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Evaluating the Case for Reduced Precious Metal Catalysts in Proton Exchange Membrane Electrolyzers

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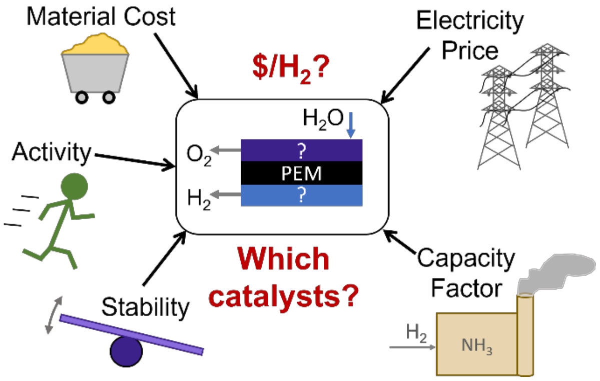
Abstract

Proton exchange membrane (PEM) water electrolyzers are a key technology in decarbonizing hydrogen production. Though the market for PEM electrolyzer systems is growing, there are concerns that the cost and availability of precious metal catalysts utilized in today's commercial systems can limit deployment. Herein, we show that while the availability of Ir should not impede deployment in the near-term, the inelasticity of the Ir commodity price is cause for immediate concern. We emphasize that diversifying catalyst materials, even with other precious metals, can reduce system costs and mitigate supply chain risk. Furthermore, we analyze the trade-offs

between catalyst capital cost and catalyst activity for a range of operating conditions (i.e. capacity factor, electricity price). The framework presented herein is a first step towards establishing performance targets (i.e. activity, stability, material cost) for reduced- and non-precious metal catalysts as a function of PEM electrolyzer operating conditions.

Table of Contents Graphic



Main Text

Electrolytic hydrogen offers a pathway to decarbonization in the transportation, industrial, and even the power sector. While today only a small fraction of the world's H_2 is produced by electrolysis,[1] the push to achieve net-zero carbon emissions coupled to abundant and cheap renewable electricity is driving the deployment of proton exchange membrane (PEM) electrolyzers. Compared to traditional alkaline electrolyzers, the solid polymer electrolyte allows PEM electrolyzers to reach high current densities with high energy efficiency, mitigate gas crossover, and respond to changes in power supply on a short time scale.[2,3] These advantages render the PEM configuration a promising avenue for widespread electrolysis at large- and small-scales. For example, at a large-scale, a 50-MW electrolyzer powered by offshore wind energy will supply 9,000 tonnes of H_2 annually to a refinery in Germany by 2024.[4] Smaller-scale electrolyzers

(~0.1-MW - 1-MW) will supply H_2 for more distributed projects, such as H_2 fuel cell vehicle fueling stations.[5] These examples illustrate the recent uptake of PEM electrolyzers to meet a diverse set of H_2 and energy demands.

Despite recent growth in the PEM electrolyzer market, recent bottom-up manufacturing technoeconomic analysis showed that the production cost of H_2 from a 1-MW PEM electrolyzer today is nearly \$5/kg (~5x the U.S. Dept. of Energy's 2030 target) for both industrial and energy storage applications (**Figure 1B**).[6] For a detailed technoeconomic analysis and breakdown of electrolyzer component and operating costs, please see Ref. 6. In brief, the capital costs shown are for the stack (including catalysts, porous transport layers, membrane, and bipolar plates) and balance of plant equipment (such as power electronics, water purification system, and hydrogen processing equipment).[6] These components can be costly owing to the materials they are made from (e.g. Ti bipolar plates) and/or low manufacturing volumes of specialized components.[6] Feedstock costs are dominated by the cost of electricity. While costs may differ around the world, in most cases, H_2 produced by PEM electrolyzers is simply not cost competitive with fossil-fuel derived H_2.[7]

Cheap electricity can significantly reduce PEM electrolyzer operating costs, with projected cost reductions of ~20-50% assuming all else constant (i.e. capital cost, capacity factor, lifetime).[8,9] However, achieving lower average electricity prices today utilizes intermittent renewable electricity and therefore coincides with a reduction in the capacity factor of the electrolyzer (**Figure 1A**).[10–13] This coupling of electricity price and capacity factor means that the overall H_2 production cost does not decrease substantially when utilizing renewable energy sources, such as for energy storage applications. Instead, researchers have shown that the effect is a re-distribution of the relative cost contributions: capital cost is of greater concern than the cost of electricity for energy storage applications, while electricity costs are of greater concern for industrial uses for H_2, such as ammonia production (**Figure 1B**).[6] Thus, we emphasize that the economic benefit of improvements in electrolyzer efficiency versus reductions in capital cost will depend on the application of the electrolyzer.

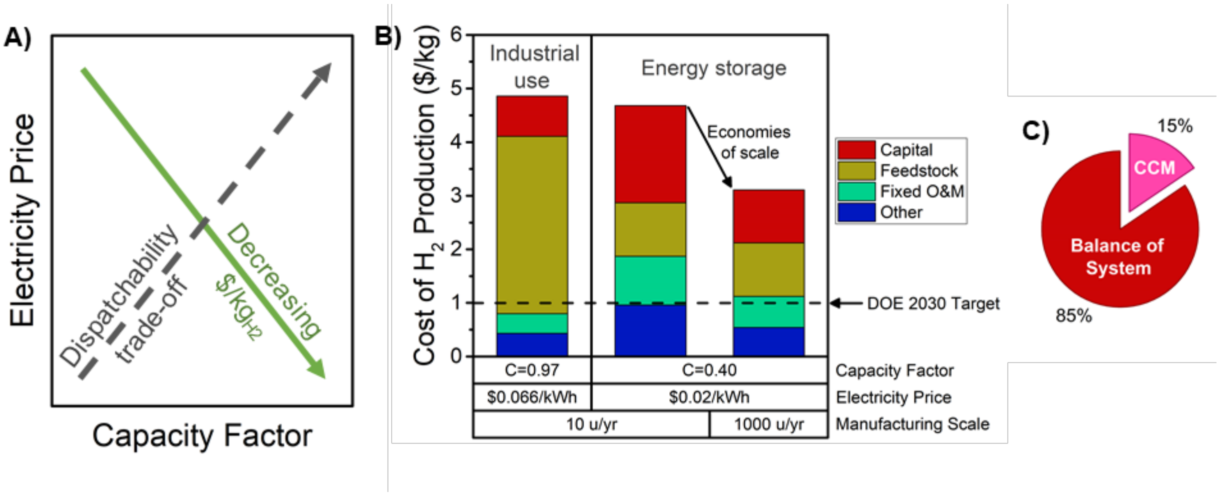


Figure 1. (A) Schematic representation of the relationship between average electricity price and capacity factor (gray dashed line). Ideal relationship for decreasing H_2 production cost shown by green solid line. (B) Production cost of H_2 under different capacity factor, electricity price, and manufacturing scale scenarios reflective of industrial or energy storage use-case of electrolyzer. Feedstock costs include electricity. Data from Ref. 6 for a 1-MW PEM electrolyzer. (C) Breakdown of PEM electrolyzer capital costs shows the relative contribution of the CCM, which is independent of manufacturing scale from 10-1000 u/yr. Data from Ref. 6.

Previous analysis has shown that H_2 production cost targets cannot be fully achieved just by reaching economies of scale in manufacturing (**Figure 1B**).[6] Producing cost competitive H_2 from PEM electrolyzers requires continued research and development to reduce the capital cost and/or improve the system efficiency. There are several components worth targeting for improvements, such as power electronics and bipolar plates.[6,7] We focus this discussion on the catalyst-coated membrane (CCM), which has received decades of attention in the field of electrocatalysis. The CCM constitutes 15% of the electrolyzer capital cost (**Figure 1C**),[6] contains scarce materials, and is the main driver of efficiency. Thus, engineering the catalysts in the CCM can have a major impact on both capital and operating costs.

Today, commercial PEM electrolyzers utilize Pt (0.5 – 1 mg/cm^2)[14] and IrO_x (2 – 2.5 mg/cm^2)[14,15] catalysts for the hydrogen evolution (HER) and oxygen evolution reaction (OER), respectively.[10] Of the limited number of materials that are stable under PEM electrolyzer operating conditions, these materials catalyze HER and OER with the highest efficiency. However, concerns about high raw material prices and material scarcity have resulted in decades of research focused on reducing precious metal loading and developing catalysts made from alternative materials that have comparable activity and stability to Pt and IrO_x.

These research efforts have aimed to optimize often competing catalyst performance metrics: activity, stability, and material cost. The ideal catalyst would be highly active and durable, and be made from cheap, earth-abundant materials. But in reality, the optimization of one or two of these metrics often sacrifices the other(s). For example, to date, no non-precious metal HER catalysts have exhibited superior intrinsic activity *and* durability relative to a state-of-the-art Pt catalyst.[16] There are similar research efforts to find alternative OER catalysts to Ir, or to simply reduce the Ir loading without compromising activity and durability.[10,14] A multitude of publications claim superior catalyst activity, durability, or cost, but it is unheard of to see simultaneous improvement of all three metrics. This begs the question: If one metric is improved while the other is sacrificed, what is the overall impact on H_2 production cost?

Herein, we address two key questions:

1. What impact does Pt and Ir scarcity have on PEM electrolyzer deployment rates?

2. How should activity, stability, and material cost metrics be optimized for novel catalysts, and how does that optimization depend on the application of the electrolyzer?

We illustrate how catalyst material scarcity concerns should be rationalized with PEM electrolyzer-derived H_2 demand. We further discuss how diversifying PEM catalysts, specifically by utilizing alternative precious metals or non-precious metals, can reduce the risk of material scarcity while reducing capital costs. We then apply levelized cost of H_2 (LCOH) analysis to establish cost-driven performance metrics for novel catalysts, such as non-precious metal catalysts, under different PEM electrolyzer operating regimes. We propose that this LCOH model be used as a framework to guide and evaluate future catalyst development.

It is well-established that the high *cost* of precious metal catalysts in electrolyzers hinders widespread PEM deployment, especially at the MW-scale.[17] It is more uncertain how the *scarcity* of precious metals will impact deployment rates. Recent supply and demand analysis for Ir, in particular, highlights the potential bottleneck that Ir may pose in the electrolyzer supply chain.[18] In addition, scarce materials can have volatile, inelastic prices that influence the rate and extent to which PEM electrolyzers are able to penetrate the H_2 market. We acknowledge that PEM electrolyzer manufacturers' research investments to reduce precious metal content is evidence that material abundance and volatile prices present a risk to future PEM electrolyzer deployment.[10] Here, we evaluate both material supply and price inelasticity as drivers of non-precious metal catalyst research.

Reliance on precious metals becomes increasingly risky with greater demand for electrolytic H_2. For current PEM electrolyzer technology to meet 100% of today's global demand for H_2 (70 million metric tonnes),[19] nearly 100,000 kg of Pt would be required (assuming 1 mg_{Pt}/cm^2_{geo}, within the range of reported commercial loading, **Figure S1**), which is ~50% of annual Pt production (see **Table S1** for annual production).[20,21] Previous analysis suggests that ~10% is a reasonable fraction of an element's annual production that could be repurposed for a new technology.[22] In other words, if 10% of the annual Pt produced was used to deploy PEM electrolyzers, material availability would limit the capacity deployment rate to 100 GW/yr (**Figure 2.2A**). Thus, it would only take ~4 years of diverting 10% of Pt production to meet the annual global H_2 demand (~400 GW) with PEM electrolyzers utilizing Pt catalysts. On the other hand, Ir availability would limit PEM deployment to 2 GW/yr (assuming 2 mg/cm^2_{geo}), meaning it would require 200 years of diverting 10% of Ir production to build enough PEM electrolyzer capacity to meet today's global H_2 demand (**Figure 2.2B**). This estimate is consistent with previous reports.[18,23]

Historically, Ir availability has not hindered deployment as rates of building PEM capacity have been far less than 2 GW/yr. As of October 2020, total PEM capacity (installed and under construction) in the U.S. was 13 MW, with most individual systems <0.2 MW.[24] By June 2021, however, this capacity had grown to 172 MW, including the announcement of a 120-MW capacity facility.[5] In Europe, PEM electrolyzers on the 100-MW scale are also under development,[25] which will help the EU achieve its goal of 40 GW of electrolysis by 2030.[7] Thus, annual deployment rates are beginning to approach the GW-scale.

As demand for carbon-neutral H_2 continues to increase, the demand for PEM electrolyzers will put more strain on the Ir supply chain. To accelerate PEM deployment beyond 2 GW/yr in the future will require reducing the Ir content, perhaps by substituting or complimenting Ir with an alternative OER catalyst material, such as Ru, thereby diversifying the catalyst material supply. Similar analyses have concluded that Ir loadings of 0.05-0.1 mg/cm^2 are necessary to achieve PEM electrolyzer deployment on the GW-scale, consistent with **Figure 2B**.[15,23,26]

We acknowledge that the estimated maximum deployment rates are sensitive to material supply, catalyst loading, and the power density of PEM electrolyzers. For example, if less than 10% of Ir annual production can be used in PEM electrolyzers, deployment rates could be even more limited than we estimate. However, if Ir loading is reduced or the operating power density is improved, deployment rates could be greater than our estimate. Our analysis also does not account for the finite lifetime of a PEM electrolyzer, and more catalyst materials will be needed to replace aging electrolyzers, which also suggests recycling and recovery of PEM electrolyzer catalysts will be essential in the future.[18]

While availability of Ir could limit PEM electrolyzer deployment rate in the future, the major limitation of using Ir today is its high and volatile cost. As a consequence of being a scarce material and produced as a by-product of Pt mining,[21] the price of Ir is also inelastic to increasing demand as can be seen in the increase in price between 2016-2020[27] and vulnerable to supply chain interruptions as seen in the sharp price increase between 2020-2021[28] (**Figure 2D**).[20,29] Growing demand for Ir comes not just from growth in PEM electrolyzer development, but also from the growing demand for 5G electronics in the telecommunications industry. In addition, the majority of global supply comes from a single country, South Africa, making the price sensitive to geopolitics.[27] For the HER, although Pt is also a precious metal, it is a primary product of mining and the price of Pt over time has remained relatively steady, although high (**Figure 2D**). Thus, the volatile price of Ir poses a greater risk to the widespread deployment of PEM electrolyzers today, even if the abundance of Ir is not a concern in the near-term.

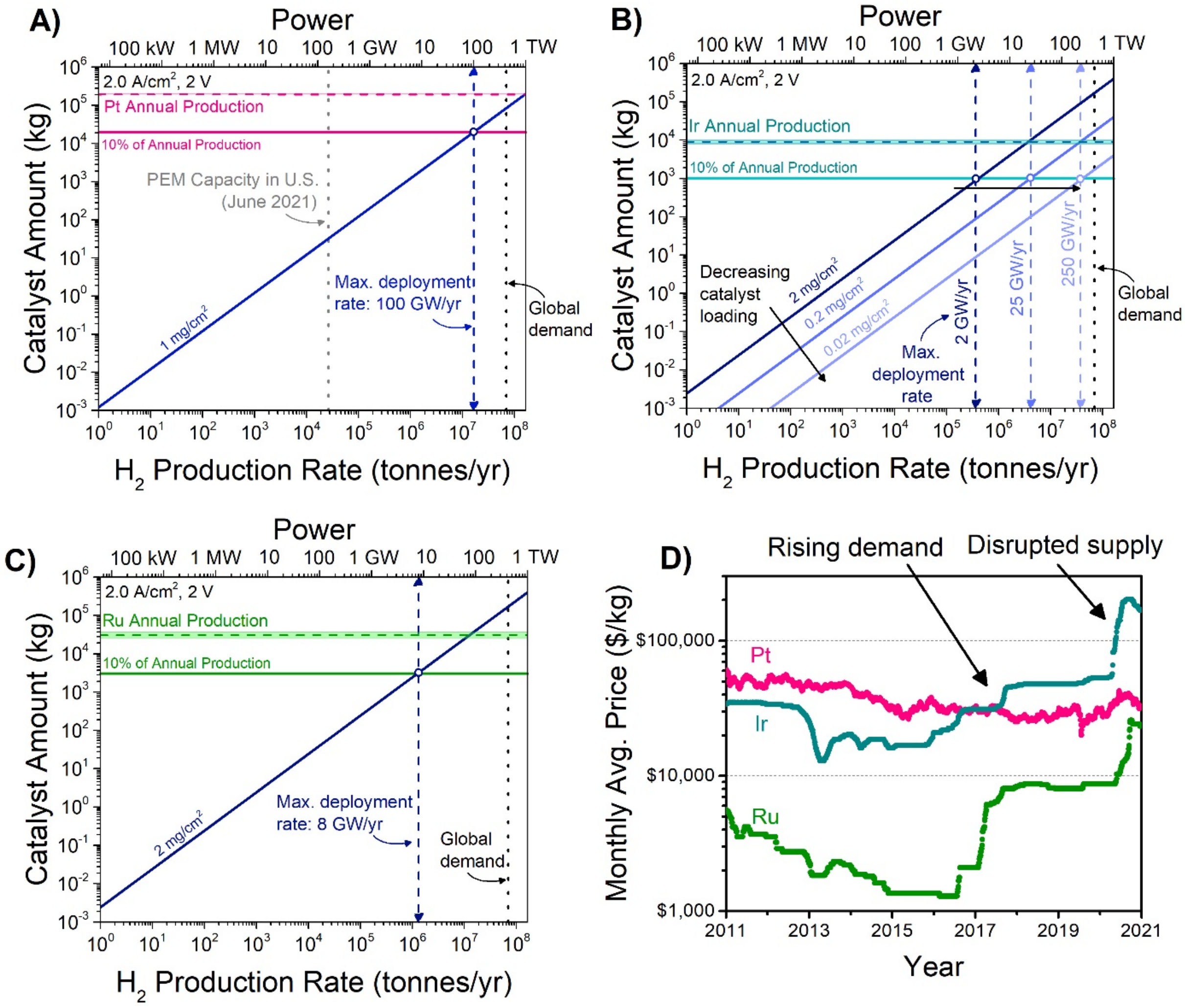


Figure 2. (A-C) Amount of catalyst required to deploy electrolyzers at a specified loading (mg/cm^2) as a function of scale (blue solid lines). Commercially relevant catalyst loadings represented by darkest blue line, with future R&D targets for Ir catalyst loading shown by lighter blue lines. See Supporting Information for methods and assumptions (**Table S2**).[14,30,31] The intersection with annual production rates for (A) Pt (pink), (B) Ir (cyan), and (C) Ru (green) visually show the feasible scale of deployment for each catalyst material and the impact of decreasing loading and diversifying catalyst materials.[20,21] U.S. PEM capacity from Ref. 5. (D) Monthly moving average prices of Pt, Ir, and Ru.[29]

Diversifying catalyst materials in PEM electrolyzers can effectively reduce risk to large-scale deployment by reducing dependence on precious metals, or at least broadening the range of precious metals used. Many such catalysts have been studied to displace both Pt and Ir catalysts in order to reduce the overall cost of H_2 from PEM electrolyzers.[26,32,33] For example, an alternative

OER catalyst material, Ru, is another by-product of Pt mining with an inelastic price, but has a lower average market price to begin with than Ir (**Figure 2C-D**). By alloying Ru with Ir or forming mixed metal oxides, researchers have demonstrated improved intrinsic OER activity relative to IrO_x while improving stability relative to RuO_2.[34–37] While many reports show reasonable activity and stability of novel catalysts at low current density in lab-scale devices, fewer demonstrate how those achievements can be sustained in a PEM electrolyzer operating at higher current densities and elevated temperature and pressure.[38–40] Even for Pt and Ir catalysts, it has been shown that performance from lab-scale measurements does not always translate to a device.[14,41]

Assessing novel catalysts in PEM electrolyzers is critical in determining the overall impact of the catalyst on H_2 production cost. As the practical goal of catalyst development is to reduce cost, we propose that performance targets (i.e. activity and stability goals) be established for a given material and set of operating conditions (i.e. electricity price and capacity factor). As a first step to establishing catalyst performance targets, we consider the trade-offs between material cost and catalyst activity to answer the question: If a catalyst is made from cheap materials, how efficient does it have to be over the lifetime of the device? We aim to answer this question by comparing the levelized cost of H_2 (LCOH) of two electrolyzers (PEM 1 and PEM 2) made with different catalyst materials, catalyst loading, and device performance.

$$LCOH_{PEM,1} = LCOH_{PEM,2} \tag{1}$$

The LCOH is the net present value (NPV) of the upfront capital cost (c_{cap}) of the electrolyzer and the operating expenses (c_{op}) over the lifetime of the electrolyzer, normalized by the discounted annual H_2 production rate ($\dot{m}_{H2}$) summed over the lifetime of the electrolyzer. This is akin to the levelized cost of energy (LCOE) metric. We make simplifying assumptions that all costs other than the catalyst material and electricity are the same between the electrolyzers (e.g. maintenance, balance of systems) and that the catalysts have the same lifetime. Additional calculation details and assumptions can be found in the Supporting Information (**Table S3-S4**).

$$LCOH = \frac{c_{cap} + \sum_{t=1}^{t_{life}} \frac{c_{op}}{(1+d)^t}}{\sum_{t}^{t_{life}} \frac{\dot{m}_{H2,t}}{(1+d)^t}} \tag{2}$$

We first exemplify this framework to understand the extent to which catalyst efficiency can achieve cost reductions given a particular use case (e.g. capacity factor, electricity price) and catalyst capital cost ($\$/m^2$). We consider an electrolyzer using an IrO_x benchmark OER catalyst. If less Ir or a cheaper material were used instead, money would be saved on the initial investment that could be spent over the lifetime of the electrolyzer to make up for increased operating costs from, for instance, a lower efficiency catalyst. The isocost curve in **Figure 3A** represents the tolerable change in voltage (relative to IrO_x at a fixed current density) for a cheaper catalyst to achieve the same LCOH as the baseline IrO_x. Any catalyst that is more efficient and falls below the isocost curve would result in a lower LCOH, and above the isocost curve would result in a higher LCOH. This same analysis can be extended to HER catalysts, using a Pt/C cathode as a baseline (**Figure 3C**).

The slope of the isocost curve is determined by the average capacity factor and electricity price over the lifetime of the electrolyzer (**Figure 3B-C**). Lower capacity factors and lower electricity prices enable the use of less efficient catalysts (relative to precious metal benchmarks) while still achieving the same or a reduced LCOH. As capacity factors and electricity prices decrease, the majority of the LCOH is increasingly attributed to capital costs, thus decreasing material cost has a larger impact on LCOH than the catalyst efficiency. This analysis shows that the electrolyzer operating parameters (i.e. electricity price, capacity factor) for a particular scenario can impact decisions for the cost-optimal catalyst; thus developing a diverse portfolio of catalyst options can facilitate wide adoption of the technology for use across the broadest range of conditions.

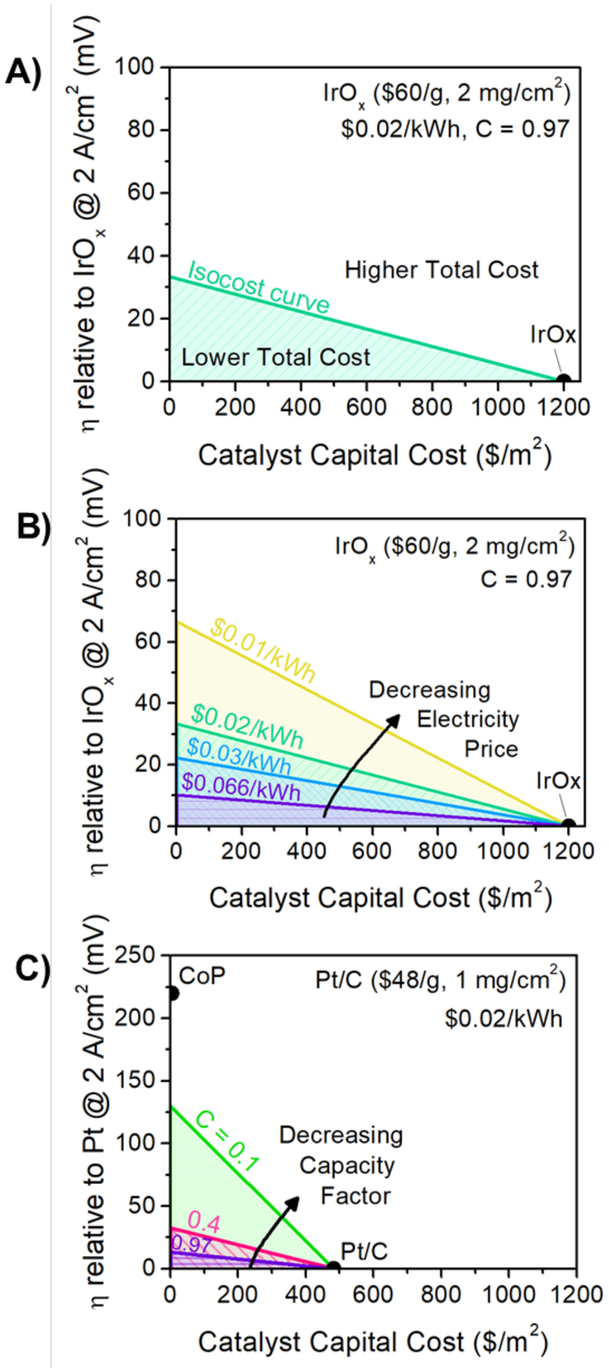


Figure 3. (A) The same LCOH, represented by the isocost curve, can be achieved with a combination of catalyst capital cost and performance, represented by an allowable increase in overpotential to achieve 2 A/cm^2. Slope of the isocost curve changes with changes in operating conditions such as electricity price (B) and capacity factor (C). Performance of a CoP catalyst ($4/m^2, 220 mV) compared to a Pt catalyst in a PEM electrolyzer shown as an example in (C).

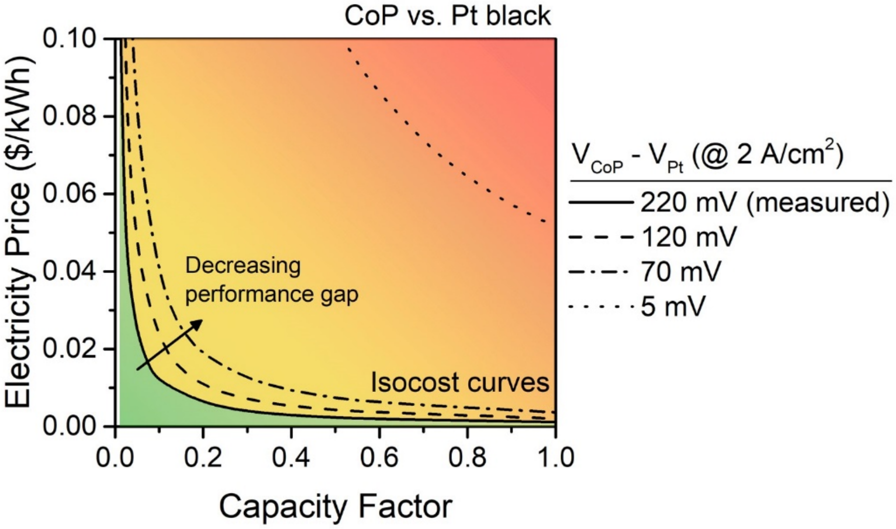


Figure 4. Isocost curve reveals capacity factors and electricity prices necessary for a PEM electrolyzer utilizing a CoP cathode to achieve the same LCOH as a Pt black cathode. Line styles indicate the effect of decreasing the performance gap (i.e. the difference in cell voltage to achieve 2 A/cm^2) on cost-effective capacity factors and electricity prices. Qualitative shading indicates which electricity price and capacity factor would result in a reduced LCOH (green) or would result in increasingly higher LCOH (yellow to red) if performance improvements not made to the 220 mV solid curve.

This framework can also be applied to a known catalyst (with pre-defined cost and electrolyzer efficiency) to determine what use cases (i.e. capacity factor and electricity price combinations) would result in the same or lower LCOH. We emphasize that this requires that non-precious metal catalysts have been evaluated in electrolyzers, of which there are only a few demonstrations at high current density to date. As one example, we show how a reported CoP HER catalyst tested in a commercial PEM performed relative to a Pt HER catalyst in an otherwise identical electrolyzer.[38] Although the CoP catalyst had a greater loading than the Pt catalyst in this study, the overall capital cost of the CoP catalyst was still much lower than Pt owing to the lower material cost of the non-precious metal material. Utilizing the same IrO_x anode and all other parameters being equal, the difference in cell voltage at ~2 A/cm^2 between the electrolyzers was 220 mV, and is shown in **Figure 3C**.[38]

Our analysis suggests that a lower LCOH for an electrolyzer utilizing this CoP catalyst rather than Pt would only be feasible with extremely low electricity prices and capacity factors, as shown by the green area under the isocost curve in **Figure 4**. We also acknowledge that the manufactured cost of this lab-scale produced CoP is unknown, and a higher cost than assumed here could result in an even more limited range of electricity prices and capacity factors. The benefits of using this non-precious metal catalyst in a PEM electrolyzer today are therefore limited to energy storage applications and underwater O_2-generation applications unless the performance gap with Pt/C catalysts can be reduced (**Figure 4**). Outside of these regimes, utilizing this CoP HER catalyst would be prohibitively expensive with today's known technology. Thus, further work to optimize the efficiency of non-precious metal catalysts (e.g. higher loading, optimized ionomer content) and close the performance gap is needed for realistic electrolyzer applications.

The framework and assumptions presented here should be considered a starting point, and there are opportunities to expand upon this model. For instance, catalyst activity is assumed to be constant over the lifetime of the electrolyzer. Future work could incorporate degradation in catalyst performance over time by considering an increasing voltage,[42] additional maintenance or replacement costs, and/or recycling costs to compare PEMs utilizing cheap, yet unstable catalysts to more stable precious metal catalysts.

We also acknowledge the challenges of adopting this kind of evaluation framework. For one, it is well-known that fabrication and operating parameters such as ionomer content and break-in procedure can significantly impact the observed performance of a catalyst in a PEM electrolyzer.[31,43] This makes it challenging to compare electrolyzer performances reported in the literature, and as such we echo the call for established benchmarking protocols.[10,31] In addition, our proposed framework relies on direct comparison of a novel catalyst to a Pt or IrO_x benchmark in an electrolyzer, thus requiring a Pt-IrO_x control experiment (as was the case for the CoP-IrO_x electrolyzer). Alternatively, integrating a reference electrode into a PEM electrolyzer to measure the relative voltage contributions of the HER and OER catalysts is an interesting way to isolate the performance of each catalyst.[44] These challenges are not insurmountable, and we hope our preliminary analysis will inspire the field to measure novel catalyst performance using standardized PEM electrolyzer protocols to enable setting performance targets.

High catalyst cost and economic risk due to material scarcity are well-known barriers to large-scale PEM electrolyzer deployment. While the PEM electrolyzer market has continued to expand in recent years, we show that there is a finite growth rate based on annual raw material production. Diversifying catalyst material supply could eliminate this barrier in the future as electrolytic H_2 demand increases rapidly. Further, using a diverse set of catalyst materials would mitigate near-term economic risks in the catalyst supply chain arising from volatile prices of precious metals. Thus, there is strong motivation for continued non-precious and reduced precious metal catalyst fundamental research and applied engineering.

Moving forward, we propose that novel catalyst research be evaluated and guided using a cost-based framework to set targets for activity and stability. While maximizing catalyst activity and stability while simultaneously reducing material cost is ideal, this goal is perhaps unrealistic. We highlight that performance targets such as activity and material cost will be strongly influenced by the operating conditions of the electrolyzer. We demonstrate, for example, that non-precious metal HER catalysts today are only cost competitive with Pt in limited use cases. This result is suggestive that future PEM electrolyzers could utilize different catalysts depending upon their different intended operating conditions. Developing such diverse catalysts for diverse electrolyzer applications is a pathway towards PEM electrolyzer cost reduction, and ultimately a step towards decarbonizing the global H_2 market.

Supporting Information Available

List of parameters, constants, data, and assumptions used in catalyst demand and cost calculations; material supply data; material price data; methods to calculate levelized cost of hydrogen and performance gap

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Notes

The authors declare no competing financial interest.

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Selected Quotes

1. Diversifying catalyst materials in PEM electrolyzers can effectively reduce risk to large-scale deployment by reducing dependence on precious metals
2. operating parameters (i.e. electricity price, capacity factor) for a particular scenario can impact decisions for the cost-optimal catalyst

3. volatile price of Ir poses a greater risk to the widespread deployment of PEM electrolyzers today, even if the abundance of Ir is not a concern in the near-term
4. Reliance on precious metals becomes increasingly risky with greater demand for electrolytic H_2.

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