV capacity) in the case of inexpensive geological H₂ storage compared with pressure vessel H₂ storage (30%–63% of PV capacity). The availability of low-cost H₂ storage (i.e., geological) makes it cost effective to use more of the PV electricity supply whenever it is available and store the produced H₂ for providing supply at other times. Consequently, system design with geological H₂ storage leads to larger relative electrolyzer size (Figure 2A), lower PV installed capacity (Figure 2C), greater H₂ storage capacity (Figure 2D), and lower PV curtailment (Figure 2E) compared with design outcomes with more expensive pressure vessel H₂ storage. PV curtailment predominantly occurs in the summer season (Figure 3), whereas plant operation in the winter nearly utilizes all available PV generation and even includes scheduled production downtimes, as illustrated in Figure 3, to minimize H₂ storage requirements and costs.

Despite the prevalence of PV curtailment (Figure 2E), battery storage is not chosen as part of the system design across any of the locations for the 2030 cost scenario (Figure S4). Even though battery storage will improve electrolyzer utilization beyond what is possible with PV alone (~30%; Figure S12), it is orders of magnitude more expensive (on a per-kilogram H₂ stored basis) than the estimated cost of pressure vessel H₂ storage for the 2030 scenario. For example, a battery storage capital cost of $350/kWh is approximately equal to $11665/kg of H₂ stored, not accounting for losses in storage and H₂ production. This makes it less valuable to deploy battery storage even when it can time-shift some or all of the curtailed PV generation and improve electrolyzer utilization. A small amount of battery storage is deployed in the most expensive H₂ storage scenario evaluated here, corresponding to the 2020 costs with pressure vessel H₂ storage (Figure S4).

In general, differences in average PV capacity factor explain lesser of the spatial variability in H₂ storage requirements than the variability in installed PV capacity and relative electrolyzer size, as noted in the coefficient of determination (R²) values in Figure 2D. For example, even among the top PV resource sites (capacity factor ≥ 25%, 128 sites), the H₂ storage requirements differ by a factor of 2.5 for both storage types considered in Figure 2. Regions with a greater difference in PV availability between summer and winter months require increased H₂ storage capacity compared with regions with smaller seasonal variations in PV availability (Figure S5). Figure 3 illustrates the use of H₂ storage to manage diurnal and daily variations in PV availability and realize near-steady H₂ production flow (Figures 3C and 3D, product flow) for a hypothetical facility located in El Paso, TX.

Figure 4 shows the spatial distribution in levelized H₂ costs in the 2030 cost scenario with pressure vessel H₂ storage, with the highest costs ($11.8/kg) and lowest costs ($2.3/kg) observed in the United States northwest and southwest regions, respectively. Similar spatial trends are observed for the 2030 cost scenario with geological
H₂ storage, although the range of levelized costs is much smaller ($1.9–$4.2/kg) than the range of costs for the 2030 scenario with pressure vessel H₂ storage (Figure S6).

Notably, the much lower cost of geological H₂ storage allows smoothening the temporal variations in PV availability at relatively low cost and leads to the average PV capacity factor being a strong indicator for levelized H₂ costs (R² value of 0.95 in Figure 2B). For the 2020 cost scenario, the spatial distribution in levelized H₂ costs is similar to the 2030 cost scenario, although the range of levelized costs is much higher ($5.7–$23.7/kg for pressure vessel H₂ storage [Figure S1] and $5.1–$11.4/kg and geological H₂ storage), indicating that the PV-electrolysis process shown in Figure 1 is currently not economically competitive with NG-based H₂ production routes.

Although the process shown in Figure 1 may not ever be an economically viable H₂ production pathway for low-quality PV resource regions like the United States northwest even in the 2030 cost scenario, there are 34 sites, mostly in the United States southwest and west Texas, with costs less than or equal to $2.5/kg and 245 sites with costs less than $3/kg while using pressure vessel H₂ storage. If geological H₂ storage is widely available, which we have not evaluated here, then many more

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Figure 3. Illustration of Modeled Hourly Operations of a PV-Electrolysis H₂ Production Facility Located in El Paso, TX

(A–F) Average PV capacity factor = 25.9%. Operations are shown for a typical week in the summer (left) and winter (right). Shown are operational trends in PV (A and B), electrolyzer (C and D), and H₂ storage levels (E and F). The modeled facility is designed to produce 4.17 tonnes H₂/h (100 tons/day, with 10% hourly tolerance) and 95% annual plant availability. The time units used for displaying H₂ storage are estimated by dividing the hourly inventory of stored H₂ (in kilograms) with the nominal design flow rate of 4.17 tonnes H₂/h. The results shown correspond to the 2030 cost scenario with pressure vessel H₂ storage defined in Table 1.
locations (621 of 1,487 locations) could meet the $2.5/kg cost threshold (Figure S6). Moreover, Figure 4 suggests that few low-cost regions, such as the Texas Gulf Coast and southern California, are also places with existing H₂ demand, as inferred by the presence of fossil fuel H₂ production facilities, making them attractive locations for practical deployment.

Figure 5 shows the breakdown of levelized H₂ costs for the 2030 scenario for 10 sites that have the highest average PV capacity factor among locations with existing fossil fuel-based H₂ production. Collectively, these sites accounted for 11.2 million tonnes of CO₂ equivalents per year or 25% of the GHG emissions associated with H₂ production in 2017 (Table S6). Because H₂ production sites are typically located close to the point of industrial consumption, these sites are promising locations for initial deployment of the PV-electrolytic H₂ process being studied here. Unsurprisingly, PV and electrolysis capital and fixed operating and maintenance (FOM) costs dominate the levelized cost across all the 10 locations, with PV costs alone accounting for between 61%–62% of total costs. Electrolyzer capital costs represent a smaller share of total costs because of their lower capital costs on a dollar per kilowatt basis versus PV and the oversizing of PV capacity relative to the electrolyzer capacity. Electrolyzer FOM costs, which include the estimated cost of periodical stack replacement (Note S2) contribute 11% of total costs across the locations. Compared with electrolyzer and PV costs, the cost of H₂ storage is a
relatively minor share of total costs even when using the more expensive H₂ storage option of pressure vessels. The costs of the inverter, H₂ compression, and feed water costs (Figure 5, electrolyzer variable operating and maintenance [VOM]) contribute a relatively minor share of overall costs and are therefore not considered for further sensitivity analysis.

**Effect of Inter-annual Variations in PV Resources**

The estimated design trends and levelized costs discussed above are based on characterizing PV resources for each hour of the year using TMY insolation data, which are synthesized from multiple years of data and are commonly used to represent typical variability in PV resources in VRE-related design studies. Here we investigate the reliability of the resulting plant design to accommodate “atypical” variations in PV availability, such as inter-annual variability, by simulating their operation over 20 years using historical PV resource data for 1998–2017. For this, we solved the design optimization model for each location and a specified cost scenario while fixing all sizing decisions to be equal to values identified from solving the model with TMY PV resource data. Figure 6 highlights the annual availability factor of TMY-based plant designs at 10 locations when simulated with PV resource data from historical weather years (1998–2017). Although inter-annual variations in PV availability result in less than a 95% annual availability factor for some years, the overall variation in annual availability is relatively narrow, with a lowest annual availability factor of 90%. Moreover, the number of hours of lost production (i.e., when plant output is below the design flow rate) is in the range of 5%–11% (Figure S7). Similar trends are observed in the case of a TMY-based plant design using geological H₂ storage (see Figure S8). These comparisons indicate that designs obtained using TMY data could yield a reasonably steady supply of H₂ even with inter-annual variations in PV availability and, thus, may be acceptable for a screening analysis to explore promising locations and general system design heuristics (e.g., an electrolyzer-to-PV ratio of less than 1). That said, use of multiple years of historical PV availability may be important for optimizing detailed plant design at a specific location.
The results from the 2030 cost scenario analysis indicate a potential for numerous United States sites to produce H₂ via the process shown in Figure 1 at costs of $2.5/kg or lower. However, there is considerable uncertainty regarding the cost and performance of individual components, particularly electrolysis and H₂ storage. Here we further explore the effect of component cost and performance as well as system design parameters on the cost competitiveness of electrolytic H₂ production at the 10 promising sites identified for initial deployment in Figure 5. The findings from sensitivity analyses at these 10 sites are meant to be illustrative of the possible outcomes at other similar resource quality locations in the United States, identified in the previous section. Given the relative immaturity of PEM electrolysis or H₂ storage compared with PV, we focus our analysis on the costs and performance of the former two technologies while keeping PV costs constant at the values assumed for 2030 ($500/kW DC).

Figure 7 highlights the combination of electrolyzer capital costs, FOM costs, energy efficiency, and H₂ storage capital costs that lead to levelized costs of $2.5/kg or lower while holding PV capital and FOM costs constant at $500/kW DC and 1% of capital costs, respectively. The values for the remaining model input parameters used in Figure 7 correspond to the 2030 scenario defined in Table 1 and Table S4.

A central finding of Figure 7 is the effect of H₂ storage costs on the magnitude of electrolyzer capital cost reductions needed to achieve levelized H₂ costs of $2.5/kg or less. This is indicated by the fewer number of green versus blue markers in each panel of Figure 7. The typical scale of geological H₂ storage, on the order of thousands of tonnes, overlaps with the storage capacity estimated for the process configurations highlighted in Figure 7. However, geological H₂ storage may be limited in its geographic availability, in which case further electrolyzer cost reductions are needed to offset the relatively high cost of pressure vessel H₂ storage. For instance, at the best PV resource location, L10, and an electrolyzer efficiency of 70%, Figure 7 highlights that achieving $2.5/kg or lower levelized costs with...
pressure vessel H₂ storage and geological H₂ storage requires electrolyzer capital cost reductions (compared with 2020 costs of $800/kW) in the range of 50%–59% and 18%–34%, respectively. As a reference, electrolyzer capital costs are estimated to have declined by 3%–7% per year during 2003–2016. Although a $2.5/kg levelized cost threshold excludes the option of pressure vessel H₂ storage in 8 of the 10 sites in Figure 7 for the plausible 2030 scenario of electrolyzer cost and performance (capital cost of $300/kW and 70% efficiency), a threshold cost of $3/kg makes the system with pressure vessel H₂ storage feasible at 7 of 10 sites (Figure S9). Additionally, $3/kg or lower levelized H₂ costs with pressure vessel H₂ storage appear to be feasible at multiple locations with 2030 electrolyzer cost and performance, even when the cost of pressure vessel storage remains the same as the 2020 estimates (Figure S10). Similarly, for geological H₂ storage, $2.5/kg or lower levelized H₂ costs are achievable at 8 of the 10 sites with 2030 electrolyzer costs and performance and 2020 H₂ storage costs (Figure S11).

A comparison of the filled and unfilled markers of the same color in Figure 7 highlights the effect of decreasing electrolyzer FOM costs on levelized H₂ costs. As modeled here, FOM costs include the annualized cost of stack replacement, and this cost is expected to decrease as stack lifetimes increase. Figure 7 suggests that scenarios with high FOM costs (5% of installed capital costs [capex]) and geological storage (blue unfilled markers) lead to higher threshold values for electrolyzer capital costs (or lower levelized costs) compared with scenarios with low FOM costs (2% capex) and pressure vessel storage (green filled markers). This finding suggests that levelized costs are more sensitive to the type of H₂ storage compared with electrolyzer FOM costs.

The effect of increasing electrolyzer efficiency increases the number of combinations of electrolyzer costs, storage type, and locations that can achieve less than $2.5/kg levelized H₂ costs (Figure 7, 24 markers in the left panel versus 32 markers in the center panel and 34 markers in the right panel). Based on the difference in maximum
electrolyzer capital cost across the panels in Figure 7, one can evaluate threshold cost increases associated with efficiency improvements that still result in levelized costs of $2.5/kg or less. For example, with geological H$_2$ storage and FOM costs equal to 5% of capex, approaches that improve efficiency from 70% to 74% without increasing capital costs more than $50–$75/kW will be able to achieve levelized costs below $2.5/kg at the 10 locations. Conversely, if electrolyzer efficiencies remain at their current levels of 58%, then electrolyzer capital costs will have to be in the range of $200–$350/kW to achieve levelized costs of $2.5/kg or less at the 10 locations (Figure 7, left panel). Finally, this analysis assumes the electrolyzer energy efficiency to be independent of the device’s power loading, whereas in practice, the system efficiency generally decreases with increasing loading levels because of resistive losses. For the process shown in Figure 1, however, the electrolyzer hourly loading is predominated by two states, at or near full operation or zero output (Figure S12). Consequently, the approximation of constant electrolyzer efficiency across loading levels has a relatively small effect on system design and cost outcomes (Figure S13).

**Effect of System Factors**

Although several studies of electrolytic H$_2$ production assume the annual plant availability to be the same as the PV capacity factor, our analysis defines it as an independent parameter. In general, increasing plant availability above the average PV capacity factor necessitates the need for additional energy storage and/or overbuilding PV capacity, both of which increase levelized costs. When H$_2$ storage is cheap, as in the case of geological H$_2$ storage, it is more cost-effective to increase H$_2$ storage capacity than overbuild PV capacity, whereas the opposite is true in case of higher H$_2$ storage costs corresponding to pressure vessel H$_2$ storage (Figures S14–S16). Figure 8 shows that plant availability requirements have a significant effect on levelized H$_2$ costs when considering more expensive pressure vessel H$_2$ storage. For instance, as plant availability is changed from 100% to 70%, the levelized costs for the highest PV capacity factor site, L10, decrease by nearly $1/kg in the case of pressure vessel H$_2$ storage compared with less than $0.2/kg in the case of underground H$_2$ storage. When contemplating H$_2$ infrastructure requirements to meet spatially distributed H$_2$ demand, the above finding suggests that it may be cost-effective to operate facilities with access to geological H$_2$ storage at or near 100% availability to compensate for the lower availability in H$_2$ supply from other facilities using pressure vessel H$_2$ storage (that may be located to closer to demand).

Because the levelized cost is nearly entirely made up by capital costs, the assumed cost of capital is a key determinant of system costs. Figure S17 quantifies the sensitivity of the levelized costs to differing assumptions regarding the cost of capital, which is used to evaluate the fraction of total capital costs included in the annualized cost calculations (via the capital charge factor; Table S4). Across the locations and storage costs, changing cost of capital from the default value of 8.1% to 12% or 5% results in an increase or decrease in costs by roughly $0.5–1/kg. The costs of H$_2$ at the highest PV resource sites show the smallest change with changing cost of capital because of the relatively small installed PV capacity, which dominates levelized costs (Figures S5A and S5B).

**Comparison with NG Pathways for the 2030 Scenario**

Currently, NG SMR without CCS is the most economical pathway for H$_2$ production in the United States, with an estimated cost near $1/kg of H$_2$ for centralized production (around 300 tonnes/day). Therefore, in the absence of any policy incentive (e.g., carbon price) for low-carbon H$_2$ production, there is no economic driver
to deploy the PV-electrolysis process shown in Figure 1, even for the range of future technology costs and performance scenarios investigated above. The NG SMR process is associated with life cycle GHG emissions of 10–17 kg CO₂ equivalents/kg H₂,39,40 of which process GHG emissions account for approximately 9 kg CO₂/kg H₂,51 whereas the remaining emissions result from upstream activities (NG production, processing, and transmission). Figure 9 shows the estimated costs of avoiding process CO₂ emissions from NG SMR by substituting with H₂ produced from the process shown in Figure 1 for the 2030 scenario at the top 10 PV resource locations with existing NG-based H₂ production. These costs, referred as avoided CO₂ costs, are estimated as the ratio of the difference in levelized costs to the difference in CO₂ emission intensity between the two processes (Equation 1), where NG SMR is characterized with a cost of $1.15/kg and 9.28 kg CO₂/kg H₂.26

\[
\text{Avoided CO}_2 \text{ cost} = \frac{\text{Levelized Cost}_{\text{PV-electrolysis}} - \text{Levelized Cost}_{\text{NG-SMR}}}{\text{Emission Intensity}_{\text{NG-SMR}} - \text{Emission Intensity}_{\text{PV-electrolysis}}}
\]  

(Equation 1)

For 2030 electrolyzer cost and performance (defined in Table 1), the avoided CO₂ costs for 6 of the 10 sites (L3 and L6–L10) in Figure 7, which collectively accounted for 14.5% of H₂-related GHG emissions in 2017 (Table S6)52 is in the range of $87–$120/ton CO₂ with geological H₂ storage and $135–$207/ton CO₂ with pressure vessel H₂ storage. The range of avoided CO₂ costs for PV-electrolysis plus geological H₂ storage overlaps well with the range of avoided CO₂ costs (including cost of capture, transport, and storage) for NG-based H₂ production ($77–$115 ton/CO₂6,39,40). Despite the cost of CO₂ capture being slightly less for an ATR plant than an SMR plant, the choice of reforming technology has a relatively minor effect on the total avoided CO₂ costs for NG-based H₂ production4,40,42 and, consequently, on the comparison with PV-electrolytic H₂. The avoided CO₂ costs can be recovered in markets with incentives for fuel emission intensity reduction, such as the LCFS program in California, to achieve cost parity against more CO₂-emitting but cheaper cost pathways, like NG SMR without CCS. The average monthly price of emission credits generated via the LCFS program, which is capped at $200/tonne CO₂, has ranged from $122/tonne CO₂ to
$190/tonne CO₂ over the period of March 2018–February 2019. This range overlaps with the range of avoided CO₂ costs estimated here.

The avoided CO₂ costs estimated here will likely be lower when calculated based on avoided life cycle GHG emissions instead of process GHG emissions because of higher upstream GHG emissions associated with NG-based H₂ compared with PV-electrolytic H₂. For example, according to Parkinson et al., the central estimate for life cycle GHG emissions for H₂ produced from NG SMR and PV-electrolysis is 13.2 kg CO₂ equivalents/kg H₂ and 2.2 kg CO₂ equivalents/kg H₂, respectively. Using these life cycle GHG emissions rather than process-based GHG emissions in the avoided CO₂ cost calculations of Equation 1 lowers the avoided CO₂ cost for PV-electrolysis with either H₂ storage option for 6 of the 10 locations (L3 and L6–L10) by ~16% ($74–$100/tonne CO₂ for geological H₂ storage and $114–$174/tonne CO₂ for pressure vessel H₂ storage).

Although the design and cost outcomes presented here for PV-electrolysis correspond to a scale of 100 tons of H₂/day, many of the system components, with the exception of the H₂ compressor (which has a relatively small contribution to total costs; Figure 5), are modular in nature above a certain scale. This implies that the levelized costs are likely to be similar if the scale of production was changed, say, to serve distributed H₂ demand from a collection of H₂ fuel cell vehicle refueling stations (1–2 tonnes/day). For these end uses, PV-electrolysis coupled with pressure vessel H₂ storage could potentially be deployed closer to demand (i.e., refueling stations) to minimize H₂ transportation costs. Low-carbon H₂ supply with NG pathways at distributed scale has yet to be demonstrated, and centralized routes will be associated with additional delivery costs which, when completed via dedicated H₂ pipelines, are estimated to be around $2/kg H₂. Consequently, the delivered cost of H₂ from NG SMR coupled with pipeline transport for distributed end uses could be as...
high as $3/kg, not accounting for the cost of CCS. This implies that PV-electrolysis coupled with pressure vessel H₂ storage could potentially also be a cost-competitive supply option for distributed end uses at the highest PV resource locations if the 2030 cost scenario is realized.

DISCUSSION

Using plausible projections of 2030 costs and performance of commodity technologies for PV, electrolysis, and H₂ storage, we identify a set of sunny United States locations and plant configurations that could supply industrial-scale quantities of H₂ round-the-clock at costs at or below $2.5/kg H₂.

The majority of the instances identified with a cost of $2.5/kg or less are contingent on (1) a reduction in electrolyzer capital costs between 28% and 62% compared with current costs for multi-megawatt systems depending on the case; (2) ~20%–28% improvements in electrolyzer efficiency beyond current levels; (3) availability of geological H₂ storage, which not only enables low H₂ storage costs but could also provide sufficient storage capacity to support supply for industrial H₂ demand; and (4) PV capital costs of $500/kW DC, which seems plausible given historical trends and available projections. Moreover, under these conditions, PV-electrolysis coupled with H₂ storage at select locations could displace NG-based H₂ supply with costs of avoiding process CO₂ emissions similar to costs estimated for deploying CCS at NG SMR facilities. These findings are made possible by the integrated design approach used in this study; notably, the costs would be considerably higher if one used the same technology cost and performance assumptions but did not optimize an individual component’s size (e.g., electrolyzer to PV ratio < 1) at each location. Our approach not only quantifies the levelized cost effects associated with choices inherent in electrolyzer design, such as increasing efficiency versus decreasing capital costs, but also compares them with changes in costs and performance of other equipment; namely, the costs of PV and energy storage.

Estimates of future production costs are always uncertain. How might different assumptions change our conclusions? Factors that might lead to an under-estimate of costs include (1) a less than anticipated decline in the cost of individual technologies by 2030, notably electrolyzer and PV; (2) the potential cost savings from DC-DC integration of electrolyzer and PV systems being outweighed by the practicality and reduced performance of coupled operation; and (3) limitations regarding land availability and/or geological H₂ storage at the best sites, perhaps based on safety concerns about H₂ storage. Factors that might lead to an over-estimate of costs include our neglect of wind power and the benefits of the negative correlation between wind and solar availability in providing low-carbon power with higher availability than PV systems alone. The higher-capacity factor of wind as well as high resource availability in regions with low-quality solar resources (e.g., the United States Midwest) makes a compelling case for studying the economics of wind-based electrolytic H₂ production integrated with on-site storage. We neglected the benefits of grid integration, which could lower costs at the expense of increasing GHG emission intensity. Potential economic benefits of grid integration include providing ancillary services via electrolyzer operation, reducing the installed on-site capacity of renewable generation, electrolyzer and H₂ storage, as well as exporting any excess renewable electricity. The GHG emission effects of complete reliance on grid electricity for electrolysis, however, could be significant in the near term. For example, in California, renewables, including wind and solar, accounted for 29% of total generation in 2017, leading to an average CO₂ emission intensity of electricity generation in
2017 of 212 kg CO₂/MWh.\textsuperscript{55} This translates into CO₂ emissions of around 10 tonnes CO₂ per ton H₂ using a 70% electrolyzer efficiency, which is similar to the life cycle CO₂ emission intensity of H₂ produced from NG SMR. We neglected the use of curtailed PV electricity for consumption within the industrial plant that is also consuming the produced H₂. This approach could reduce electricity demand from the grid or onsite fossil-based generation, which reduces electricity supply costs for industrial application while also lowering plant direct and/or indirect CO₂ emissions. Finally, we only examined the United States, but the PV-electrolytic H₂ system may be even more cost effective in other regions with higher quality solar resources, such as Chile and India, regions with rapidly growing energy demands.

Our estimates of levelized H₂ cost and avoided CO₂ costs ignore the effect of existing policies supporting low-carbon H₂ or fuel production. As noted earlier, existing policies supporting renewable energy, like the LCFS and modified accelerated cost recovery system in the United States available for PV,\textsuperscript{56} could further improve the cost effectiveness of dedicated PV-based electrolytic H₂. Such policies could also reduce the costs of competing H₂ supply technologies, such as NG SMR or ATR with CCS, so the effect on carbon-avoided costs is less clear.

Explicit treatment of the variability of PV output on timescales from hours to years is needed to understand the optimal system design and resulting H₂ production costs. In the analysis for the 2030 scenario with pressure vessel H₂ storage spanning nearly 1,500 locations, for example, the average PV capacity factor explains 61%, 61%, 58%, and 55% of the variation observed in, respectively, the H₂ production cost, installed PV capacity, relative electrolyzer size, and duration of installed H₂ storage capacity. Moreover, these values are based on characterizing annual PV resources at an hourly resolution using TMY data, but our simulations of plant availability using PV resource from individual years suggest that use of longer historical time series (or more judiciously selected annual time series) could be important to minimize costs in the practical design of high-availability, VRE-based H₂ production systems.

Future work could re-assess the promising sites identified for H₂ production in this study after factoring in the historical inter-annual variability in PV resources as well as the potential for geological H₂ storage sites and their various attributes (e.g., formation pressure, cushion gas requirements\textsuperscript{15}). Further analysis is also needed to estimate the total potential supply of H₂ at each site that considers land availability constraints (e.g., excluding urban areas and preservation lands), manufacturing supply chain considerations, as well as the cost of importing H₂ from neighboring locations.

Previous attempts to expand the role of H₂ across the economy generally focused on transportation as the initial-use case. Instead, we argue for expanding use of H₂ in the industrial sector as a way to rapidly scale up electrolysis technologies and kickstart sectoral emission reduction efforts by 2030 to be consistent with mid-century deep decarbonization goals. Under a strong climate policy, our analysis suggests that electrolytic production of H₂ integrated with large solar PV arrays could, in areas of good solar resources, be cost competitive as an industrial feedstock by 2030.

EXPERIMENTAL PROCEDURES

Resource Availability

Lead Contact

Further information and requests for resources should be directed to the Lead Contact, Dharik Mallapragada (dharik@mit.edu).
Materials Availability
All of the data and methods used, including optimization models, are available from
the Lead Contact upon reasonable request.

Data and Code Availability
The parameter inputs to characterize cost and performance technologies are docu-
mented in the study, with the exception of PV resource availability, which is drawn
from a publicly available data source. The scripts used to perform the modeling
and a complete sample dataset are available at https://www.dropbox.com/sh/ros1svyybw09xhz/AADEajd-LPhYqRKeLQpDNyZAa?dl=0.

Modeling Approach and Data Inputs
We use an integrated design and operations optimization model to evaluate the
levelized cost of H2 production across the continental United States. The model
determines the cost-optimal size and hourly operation of all components
throughout the year in the process shown in Figure 1 to meet the specified hourly
H2 production requirements while minimizing total annualized capital and oper-
ating costs. The model includes the following constraints associated with hourly
plant operation: (1) inter-temporal constraints governing energy storage (H2, bat-
tery) operation; (2) hourly limits on PV resource availability; (3) for each component,
hourly power flows cannot exceed the installed power capacity; (4) throughput-
based energy requirements for H2 compression prior to storage; (5) minimum
downtime requirements for the entire plant (12 h), and (6) annual plant availability
requirements.

The model makes the following assumptions about individual component opera-
tion: (1) constant specific power consumption for the electrolyzer and compressor
irrespective of loading; (2) fully flexible operation of the electrolyzer, compressor,
H2 storage, and battery energy storage, implying that each component can go
from zero to the maximum power rating within an hour; (3) no minimum stable
operating level for the electrolyzer; and (4) no minimum state of charge require-
ments for H2 or battery storage. A complete mathematical description of the opti-
mization model is available in Note S1. Unless stated otherwise, all results corre-
spond to solutions where the optimization model was terminated with a 1% or
lower optimality gap.

Annual hourly PV capacity factor data for the various United States locations evalu-
ated was derived using TMY insolation data available from the National Solar Radia-
tion Database (NSRDB) in conjunction with the pvlib simulation toolbox. The
pvlib simulation toolbox converts the insolation time series into a capacity factor
time series (DC values) based on a pre-specified PV system configuration, which,
in this analysis, is assumed to be a single-axis tracking system that is oriented hori-
zontally. The cost and performance assumptions used to characterize operating and
capital costs of various components across the 2020 and 2030 scenarios is sum-
marized in Table 1 and Table S4.

The spatial distribution of levelized H2 production costs shown in Figures 2 and 4 was
developed based on evaluating the optimization model for 1,487 locations across
the United States. These locations correspond to points on a grid developed from
evenly spaced latitudes and longitudes spanning the continental United States
land area. The levelized H2 production costs estimated for the 1,487 locations
were translated into a smooth color map for the continental United States using a
Voronoi diagram (Note S3).
SUPPLEMENTAL INFORMATION
Supplemental Information can be found online at https://doi.org/10.1016/j.xcrp.2020.100174.

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AUTHOR CONTRIBUTIONS
Conceptualization, D.W.K., D.S.M., E.G., and F.M.O.; Methodology, D.S.M. and E.G.; Investigation, D.S.M., E.G., and P.I.; Writing—Original Draft, D.S.M.; Visualization, D.S.M. and P.I.; Project Administration and Funding Acquisition, D.W.K., D.S.M., and F.M.O.

DECLARATION OF INTERESTS
F.M.O. is Senior Vice President for Strategy at Orsted Onshore North America, a developer and owner of wind and solar projects in the United States. D.W.K. is a founder and board member of Carbon Engineering, a developer of direct air capture technologies that might be used to produce fuels using solar hydrogen as an input.

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REFERENCES
1. U.S. Energy Information Administration (2019). Annual Energy Outlook 2019: with projections to 2050. https://www.eia.gov/outlooks/aeo/pdf/aeo2019.pdf.
2. Balcombe, P., Brierley, J., Lewis, C., Skatvedt, L., Spera, J., Hawkes, A., and Staffell, I. (2019). How to decarbonise international shipping: Options for fuels, technologies and policies. Energy Convers. Manag. 182, 72–88.
3. Schafer, A.W., Barrett, S.R.H., Doyme, K., Dray, L.M., Gnadt, A.R., Self, R., O’Sullivan, A., Symondos, A.P., and Tonja, A.J. (2019). Technological, economic and environmental prospects of all-electric aircraft. Nat. Energy 4, 160–166.
4. World Energy Council Netherlands (2018). Hydrogen- Industry as catalyst: Accelerating the decarbonisation of our economy to 2030. http://www.wereldenergieraad.nl/wp-content/uploads/2019/02/190207-WEC-brochure-2019-A4.pdf.
5. Davis, S.J., Lewis, N.S., Shaner, M., Aggarwal, S., Arent, D., Azevedo, I.L., Benson, S.M., Bradley, T., Brouwer, J., Chiang, Y.-M., et al. (2018). Net-zero emissions energy systems. Science 360, eaas9793.
6. International Energy Agency (2019). The Future of Hydrogen: Seizing today’s opportunities. https://www.iea.org/reports/the-future-of-hydrogen.
7. International Energy Agency (2020). Hydrogen Projects Database. https://www.iea.org/reports/hydrogen-projects-database.
8. IPCC (2018). Global Warming of 1.5°C. https://www.ipcc.ch/sr15/
9. International Renewable Energy Agency (2019). Hydrogen: A Renewable Energy Perspective. https://www.irena.org/-/media/Files/IRENA/Agency/Publication/2019/Sep/IRENA_Hydrogen_2019.pdf.
10. Thoma, M., Bauer, F., and Sterner, M. (2019). Power-to-Gas: Electrolysis and methanation: status review. Renew. Sustain. Energy Rev. 112, 775–787.
11. ITM Power (2019). Interim Results Presentation. https://www.itm-power.com/images/Investors/PresentationsAndResearch/Interim-Results-presentation_18.pdf.
12. Bloomberg New Energy Finance (2019). New Energy Outlook 2019. https://about.bnef.com/new-energy-outlook/.
13. National Renewable Energy Laboratory (2018). Annual Technology Baseline. https://atb.nrel.gov/electricity/2018/.
14. Shaner, M.R., Atwater, H.A., Lewis, N.S., and McFarland, E.W. (2016). A comparative techno-economic analysis of renewable hydrogen production using solar energy. Energy Environ. Sci. 9, 2358–2371.
15. Tietze, V., Luhr, S., and Stolten, D. (2016). Bulk Storage Vessels for Compressed and Liquid Hydrogen. In Hydrogen Science and Engineering: Materials, Processes, Systems and Technology, D. Stolten and B. Emonts, eds. (Wiley-VCH), pp. 659–690.
16. Air Products and Chemicals Inc. (2020). Typical Bulk Gas Storage Systems. http://www.airproducts.com/Products/Gases/supply-options/bulk-deliveries-and-storage-systems/typical-bulk-gas-storage-systems.aspx.
17. U.S. Department of Energy (2017). US DRIVE Hydrogen Delivery Technical Team Roadmap. https://www.energy.gov/eere/vehicles/downloads/us-drive-hydrogen-delivery-technical-team-roadmap.
18. Lord, A.S., Kobos, P.H., and Borns, D.J. (2014). Geologic storage of hydrogen: Scaling up to meet city transportation demands. Int. J. Hydrogen Energy 39, 15570–15582.
19. Forsberg, C. (2006). Assessment of Nuclear-Hydrogen Synergies with Renewable Energy Technologies that might be used to produce fuels using solar hydrogen as an input.
20. Lord, A.S. (2009). Overview of Geologic Storage of Natural Gas with an Emphasis on Assessing the Feasibility of Storing Hydrogen (Sandia National Laboratories).

21. Sepulveda, N.A., Jenkins, J.D., de Sisternes, F.J., and Lester, R.K. (2018). The Role of Firm Low-Carbon Electricity Resources in Deep Decarbonization of Power Generation. Joule 2, 2003–2420.

22. Denholm, P., O’Connell, M., Brinkman, G., and Jorgenson, J. (2013). Overgeneration from Solar Energy in California: A Field Guide to the Duck Chart (NREL).

23. Schoenung, S.M., and Keller, J.O. (2017). Cell Reports Physical Science 3, 358–368.

24. Jacobson, M.Z., and Chen, Z. (2017). Optimization of investments in coupled offshore wind– electrolytic hydrogen storage systems in Denmark. J. Power Sources 359, 186–197.

25. Gillelsen, B., Heinrichs, H.U., Stenzel, P., and Lissens, J. (2017). Hybridization strategies of power-to-gas systems and battery storage using renewable energy. Int. J. Hydrogen Energy 42, 13554–13567.

26. National Renewable Energy Laboratory (2018). Hydrogen Station Compression, Hydrogen Storage Options (Argonne National Laboratory).

27. Ramsden, T., Ruth, M., Diakov, V., Laffen, M., and Jorgenson, J. (2013). Land-Use Requirements for Solar Power Plants in the United States. (NREL).

28. Ramsden, T., Ruth, M., Diakov, V., Laffen, M., and Jorgenson, J. (2013). Land-Use Requirements for Solar Power Plants in the United States. (NREL).

29. Eichman, J., Townsend, A., and Melaina, M. (2016). Economic Assessment of Hydrogen Technologies Participating in California Electricity Markets (NREL).

30. Guerra, O.J., Eichman, J., Kurtz, J., and Hodge, B.M. (2019). System Level Analysis of power-sector-decarbonization. https://energy.mit.edu/publication/system-implications-of-continued-cost-declines-for-wind-solar-on-driving-power-sector-decarbonization/.

31. Kopp, M., Coleman, D., Stiller, C., Scheffer, K., Aichinger, J., and Scheppat, B. (2017). Energiepark Mannz. Technical and economic analysis of the worldwide largest Power-To-Gas plant with PEM electrolysis. Int. J. Hydrogen Energy 42, 13311–13320.

32. Keipi, T., Tolvanen, H., and Konttinen, J. (2018). Economic analysis of hydrogen production from natural gas using current and emerging technologies. Int. J. Hydrogen Energy 43, 216–222.

33. Muradov, N. (2017). Low to near-zero CO2 production of hydrogen from fossil fuels. Status and perspectives. Int. J. Hydrogen Energy 42, 14058–14088.

34. Linssen, J. (2017). Hybridization strategies of Solar Power Plants and Battery Storage Towards Low Cost, High Efficiency PEM Electrolysis. In ECS Transactions (The Electrochemical Society), pp. 3–15.

35. Eichman, J., Townsend, A., and Melaina, M. (2016). Economic Assessment of Hydrogen Technologies Participating in California Electricity Markets (NREL).

36. Gru¨ ger, F., Hoch, O., Hartmann, J., Robinius, M., and Stolten, D. (2019). Optimized electrolyzer operation: Employing forecasts of wind energy availability, hydrogen demand, and electricity prices. Int. J. Hydrogen Energy 44, 4387–4397.

37. Zhao, L., and Brouwer, J. (2015). Dynamic operation and feasibility study of a self-sustainable hydrogen fueling station using renewable energy sources. Int. J. Hydrogen Energy 40, 3822–3837.

38. van Leeuwen, C., and Zauner, A. (2018). The investment costs of Electrochemical Society, pp. 3–15.

39. Parkinson, B., Balcombe, P., Speirs, J.F., Hawkes, A.D., and Hellgardt, K. (2019). Levelized cost of CO2 mitigation from hydrogen production routes. Energy Environ. Sci. 12, 19–40.

40. Hydrogen Council (2020). Path to hydrogen competitiveness: carbon-neutral hydrogen technologies. https://hydrogencouncil.com/en/path-to-hydrogen-competitiveness-a-cost-perspective/.

41. Hydrogen Council (2020). Path to hydrogen competitiveness: carbon-neutral hydrogen technologies. https://hydrogencouncil.com/en/path-to-hydrogen-competitiveness-a-cost-perspective/.

42. Mallapragada, D.S., Pilas, D.D., Fernandez, P.G., and Martin, A.D. (2020). System design of a 10 MW daily hydrogen production pilot plant. Int. J. Hydrogen Energy 45, 8490–8497.

43. National Renewable Energy Laboratory (NREL) (2019). National Solar Radiation Database (NSRDB). https://nsrdb.nrel.gov/.

44. National Renewable Energy Laboratory (NREL) (2019). National Solar Radiation Database (NSRDB). https://nsrdb.nrel.gov/.

45. Parks, G., Boyd, R., Cornish, J., and Remick, R. (2019). Utility-scale Solar: Empirical Trends in Project Technology, Cost, Performance, and PPA Pricing in the United States – 2019 Edition (Berkeley Lab).

46. Penev, M., Rustagi, N., Hunter, C., and Eichman, J. (2019). Energy Storage: Days of Service Sensitivity Analysis (NREL).

47. Penev, M., Rustagi, N., Hunter, C., and Eichman, J. (2019). Energy Storage: Days of Service Sensitivity Analysis (NREL).

48. Penev, M., Hunter, C. (2019). Energy Storage Analysis (NREL).
Supplemental Information

Can Industrial-Scale Solar Hydrogen Supplied from Commodity Technologies Be Cost Competitive by 2030?

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Supporting information

Note S1. Model description

We evaluate the levelized cost of H₂ production for the process of Figure 1 using an integrated design and operations optimization model, described in Equations S1-S21. The model determines the capacity of individual components (e.g. PV, electrolyzer) and their hourly operating profile that minimizes the total cost of producing H₂ at the specified hourly rate, while considering various operational constraints. The objective function (Eq. S1) to be minimized includes: 1) annualized capital costs of PV, electrolysis, inverter battery energy storage, inverter, compressor and H₂ storage tanks, 2) annual fixed operating costs of PV, battery energy storage, and electrolyzer, 3) variable operating costs of battery operation and electrolyzer operation (feed water cost) 4) the cost penalty of not meeting specified hourly H₂ production targets, and 5) revenue obtained from sale of excess electricity to the grid as per the pre-specified hourly electricity prices. The results presented in this study do not consider any revenue from grid electricity exports. Similar to other studies on preliminary economics of electrolytic H₂ production 1,2, we assume that the cost of feed water as being constant across for all locations. As an example, feed water cost of $0.002375/gal, which is the value assumed for the H₂A analysis 3, translates into $0.08/kg of H₂ produced for the assumed plant size

\[
\text{Minimize} \ (1000 \cdot \text{CAPEX}_{PV} \cdot v_{PVCap} + 1000 \cdot \text{CAPEX}_{PowerBat} \cdot v_{BatPowCap} + 1000 \cdot \text{CAPEX}_{EnergyBat} \cdot v_{BatEnergyCap} + 1000 \cdot \text{CAPEX}_{Ely} \cdot v_{ElyCap} + 1000 \cdot \text{CAPEX}_{Inv} \cdot v_{InvCap} + 1000 \cdot \text{CAPEX}_{Comp} \cdot v_{CompCap} + \text{CAPEX}_{H2st} \cdot \text{H2stTankCap} \cdot v_{NumTanks}) \times CCF
\]

\[
+ 1000 \cdot \text{FOM}_{PV} \cdot v_{PVCap} + 1000 \cdot \text{FOM}_{Bat} \cdot v_{BatPowCap} + 1000 \cdot \text{FOM}_{Ely} \cdot v_{ElyCap} + \sum_{t \in T} VOM_{PV} \cdot v_{PV,Tot,t} + \sum_{t \in T} VOM_{Ely} \cdot v_{PDCBk,Ely,t} + \sum_{t \in T} VOM_{Bat} \cdot (\eta_c \cdot vStCharge_t + \eta_D^{-1} \cdot vStDischarge_t)
\]

\[
\sum_t (vFH_{Ely,Prod,t} + vFH_{Ely,H2st,t}) \cdot vFeedH2OCostEly
\]

\[
\sum_{t \in T} v_{Slack,t} - \sum_{t \in T} v_{PACPOw,Grid,t} \cdot LMP_t
\]

We model continuous H₂ production to normally be within a band but allow the plant to shut down, defined via Eq. S2. We allow infeasible models to deviate from the required band and downtime constraints via the slack variables in Eq. S2. The high cost penalty ($10^6$/kg) on the slack variables ensures that the model prioritizes feasibility over reducing costs by violating production commitments. The power output from the PV unit at each hour is either directly utilized or used to charge battery storage for later use (Eq. S3). The hourly output of the PV arrays is limited by their resource availability as per Eq. S4. Inter-temporal constraints given by Eq. S5-S9 characterize the operation of the battery, where Eq. S5 governs that the charge at the end of time period t is equal to the sum of the charge at the end of the previous time period (t-1) and the net charging, after accounting for any discharging, occurring during period t. Further, the state of charge in the first period of the year (t=1) is endogenously determined by relating it to the state of charge for the last period of the year (t=8760) via Eq. S6. This “wrapping” constraint is often used to initialize the state of charge of energy storage devices when modeling a single
year of operations. Eq. S7-S8 limit the rate of charge and discharge of battery storage to be less than the installed battery power rating at all times, while Eq. S9 ensures that the total stored energy does not exceed the installed capacity at all times. Eq. S10 constrains the maximum energy capacity of the battery such that it can be provide $p_{DurUB}$ hours of power at the rated power capacity, $v_{BatPowerCap}$.

As per Eq. S11, the DC power supplied from the PV array and battery storage at each hour is balanced against the power demand from the electrolyzer and the compressor (via the inverter). It is worth noting that the DC coupling of PV and electrolyzer systems assumed here, is not yet commercially proven. H2 production from the electrolyzer is modeled using a constant specific power consumption and the produced H2 is distributed to between end use and storage to meet production requirements at a later time (Eq. S12). We don’t explicitly model the cost or energy requirements for purification of feed water or produced H2 (e.g. drying), but rather assume the cost and specific energy consumption of the electrolysis system are inclusive of these conditioning units. Eq. S13 stipulates that the power input to the electrolyzer cannot exceed the installed capacity at all times.

Eq. S14 enforces that the AC power output from the inverter is either consumed for operating the H2 compressor or exported to the grid. The inverter and compressor capacities are sized to meet the maximum power flows through each device (Eq. S15-S16). Eq. S17 calculates the compressor power requirement for each time period as a function of the H2 flow rate sent to storage. We assume constant specific compression power for compressing H2 from the electrolyzer pressure (20-30 bar as per state-of-art PEM electrolyzers) to the design pressure for H2 storage (~100 bar), although in practice, the dynamics of storage charging/discharging may result in time-varying specific compression power. The effect of this approximation on model results is partly mitigated by two factors: 1) the compression energy requirements are approximately an order magnitude smaller than the electrolyzer energy requirements and 2) the prospect of excess electricity from PV during times of compressor operation, especially in the summer season, since the PV array is sized larger than the electrolyzer (Figure 2). The constraints defining the state of charge of H2 storage (Eq. S18-S20) are similar to the constraints used to model battery energy storage, with the only distinction being that we do not account for any energy losses during charging and discharging. The parasitic losses associated with H2 compression, however, are accounted via Eq. S17. Note that this analysis assumes that the H2 storage can fully discharged, even though operating protocols for pressurized gas storage may mandate a minimum H2 storage level to maintain a minimum pressure level in the storage. Eq. S20 constraints the maximum amount of H2 stored at any time period to be limited by the installed capacity of H2 storage.

The requirement on annual plant availability is enforced via Eq. S21, which states that the number of hours when the plant is online should be at least equal to the stipulated availability requirements. Further, we enforce via Eq. S22-S24, that plant downtime periods must be at least duration defined by the parameter, $MinOffline$, to mimic typical outage schedules for existing H2 production facilities for maintenance etc.

\[ v_{Prod_t} \times DesignFH2 \times UtilizationFactor - v_{Slack_t} \leq v_{FH2_{H2st.Prod_t}} + v_{FH2_{Ely.Prod_t}} \leq v_{Prod_t} \times DesignFH2 + v_{Slack_t} \\forall t \]  
\[ v_{StCharge_t} + v_{P_{PV,DCBkt}} = v_{P_{PV,Tot,t}} \forall t \]  
\[ v_{P_{PV,Tot,t}} \leq CF_t \times v_{PVCap} \forall t \]  
\[ v_{StSoC_{t,st}} = v_{SoC_{t-1,st}} + \eta_{c,rt} v_{StCharge_{t,st}} - \eta_{D}^{-1} v_{StDischarge_t} \forall t \in [2,8760] \]
\[ \nu_{\text{StSoC}_t} = \nu_{\text{StSoC}_{8760}} + \eta_c \nu_{\text{StCharge}}_t - \eta_D^{-1} \nu_{\text{StDischarge}}_t \ \forall \ t = 1 \quad (S6) \]

\[ \eta_c \nu_{\text{StCharge}}_t \leq \nu_{\text{BatPowCap}} \ \forall \ t \quad (S7) \]

\[ \eta_D^{-1} \nu_{\text{StDischarge}}_t \leq \nu_{\text{BatPowCap}} \ \forall \ t \quad (S8) \]

\[ \nu_{\text{StSoC}}_t \leq \nu_{\text{BatEnergyCap}} \ \forall \ t \quad (S9) \]

\[ \nu_{\text{StSoC}}_t \leq \text{DurUB} \times \nu_{\text{BatPowCap}} \ \forall \ t \quad (S10) \]

\[ \nu_{P_{\text{PV,DCBk},t}} + \nu_{\text{StDischarge}}_t = \nu_{P_{\text{DCBk,Ely},t}} + \nu_{P_{\text{DCBk,Inv},t}} \ \forall \ t \quad (S11) \]

\[ \frac{1000 \nu_{P_{\text{DCBk,Ely},t}}}{\text{SpecPower}_{\text{Ely}}} = \nu_{FH2_{\text{Ely,Prod},t}} + \nu_{FH2_{\text{Ely,2st},t}} \ \forall \ t \quad (S12) \]

\[ \nu_{P_{\text{DCBk,Ely},t}} \leq \nu_{Ely\text{Cap}} \ \forall \ t \quad (S13) \]

\[ \eta_{\text{inv}} \nu_{P_{\text{DCBk,Inv},t}} = \nu_{P_{\text{AC Pow,Comp},t}} + \nu_{P_{\text{AC Pow,Grid},t}} \ \forall \ t \quad (S14) \]

\[ \nu_{P_{\text{DCBk,Inv},t}} \leq \nu_{\text{Inv Cap}} \ \forall \ t \quad (S15) \]

\[ \nu_{P_{\text{AC Pow,Comp},t}} \leq \nu_{\text{Comp Cap}} \ \forall \ t \quad (S16) \]

\[ \frac{\text{SpecPower}_{\text{Comp}} \nu_{FH2_{\text{Ely,2st},t}}}{1000} = \nu_{\text{AC PowToComp},t} \ \forall \ t \quad (S17) \]

\[ \nu_{\text{H2stSoC}}_t = \nu_{\text{H2stSoC}_{8760}} + \nu_{FH2_{\text{Ely,2st},t}} - \nu_{FH2_{\text{H2st,Prod},t}}, t = 1 \quad (S18) \]

\[ \nu_{\text{H2stSoC}}_t = \nu_{\text{H2stSoC}_{t-1}} + \nu_{FH2_{\text{Ely,2st},t}} - \nu_{FH2_{\text{H2st,Prod},t}} \ \forall \ t \in [2, 8760] \quad (S19) \]

\[ \nu_{\text{H2stSoC}}_t \leq \nu_{\text{H2stTankCap}} \ \forall \ t \quad (S20) \]

\[ \sum_{t \in T} \nu_{\text{Prod}_t} \geq 8760 \text{AvailReq} \quad (S21) \]

\[ \nu_{\text{Prod}_{t-i}} - \nu_{\text{Prod}_{t-i-1}} \leq 1 - \nu_{\text{Prod}_t} \ \forall \ t \in T \ \forall \ i \in \{1, ..., \text{MinOffline}\} \ | \ t-i > 1 \quad (S22) \]

\[ \nu_{\text{Prod}_1} - \nu_{\text{Prod}_{8760}} \leq 1 - \nu_{\text{Prod}_t} \ \forall \ t \in T \ \forall \ i \in \{1, ..., \text{MinOffline}\} \ | \ t-i = 1 \quad (S23) \]

\[ \nu_{\text{Prod}_{8760+t-i}} - \nu_{\text{Prod}_{8760+t-i-1}} \leq 1 - \nu_{\text{Prod}_t} \ \forall \ t \in T \ \forall \ i \in \{1, ..., \text{MinOffline}\} \ | \ t-i < 1 \quad (S24) \]

**Table S 1. Indices and sets**

| Symbol | Description |
|--------|-------------|
| st     | Set of battery energy storage technologies |
| t \in T | Time periods of facility operation (default: 8760 hours per year) |

**Table S 2. Model parameters**

| Symbol             | Units | Description                                      |
|--------------------|-------|-------------------------------------------------|
| \( \text{CAPEX}_{\text{PV}} \) | $/kW | Capital cost of PV (DC)                           |
| \( \text{CAPEX}_{\text{PowerBat}} \) | $/kW | Power capital cost of battery energy storage technology |
| \( \text{CAPEX}_{\text{EnergyBat}} \) | $/kW | Energy capital cost of battery energy storage technology |
| \( \text{CAPEX}_{\text{Ely}} \) | $/kW | Capital cost of electrolyzer (PEM)               |
Table S 3. Model decision variables

| Symbol               | Units   | Description                                                                 |
|----------------------|---------|-----------------------------------------------------------------------------|
| $CAPEX_{Inv}$        | $/kW$   | Capital cost of DC to AC inverter                                           |
| $CAPEX_{Comp}$       | $/kW$   | Capital cost of H$_2$ compressor                                            |
| $CAPEX_{H2st}$       | $/kg$   | Capital cost of H$_2$ storage tanks                                         |
| $FOM_{pv}$           | $$/kW/yr$ | Fixed operating cost of PV system                                          |
| $FOM_{Bat}$          | $$/kW/yr$ | Fixed operating cost of battery storage system of type $st$                |
| $FOM_{Ely}$          | $$/kW/yr$ | Fixed operating cost of electrolyzer (PEM)                                  |
| $VOM_{pv}$           | $$/MWh$ | Variable operating cost of PV system                                       |
| $VOM_{Ely}$          | $$/MWh$ | Variable operating cost of electrolyzer (PEM)                              |
| $VOM_{Bat, st}$      | $$/MWh$ | Variable operating cost of battery storage of type $st$                    |
| $VOM_{comp}$         | $$/MWh$ | Variable operating cost of compressor                                       |
| $VOM_{H2st}$         | $$/hr/kg$ | Variable operating cost of compressor                                      |
| $CP_t$               | %       | Hourly PV availability as a percentage of its peak capacity                |
| $\eta_c$             | %       | Charging efficiency of battery energy storage of type $st$                 |
| $\eta_d$             | %       | Discharging efficiency of battery energy storage of type $st$              |
| $pDur_{UB}$          | Hours   | Maximum duration of battery storage                                         |
| $SpecPower_{Ely}$    | kWh/kg  | Electrical energy consumption of electrolyzer (PEM)                        |
| $SpecPower_{Comp}$   | kWh/kg  | Electrical energy consumption to compress H$_2$ from electrolyzer pressure (20-30 bar) to storage pressure (350-400 bar) |
| $\eta_{inv}$         | %       | Inverter efficiency                                                        |
| $DesignFH2$          | kg/hr   | Design H$_2$ production capacity                                           |
| UtilizationFactor    | %       | Minimum hourly utilization factor for the entire facility                  |
| $CCF$                | %       | Capital charge factor, defined as the ratio of the levelized cost of capital to the overnight capital cost |
| $AvailReq$           | %       | Fraction of the time that the plant must be online                         |
| $MinOfftime$         | hours   | Number of time periods the facility must be down if it goes offline         |
| $LMP_t$              | $$/MWh$ | Wholesale electricity price at time $t$                                     |
| SlackCost            | $$/kg$  | Cost penalty for not meeting hourly H$_2$ production targets (default =10$^6$) |
Note S2. Model data inputs

Hourly PV resource availability across the U.S. is characterized as per typical meteorological year (TMY) insolation data from the NREL solar radiation database (NSRDB) in conjunction with the pvlib toolbox simulation for a single-axis PV array that is oriented horizontally. The TMY data is preferred over historical insolation data from a particular year to avoid biasing results from transitory weather effects in a given year. Table S 4 summarizes the additional cost and performance assumptions for the various components for the 2020 and 2030 scenario. All dollar values are presented in 2016 U.S. dollars, unless noted otherwise.

There is considerable variation in reported costs of electrolyzer systems, partly due to differences in assumed system size. Our estimates for current capital costs rely on vendor information for costs for multi-MW systems. For example, cites data from two vendor on stack costs, to estimate system costs of $800/kW in 2014 dollars. Other more recent publications also support our capital cost estimate for 2020.

The annualized electrolyzer stack replacement costs are estimated by calculating the present value of periodical stack replacement through the project lifetime (i.e. stack replaced in year 5, 10, 15 for system lifetime of 20 years and cell lifetime of 5 years) and assuming stack cost are 50% of total system capital costs.

Table S 4. Additional technology cost and performance assumptions across 2020 and 2030 scenarios. FOM= Fixed Operation and Maintenance, VOM= Variable Operation and Maintenance. Dollar values, unless otherwise stated in 2016 dollars.

| Parameters                      | 2020  | 2030  | Data source/comments                                      |
|---------------------------------|-------|-------|----------------------------------------------------------|
| **Capital costs**               |       |       |                                                          |
| Inverter ($/kW)                 | 60    | 60    | Table 4 of 14                                            |
| Capital charge factor (CCF)     | 10.3  | 10.3% | Ratio of annualized capital cost to total capital cost. Default value based on cost of capital of 8.1% and project lifetime of 20 years. |
| **FOM costs**                   |       |       |                                                          |
| Battery storage ($/kW/yr)       | 7.8   | 5.3   | 15                                                       |
| **VOM costs**                   |       |       |                                                          |
| PV ($/MWh)                      | 0     | 0     | 15                                                       |
| Feed water costs ($/kg)         | $0.015| $0.015| 15                                                       |
| Storage charge/discharge ($/MWh)| 3     | 3     | Assumption                                              |
| **Performance parameters**      |       |       |                                                          |
| Minimum plant downtime (hours)  | 12    |       |                                                          |
| H₂ storage tank capacity (kg)   | 1000  |       |                                                          |
| Inverter efficiency (%)         | 96    |       | Assumption                                              |
Table S 5. Brief literature review of estimated capital cost for bulk H₂ storage either in pressure vessel or geological formations.

| Reference | Type | Description | Pressure range (bar) | Estimated capacity (tonnes) | Working capacity (%) | Estimated capital cost ($/kg) |
|-----------|------|-------------|----------------------|-----------------------------|----------------------|-------------------------------|
| 16        | Pressure vessel | Storage tanks (generic) | NA | NA | NA | 1000 |
| 17        | Pressure Vessel | Spherical vessels | 1.20 | 0.3 | 100 | 1126 |
| 17        | Pressure Vessel | Spherical vessels | 2 | 0.5 | 100 | 874 |
| 17        | Pressure Vessel | Spherical vessels | 2 | 1.5 | 100 | 726 |
| 17        | Pressure Vessel | Spherical vessels | 2 | 4.6 | 100 | 548 |
| 17        | Spherical vessels | Pipe storage (buried underground) | 100 | 64,714 | 100 | 346 |
| 18        | Pressure vessel | Pipe storage | ~100 | 50 | 100 | 516 |
| 18        | Geological | Salt cavern | 70-190 | 6000 | 62 | 33 |
| 18        | Geological | Underground Lined Rock Cavern | 150 | 672 | 95 | 60 |
| 19        | Pressure vessel | Cylindrical tanks | 200 | 10-100 | - | 283-503 |
| 19        | Geological | Salt cavern | 200 | - | - | 8.8 |
| 20        | Geological | Salt cavern | ~100 | 2486 | 77 | 18.7 |
| 20        | Geological | Depleted Oil & gas reservoir | ~100 | 2868 | 67 | 11.4 |
| 20        | Geological | Hard rock | ~100 | 2486 | 77 | 32.5 |
| 21        | Geological | Aquifer | ~100 | 2868 | 67 | 11.8 |
| 22        | Geological | Salt cavern | ~100 | 2520 | - | 0.8-1.6 |
| 22        | Geological | Salt dome | - | - | - | 2.69 |

Table S 6. Summary of average PV capacity factor and H₂ production related GHG emissions in 2017 for the evaluated sites in Figure 5 - Figure 9. PV availability is characterized using Typical Meteorological Year insolation data available from the National Solar Radiation Database. H₂ related GHG emissions from existing H₂ production facilities as per the 2017 edition of the GHG reporting program. The selected sites represent the top 10 sites in terms of PV capacity factor with existing H₂ production.

| Location label | Average annual PV capacity factor | H₂ related GHG emissions in 2017 (Million tonnes CO₂eq per year) | Share of total H₂-related GHG emissions (%) | State | Latitude | Longitude |
|----------------|---------------------------------|---------------------------------------------------------------|--------------------------------------------|-------|----------|----------|
| L1             | 0.22                            | 0.53                                                          | 1.19                                       | TX    | 27.93    | -97.34   |
### Note S3. Solution methodology

The integrated operations and design optimization model was implemented in Pyomo\(^4\) and solved using a commercial mixed-integer linear programming (MILP) model solver, Gurobi\(^5\) on a high performance computing cluster available at MIT.

The results on levelized H\(_2\) productions for the continental U.S., are based on outputs of the integrated design and operations optimizations model for 1487 terrestrial locations. These results assign zero value to the excess electricity available from the sized PV system that is not utilized for H\(_2\) production. The 1487 locations studied were identified as grid points of a 2-dimensional grid consisting of 60 uniformly spaced latitudes and 45 uniformly spaced latitude covering the entire continental U.S. land area. For each location, we solved the optimization model described in S.1 while fixing the variable corresponding to grid exports \((v_{P_{ACPow,Grid,t}})\) to be zero. Subsequently, we generated the spatial maps for levelized H\(_2\) production costs, shown in Figure 4, by generating a Voronoi diagram over the evaluated grid points. The Voronoi diagram creates a visualization in which the color of each point is representative of the levelized H\(_2\) cost of the nearest point evaluated via the optimization model. For high density grids, this is a good approximation and is easier to read than a scatter plot.

|   |   |   |   |   |   |
|---|---|---|---|---|---|
| L2 | 0.22 | 4.1 | 9.31 | CA | 38.09 | -121.82 |
| L3 | 0.23 | 4.3 | 9.74 | CA | 34.13 | -117.9 |
| L4 | 0.23 | 0.05 | 0.10 | CA | 38.65 | -121.82 |
| L5 | 0.24 | 0.03 | 0.07 | CA | 35.25 | -118.9 |
| L6 | 0.24 | 0.51 | 1.14 | TX | 35.81 | -101.26 |
| L7 | 0.24 | 0.23 | 0.51 | TX | 35.81 | -102.22 |
| L8 | 0.24 | 1.19 | 2.67 | CA | 34.13 | -118.9 |
| L9 | 0.26 | 0.15 | 0.34 | NM | 33.01 | -104.18 |
| L10 | 0.27 | 0.03 | 0.06 | TX | 31.85 | -106.1 |
Figure S1. Cost-optimal design trends for continuous H₂ production of 100 tonnes/day (4.17 tonnes/hour) with 95% availability for various locations in the U.S., characterized by annual average PV capacity factor. Results based on co-optimizing facility design and operation over the entire year at an hourly resolution for the 2020 cost scenario with pressure vessel H₂ storage defined in Table 1 and Table S4. Each point represents the design outcome for a different location in the U.S. and the line corresponds to the least-square linear fit of the data. a) Ratio of installed electrolyzer capacity to PV capacity, b) levelized H₂ production cost, c) PV installed capacity (MW), d) H₂ storage duration, e) PV curtailment as a percent of available generation. r: correlation coefficient; R²: coefficient of determination of the linear fit shown for each figure. In all cases, the model deploys zero battery storage capacity and hence the trends in battery storage size are not shown. PV availability characterized using Typical Meteorological Year insolation data available from the National Solar Radiation Database. Duration of H₂ storage calculated by dividing the capacity of installed H₂ storage (in tonnes) with the design flow rate (4.17 tonnes/hour).
Figure S 2. Distribution in the number of hours with high PV capacity factor (CF) across 1487 U.S. locations evaluated in this study. PV availability characterized using Typical Meteorological Year insolation data available from the National Solar Radiation Database.

Figure S 3. Share of total annual H2 produced at different hours of the day across three different locations with differing PV resource quality. Results based on outputs of integrated design and optimization model (see S.1) using 2030 cost scenario with pressure vessel H2 storage, defined in Table 1 and Table S 4. PV resource in each location characterized using insolation data for Typical Meteorological Year (TMY) available from the National Solar Radiation Database. PV CF = PV capacity factor, annual average value.
Figure S4. Installed battery storage power capacity (reported relative to PV capacity) for the cost-optimal design of a PV-electolytic H₂ production facility, as a function of location, characterized by annual average PV capacity factor (x-axis), cost scenario (2020, 2030) and storage type (pressure vessel or geological). Results based on modeling continuous H₂ production of 100 tonnes/day (4.17 tonnes/hour, with 10% hourly tolerance) with 95% annual availability at each location. Each point represents the design outcome for a different location in the U.S.

Figure S5. Annual variations in H₂ storage levels (top) and PV availability (bottom) for two hypothetical PV-electrolysis facilities with similar average PV capacity factor, producing 4.17 tonnes/hour H₂ (100 tonnes/day, with 10% hourly tolerance and 95% annual availability). The labels “L5” and “L6” refer to the location with same labels defined in Figure S5 and correspond to sites with annual average capacity factor of 23.6% and 23.7%, respectively. Left and right charts on the top row correspond to model results with pressure vessel H₂ storage and geological H₂ storage, respectively. Dotted lines in the top row refer to monthly average storage inventory levels for the two sites. The time units used for displaying H₂ storage are estimated by dividing the hourly inventory of stored
H₂ (in kg) with the nominal design flow rate of 4.17 tonnes H₂ per hour. Results shown correspond to the 2030 scenario defined in Table 1.

**Figure S 6.** Spatial distribution in levelized costs of round-the-clock H₂ production for an integrated PV-electrolysis-storage facility for the 2030 scenario with geological H₂ storage, defined in Table 1 and Table S 4. The visualization is based on defining Voronoi polygons (see SI (section S.3.1)) from cost estimated at 1487 grid points using the integrated design and optimization model. PV resource in each location characterized by typical meteorological year insolation data available from the NREL solar radiation database [48]. Pink markers indicate location of existing H₂ production facilities as per the 2017 edition of the EPA GHG reporting program [49], with size of the marker proportional to annual GHG emissions attributed H₂ production at the facility in 2017.
Figure S 7. Impact of inter-annual variations in PV availability (1998-2017) on the number of hours with production less than minimum design specification (90% of 4.17 tonnes/hour) for a H₂ production facility sized using Typical Meteorological Year (TMY) data. Results are shown for 10 locations, identified in Figure 5, for the 2030 cost scenario with for pressure vessel H₂ storage, as defined in Table 1.

Figure S 8. Simulated annual plant availability factor for a H₂ production facility sized using solar resource characterized using Typical Meteorological Year (TMY) data using historical PV resource availability profiles for 1998-2017 (colored circles). Plant availability factor is defined as the ratio of total annual H₂ production of the facility for each weather year (historical or TMY) relative to the design amount (after derating for maximum deviation in hourly flow rate of 10%). Results are shown for 10 locations, identified in Figure 5, for the 2030 cost scenario with for geological H₂ storage, as defined in Table 1.

Figure S 9. Combination of parameter values for electrolyzer capital costs, fixed operating and maintenance (FOM) costs, energy efficiency (based on lower heating value (LHV)) and H₂ storage capital costs that result in levelized
costs less than or equal to $3/kg. Cost of geological and pressure vessel H₂ storage are equal to $33/kg and $516/kg, respectively, corresponding to the 2020 cost scenario. Cost of remaining parameters are defined under the “2030” column in Table 1 and Table S 4. For each location, points are marked for only those combination of parameter values which results in costs lower than $3/kg. Filled and empty circles correspond to FOM costs equal to 2% and 5% of capital costs, respectively. The circle colors are used to designate whether system uses pressure vessel or geological H₂ storage.

Figure S 10. Combination of parameter values for electrolyzer capital costs, fixed operating and maintenance (FOM) costs, energy efficiency (based on lower heating value (LHV)) and H₂ storage capital costs that result in levelized costs less than or equal to $3/kg. Cost of geological and pressure vessel H₂ storage are equal to $33/kg and $516/kg, respectively, corresponding to the 2020 cost scenario. Cost of remaining parameters are defined under the “2030” column in Table 1 and Table S 4. For each location, points are marked for only those combination of parameter values which results in costs lower than $3/kg. Filled and empty circles correspond to FOM costs equal to 2% and 5% of capital costs, respectively. The circle colors are used to designate whether system uses pressure vessel or geological H₂ storage.

Figure S 11. Combination of parameter values for electrolyzer capital costs, fixed operating and maintenance (FOM) costs, energy efficiency (based on lower heating value (LHV)) and H₂ storage capital costs that result in levelized costs less than or equal to $3/kg. Cost of geological and pressure vessel H₂ storage are equal to $33/kg and $516/kg, respectively, corresponding to the 2020 cost scenario. Cost of remaining parameters are defined under the “2030” column in Table 1 and Table S 4. For each location, points are marked for only those combination of parameter values which results in costs lower than $3/kg. Filled and empty circles correspond to FOM costs equal to 2% and 5% of capital costs, respectively. The circle colors are used to designate whether system uses pressure vessel or geological H₂ storage.
costs less than or equal to $2.5/kg. Cost of geological and pressure vessel H\textsubscript{2} storage are equal to $33/kg and $516/kg, respectively, corresponding to the 2020 cost scenario. Cost of remaining parameters are defined under the “2030” column in Table 1 and Table S4. For each location, points are marked for only those combination of parameter values which results in costs lower than $2.5/kg. Filled and empty circles correspond to FOM costs equal to 2% and 5% of capital costs, respectively. The circle colors are used to designate whether system uses pressure vessel or geological H\textsubscript{2} storage.

Figure S12. Trends in electrolyzer capacity utilization for producing 4.17 tonnes H\textsubscript{2} per hour (within 10% tolerance) with 95% availability at various locations under the 2030 scenario using pressure vessel H\textsubscript{2} storage (see Table S4). a) annual average electrolyzer capacity factor and b) distribution of hourly capacity factor for electrolyzer. Location labels, L1 to L10, refer to the locations denoted in the map of Figure 5.

Figure S13. Impact of varying electrolyzer energy efficiency with loading on electrolyzer hourly power consumption at a single location for the 2030 cost scenario with pressure vessel H\textsubscript{2} storage (see Table S4). Results based on process design criteria of producing 4.17 tonnes /hour (within 10% tolerance) with 95% availability. a) Assumed variation in efficiency as a function of loading, b) Distribution of hourly power consumption under the constant efficiency case and the case with efficiency variation with loading level, c) difference between modeled power with constant efficiency assumption and power consumption based on efficiency variation with loading as per panel a. Location labels L10, correspond to the location with the same name defined Figure 5.
Figure S 14. Impact of changes in minimum plant availability requirements on the duration of installed H2 storage capacity for different H2 storage capital costs and at various locations in the U.S. Location labels, L1 to L10, refer to the locations with the same name defined in Figure 5. Aside from storage capital costs, cost of other input parameters correspond to the 2030 scenario defined in Table 1 and Table S 4. Hourly H2 production requirement held constant across the differing plant availability requirement cases at 4.17 tonnes per hour (with 10% hourly tolerance). Duration of H2 storage calculated by dividing the capacity of installed H2 storage (in kg) with the design flow rate (4.17 tonnes /hour).

Figure S 15. Impact of changes in minimum plant availability requirements on the ratio of electrolyzer to PV capacity for different H2 storage capital costs and at various locations in the U.S.. Location labels, L1 to L10, refer to the locations with the same name defined in Figure 5. Aside from storage capital costs, cost of other input parameters correspond to the 2030 scenario defined in Table 1 and Table S 4. Hourly H2 production requirement held constant across the differing plant availability requirement cases at 4.17 tonnes per hour (with 10% hourly tolerance).
Figure S 16. Impact of changes in minimum plant availability requirements on annual PV curtailment for different H₂ storage capital costs and at various locations in the U.S. Location labels, L1 to L10, refer to the locations with the same name defined in Figure 5. Aside from storage capital costs, cost of other input parameters correspond to the 2030 scenario defined in Table 1 and Table S 4. Hourly H₂ production requirement held constant across the differing plant availability requirement cases at 4.17 tonnes per hour (with 10% hourly tolerance).

Figure S 17. Sensitivity of levelized H₂ costs to the assumed cost of capital (and consequently, the capital charge factor (CCF)) at 10 locations identified in Figure 5, for the 2030 cost scenario described in Table 1 and Table S 4. The capital charge factor, which is used to calculate annualized capital costs of various technologies, is derived from the cost of capital using a 20 year technology/project lifetime. The value of CCF for the cost of capital of 5%, 8.1% and 12% corresponds to 8.0%, 10.3% and 13.3%, respectively.
Supplemental References

1. Shaner, M.R., Atwater, H.A., Lewis, N.S., and McFarland, E.W. (2016). A comparative technoeconomic analysis of renewable hydrogen production using solar energy. Energy Environ. Sci. 9, 2354–2371.

2. Eichman, J., Townsend, A., and Melaina, M. (2016). Economic Assessment of Hydrogen Technologies Participating in California Electricity Markets (National Renewable Energy Laboratory (NREL)).

3. National Renewable Energy Laboratory (NREL) (2018). H2A: Hydrogen Analysis Production Case Studies. https://www.nrel.gov/hydrogen/h2a-production-case-studies.html.

4. Denholm, P., and Hand, M. (2011). Grid flexibility and storage required to achieve very high penetration of variable renewable electricity. Energy Policy 39, 1817–1830.

5. Kopp, M., Coleman, D., Stiller, C., Scheffer, K., Aichinger, J., and Scheppat, B. (2017). Energiepark Mainz: Technical and economic analysis of the worldwide largest Power-to-Gas plant with PEM electrolysis. Int. J. Hydrogen Energy 42, 13311–13320.

6. National Renewable Energy Laboratory (NREL) (2019). National Solar Radiation Database (NSRDB). https://nsrdb.nrel.gov/.

7. Sandia National Laboratories (2018). PV Performance Modeling Collaborative.

8. Leeuwen, C. van, and Zauner, A. (2018). Report on the costs involved with PtG technologies and their potentials across the EU.

9. Mayyas, A., Ruth, M., Pivovar, B., Bender, G., and Wipke, K. (2019). Manufacturing Cost Analysis for Proton Exchange Membrane Water Electrolyzers (National Renewable Energy Laboratory).

10. International Renewable Energy Agency (2019). Hydrogen: A Renewable Energy Perspective.

11. Saba, S.M., Müller, M., Robinius, M., and Stolten, D. (2018). The investment costs of electrolysis – A comparison of cost studies from the past 30 years. Int. J. Hydrogen Energy 43, 1209–1223.

12. Thema, M., Bauer, F., and Sterner, M. (2019). Power-to-Gas: Electrolysis and methanation status review. Renew. Sustain. Energy Rev. 112, 775–787.

13. ITM Power (2019). Interim Results Presentation.

14. Fu, R., Feldman, D., Margolis, R., Woodhouse, M., and Ardani, K. (2017). U.S. Solar Photovoltaic System Cost Benchmark: Q1 2017.

15. National Renewable Energy Laboratory (NREL) (2018). Annual Technology Baseline. https://atb.nrel.gov/electricity/2018/.

16. Eichman, J., and Flores-Espino, F. (2016). California Power-to-Gas and Power-to-Hydrogen Near-Term Business Case Evaluation (National Renewable Energy Laboratory (NREL)).

17. Tietze, V., Luhr, S., and Stolten, D. (2016). Bulk Storage Vessels for Compressed and Liquid Hydrogen. In Hydrogen Science and Engineering: Materials, Processes, Systems and Technology (Wiley-VCH Verlag GmbH & Co. KGaA), pp. 659–690.

18. Ahluwalia, R.K., Papadias, D.D., Peng, J.-K., and Roh, H.S. (2019). System Level Analysis of
Hydrogen Storage Options (Argonne National Laboratory).

19. Amos, W. (1998). Costs of Storing and Transporting Hydrogen (National Renewable Energy Laboratory).

20. Lord, A.S., Kobos, P.H., and Borns, D.J. (2014). Geologic storage of hydrogen: Scaling up to meet city transportation demands. Int. J. Hydrogen Energy 39, 15570–15582.

21. Forsberg, C. (2006). Assessment of Nuclear-Hydrogen Synergies with Renewable Energy Systems and Coal Liquefaction Processes (Oak Ridge National Laboratory).

22. Penev, M., Rustagi, N., Hunter, C., and Eichman, J. (2019). Energy Storage: Days of Service Sensitivity Analysis (National Renewable Energy Laboratory (NREL)).

23. U.S. Environmental Protection Agency (2018). Greenhouse Gas Reporting Program (GHGRP). https://www.epa.gov/ghgreporting/ghg-reporting-program-data-sets.

24. Hart, W.E., Laird, C.D., Watson, J.-P., Woodruff, D.L., Hackebeil, G.A., Nicholson, B.L., and Sirola, J.D. (2017). Pyomo — Optimization Modeling in Python (Springer International Publishing).

25. Gurobi Optimization, L. (2018). Gurobi Optimizer Reference Manual. http://www.gurobi.com.