Techno-economic Comparison of Catalysts for Proton-Exchange Membrane Electrolysis

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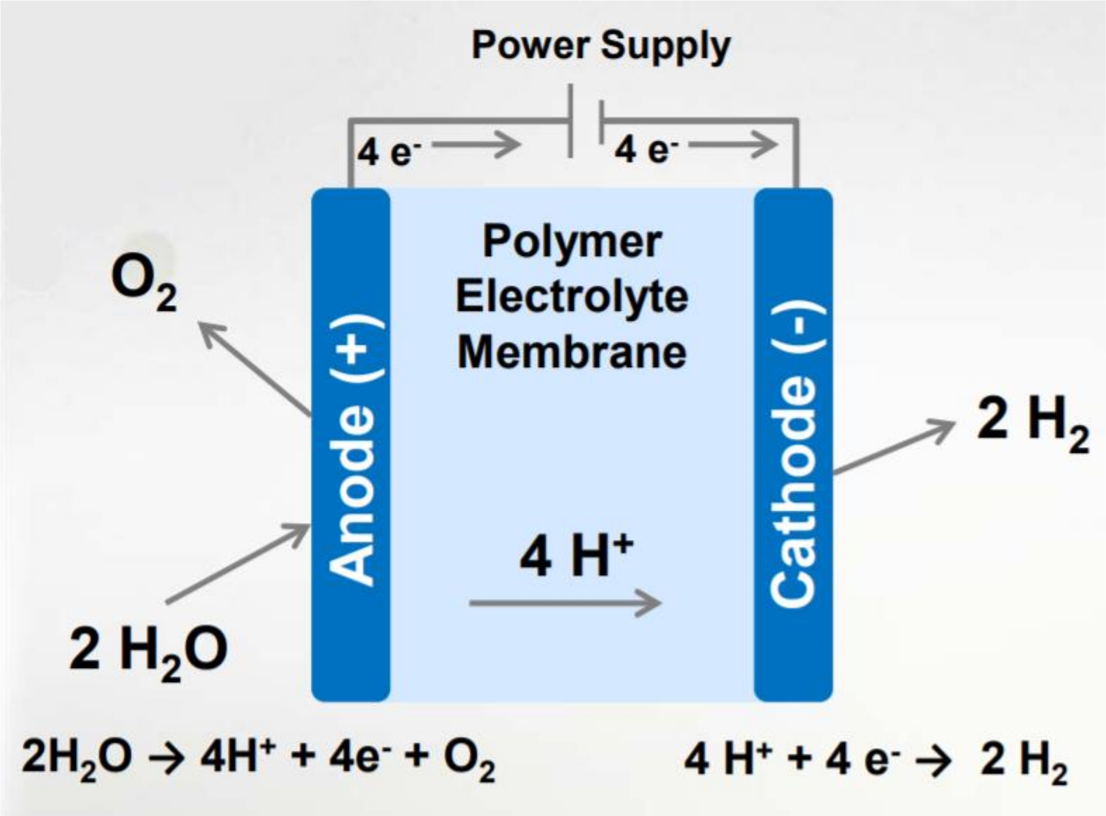
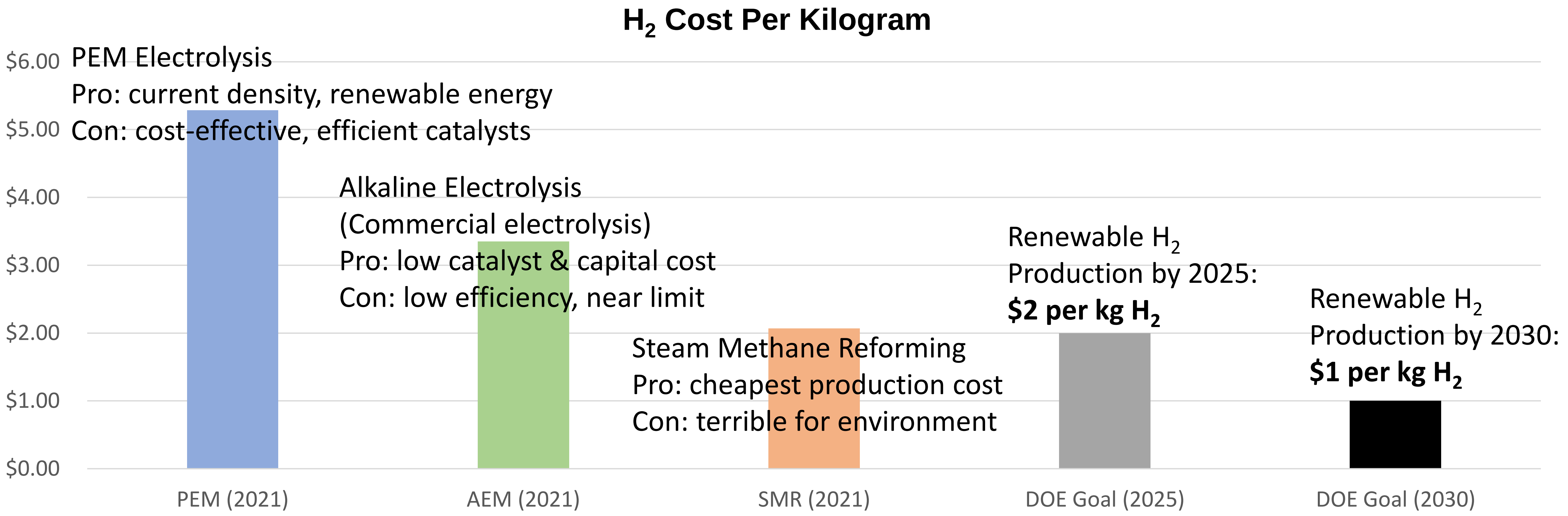
What is Proton Exchange Membrane (PEM) Electrolysis?



Colella et al., NREL, 2014

- Uses electrical power to split water into oxygen & hydrogen gas
- Zero-carbon hydrogen production
- 3 components: electrodes, membrane, and electrolyte (acidic)
- 2 reactions: OER (anode) & HER (cathode)
- Sluggish OER → need high performance, cost effective catalyst to improve efficiency
- Versatile & high performance
- Needs corrosion-resistant catalyst

Current Hydrogen Production Costs



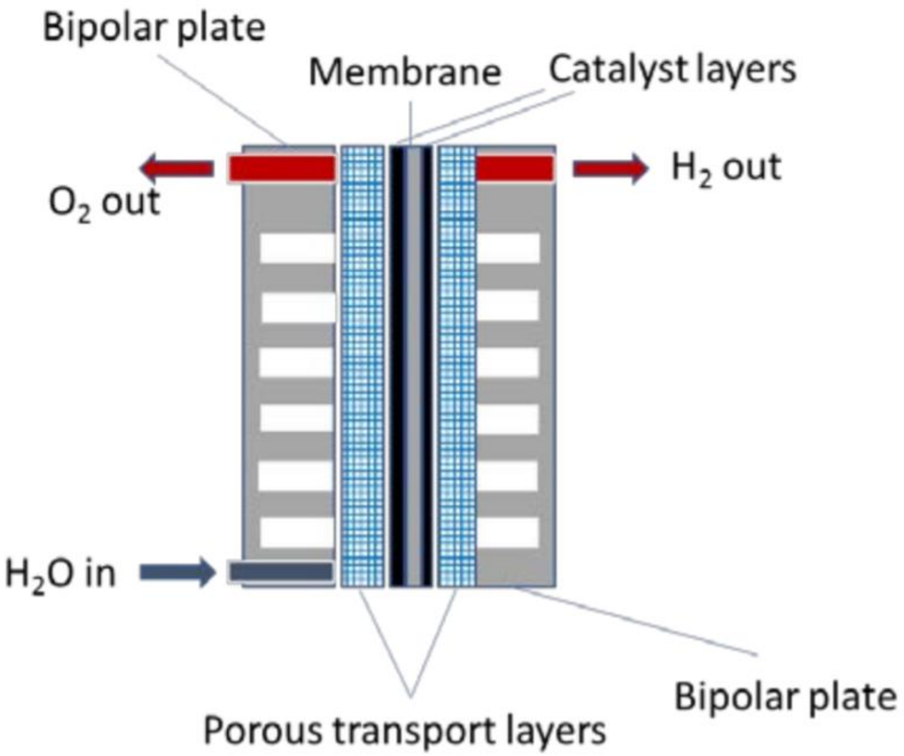
[1] Yates et al., Cell Reports Physical Science, 2020, Volume 1, Issue 10
[2] IRENA, 2019
[3] Muhammet Kayfeci, Ali Keçebaş, Mutlucan Bayat, Science, 2019, 45-83
[4] Mayyas et al., NREL, 2019
[5] James Vickers, David Peterson, Katie Randolph, DOE, 2020, 20004
[6] David Peterson, James Vickers, Dan DeSantis, DOE, 2019, 19009
[7] https://www.energy.gov/eere/fuelcells/hydrogen-shot
[8] https://www.energy.gov/eere/fuelcells/hydrogen-production

Purpose of Techno-Economic Analysis

- Accurately model hydrogen production costs
- Assess the progress of state-of-the-art electrolysis
- Analyze the most economically & environmentally feasible catalyst for PEM electrolysis
- Identify key bottlenecks in H_2 production cost with a focus on catalysts
- Determine research & development priorities for cost reductions
- Provide performance targets for renewable electrolysis to reach DOE goals

Decomposition of H_2 Production Cost

- Electricity Costs
  - $/kWh
  - Electrolyzer efficiency (depends on catalyst)
  - Other systems
- Capital Costs
  - Catalyst Coated Membrane (CCM)
    - Nafion membrane
    - Catalyst loading
  - Porous Transport Layer (PTL)
  - Bipolar Plates
  - Frame
- Replacement Costs
- Operating & Maintenance Costs



Mayyas et al., NREL, 2019

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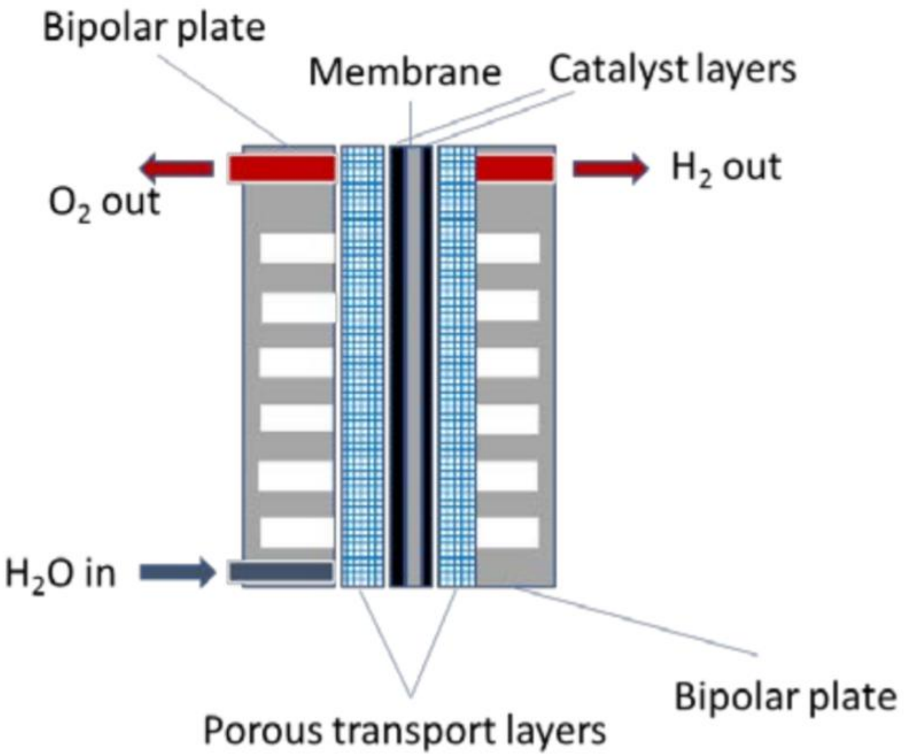
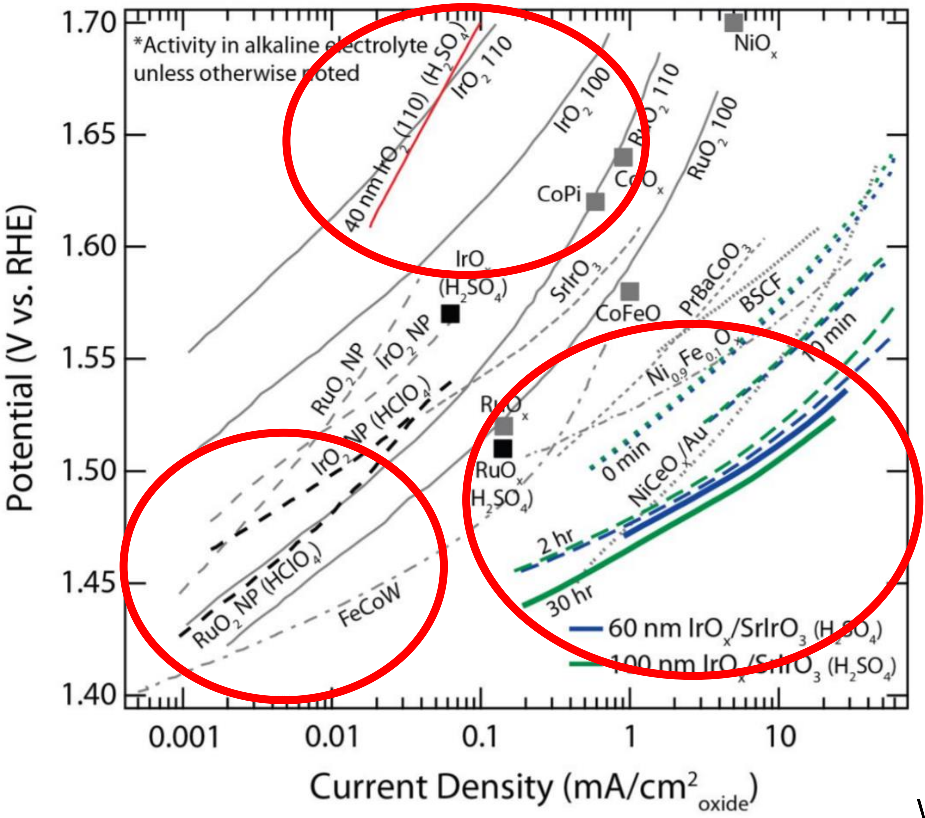


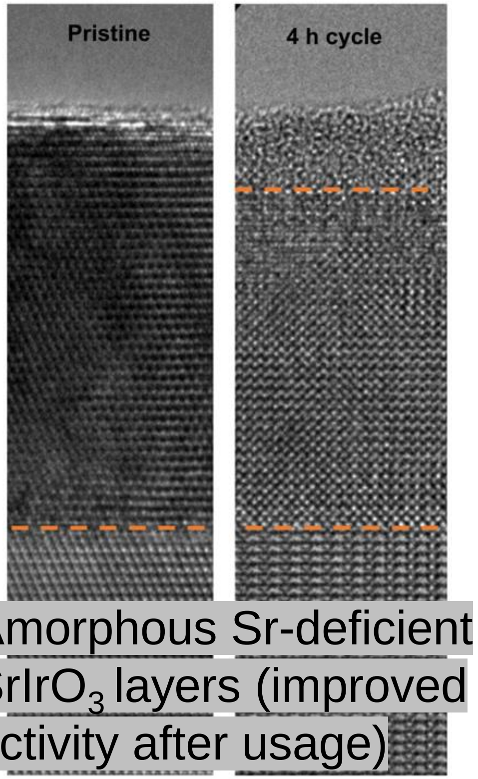
Mayyas et al., NREL, 2019

OER Catalysts for PEM Electrolysis

- High performing catalysts: low overpotentials (Operation voltage - 1.23V)
- Tradeoff between voltage and current density – electricity vs capital costs
- As current density increases, so does its voltage; commercial standard is $1 A/cm^2$
- Best catalysts: RuO_2, IrO_2, $SrIrO_3$ (analyzed with our techno-economic model)



Seitz et. al., *Science*, 2016, 353, 1011-1014



Amorphous Sr-deficient $SrIrO_3$ layers (improved activity after usage)

Wan et al., *Science*, 2021, Vol 7, Issue 2,

	Relative Performance (V at $1 A/cm^2$)	
Relative Capital Cost ($/m²)	High (<1.7)	Low (≥1.7)
High (>1000)	IrO_2, Ir-Ru based catalysts, $SrIrO_3$	RuO_2
Low (≤1000)	N/A	Pt, MoS_2

S. Shiva Kumar, V. Himabindu, Materials Science for Energy Technologies, 2019, Vol. 2, Issue 3, 442-454

Parameters & Assumptions for Our Model

Parameter	Value Used
Operating Capacity	97%
Nafion Membrane Cost ($/m^2)	0.05
Balance of Plant (% of Capital + BoP Cost)	60%
CCM Cost (% of non-BoP Capital Cost)	40%
Maintenance Cost (% of Capital Cost)	2.5%
BoP Electrical Usage (kWh/kg)	5
Input Water Cost ($/kL)	1.44
Production Rate (kg H_2/day)	1500
Installation Factor	15%
Cell Active Area (cm^2)	450
Cathode Catalyst (HER)	Pt

Total BoP/CCM costs are dependent on the cost of the catalyst

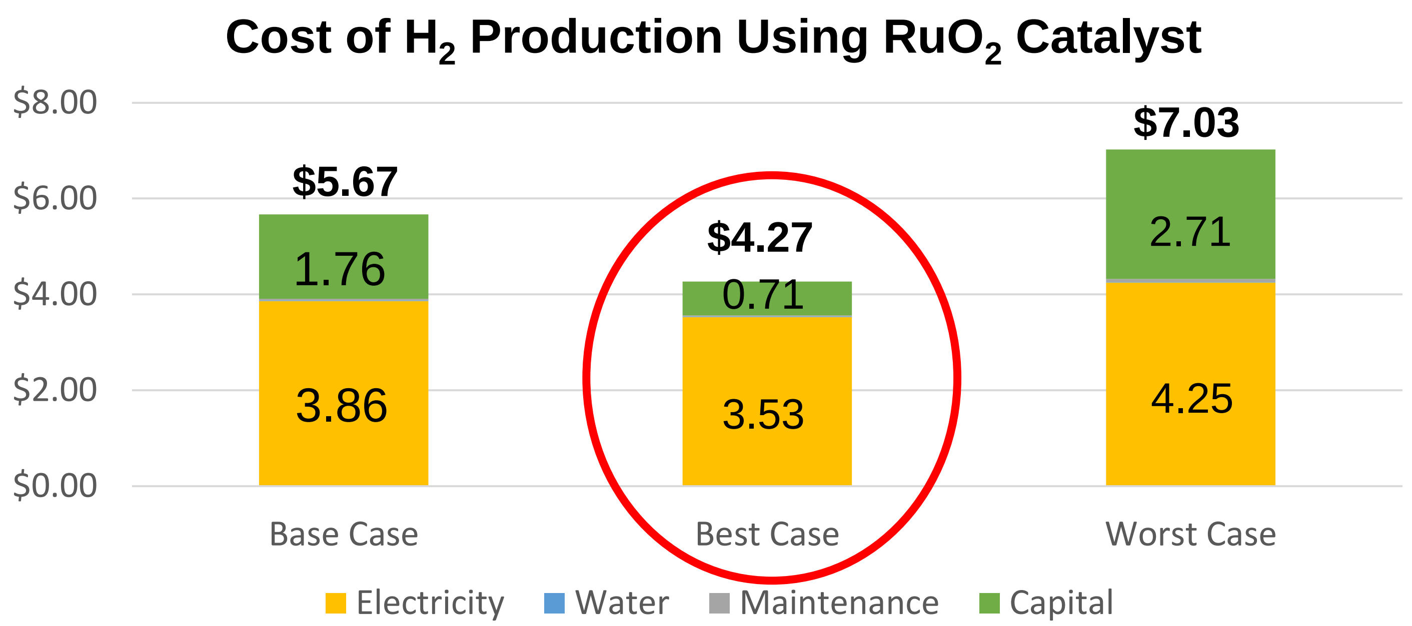
Parameter & Assumptions (cont.)

Parameter	Base Value	Renewable Energy Value
Electricity Price ($/kWh)	0.073	0.03

Assumptions:

- $SrIrO_3$ catalyst lifetime is equal to that of the IrO_2
- $SrIrO_3$ is 27% less expensive than IrO_2 since it has less iridium
- We use the electrolyzer's average potential over its lifetime

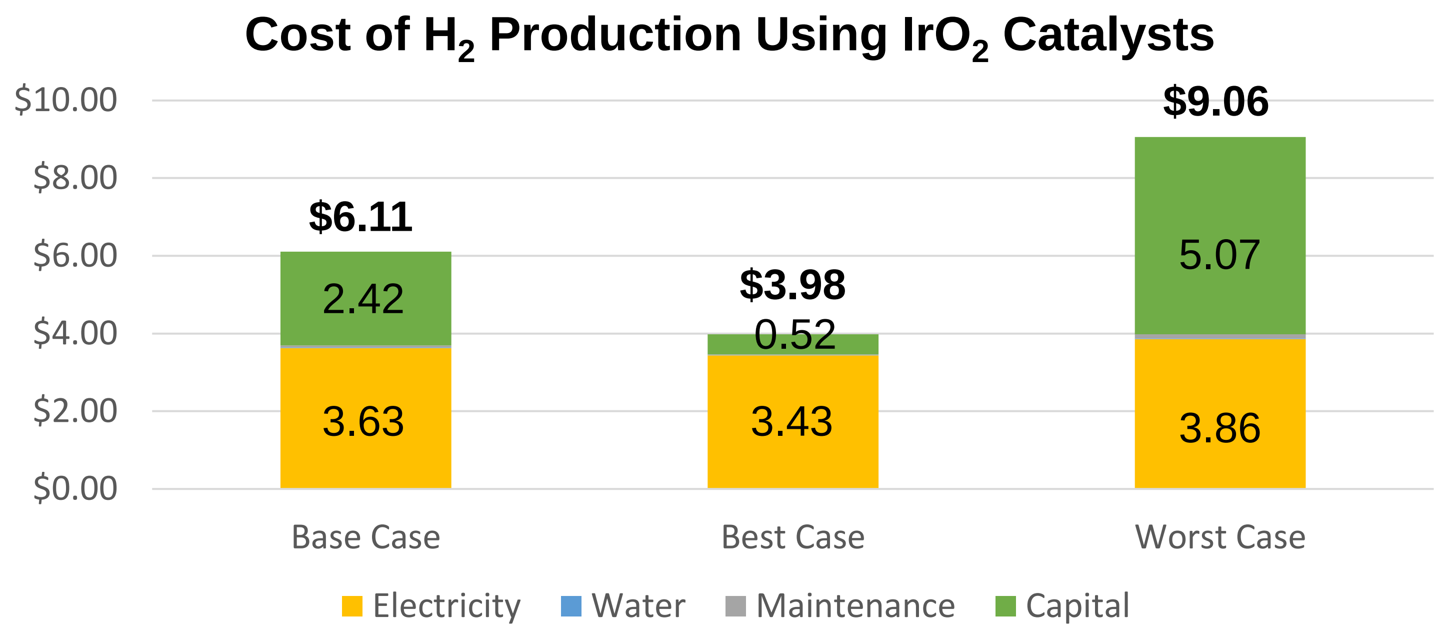
RuO_2 Catalyst Analysis



Poor best-case Scenario
Unstable catalyst

Parameter	Base Case	Best Case	Worst Case
Voltage (V)	1.8	1.63	2
Lifetime (hrs)	80000	100000	60000
Catalyst Loading (g/m^2)	25	10	30
Catalyst Cost ($/g)	100		

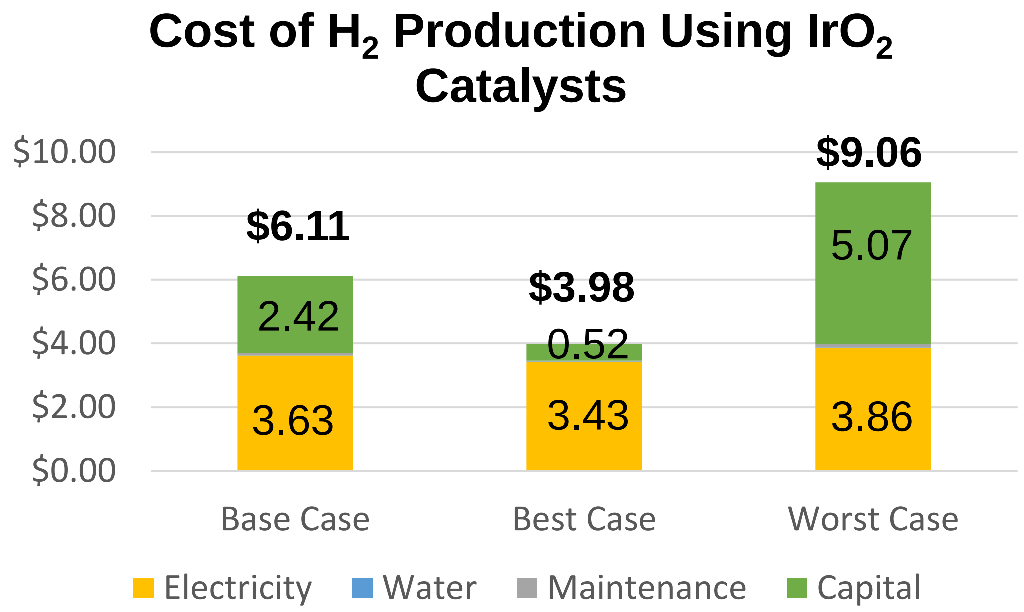
IrO_2 Catalyst Analysis

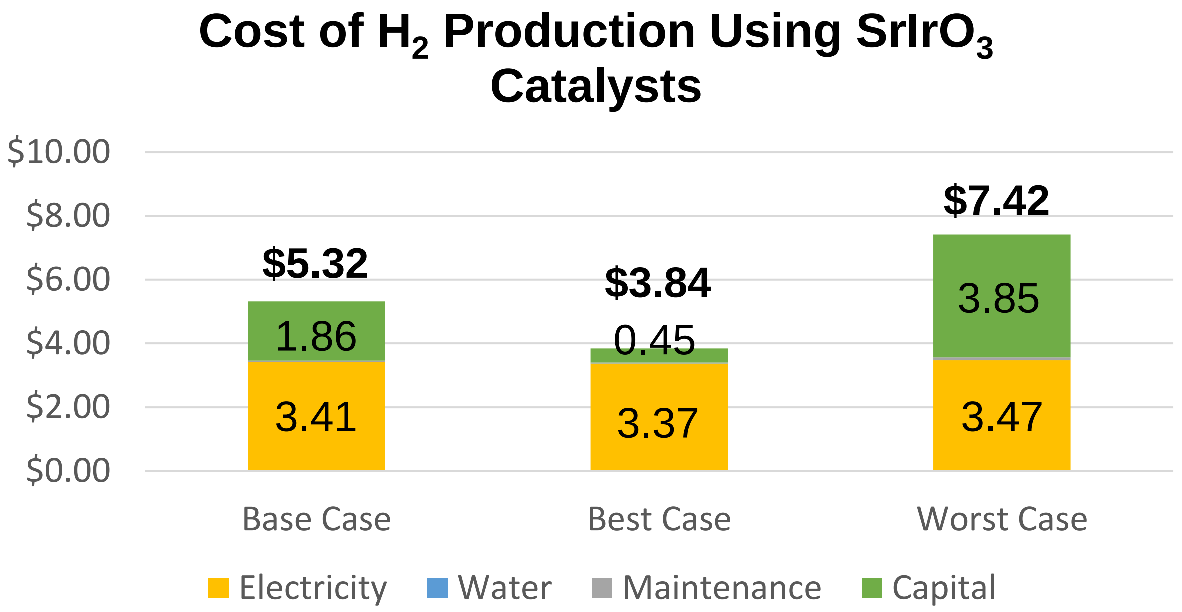


Parameter	Base Case	Best Case	Worst Case
Voltage (V)	1.68	1.58	1.80
Lifetime (hrs)	80000	100000	60000
Catalyst Loading (g/m^2)	18	3	30
Catalyst Cost ($/g)	200		

Bernt et al., *Chemie Ingenieur Technik*, 2020, 92, 31-39

IrO_2 vs $SrIrO_3$ – Same Loading





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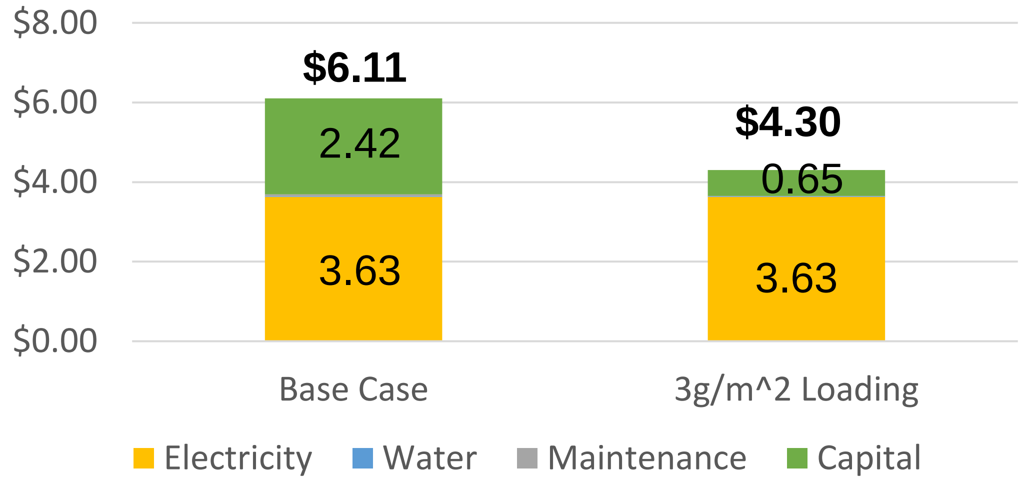
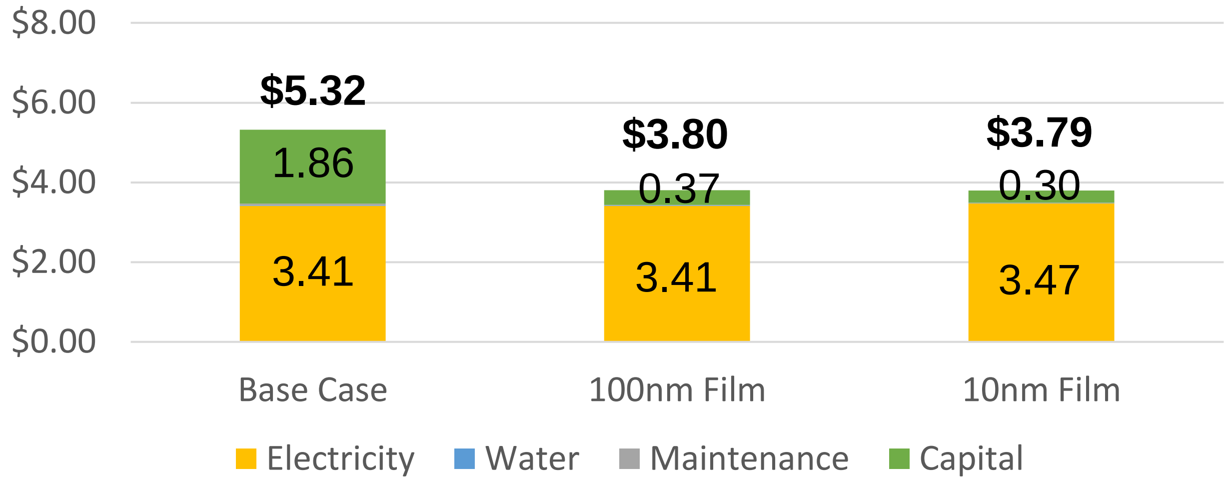
Parameter	Base Case	Best Case	Worst Case
Voltage (V)	1.57	1.55	1.60
Lifetime (hrs)	80000	100000	60000
Catalyst Loading (g/m^2)	18	3	30
Catalyst Cost ($/g)	146		

IrO_2 vs $SrIrO_3$ – Best Loading

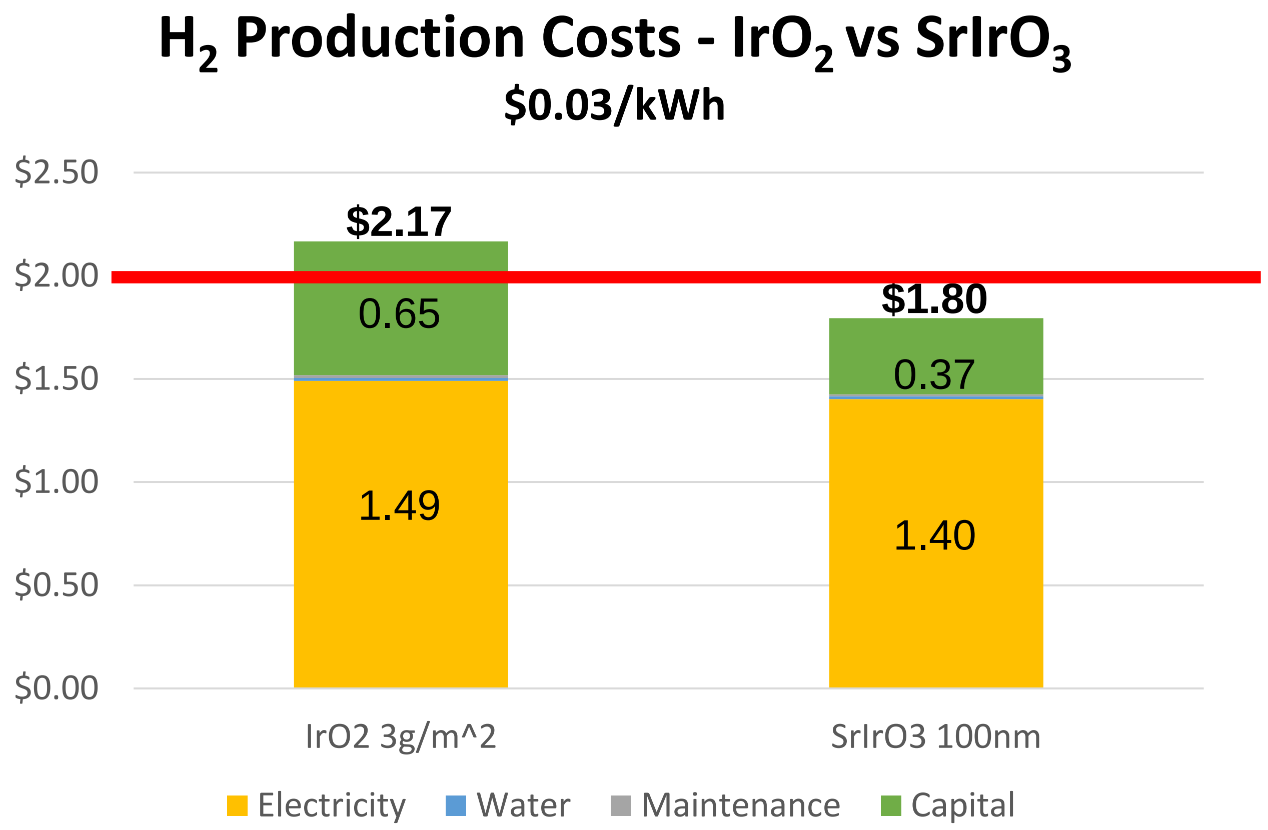




Parameter	Base Case	3g Loading
Voltage (V)	1.68	1.68
Lifetime (hrs)	80000	80000
Catalyst Loading (g/m^2)	18	3
Catalyst Cost ($/g)	200	200

Parameter	Base Case	100nm Film	10nm Film
Voltage (V)	1.57	1.57	1.60
Lifetime (hrs)	80000	80000	80000
Catalyst Loading (g/m^2)	18	0.85	0.085
Catalyst Cost ($/g)	146	146	146

IrO_2 vs $SrIrO_3$ - Best Loading & Cheap Energy



DOE 2025 Renewable Hydrogen Cost Goal

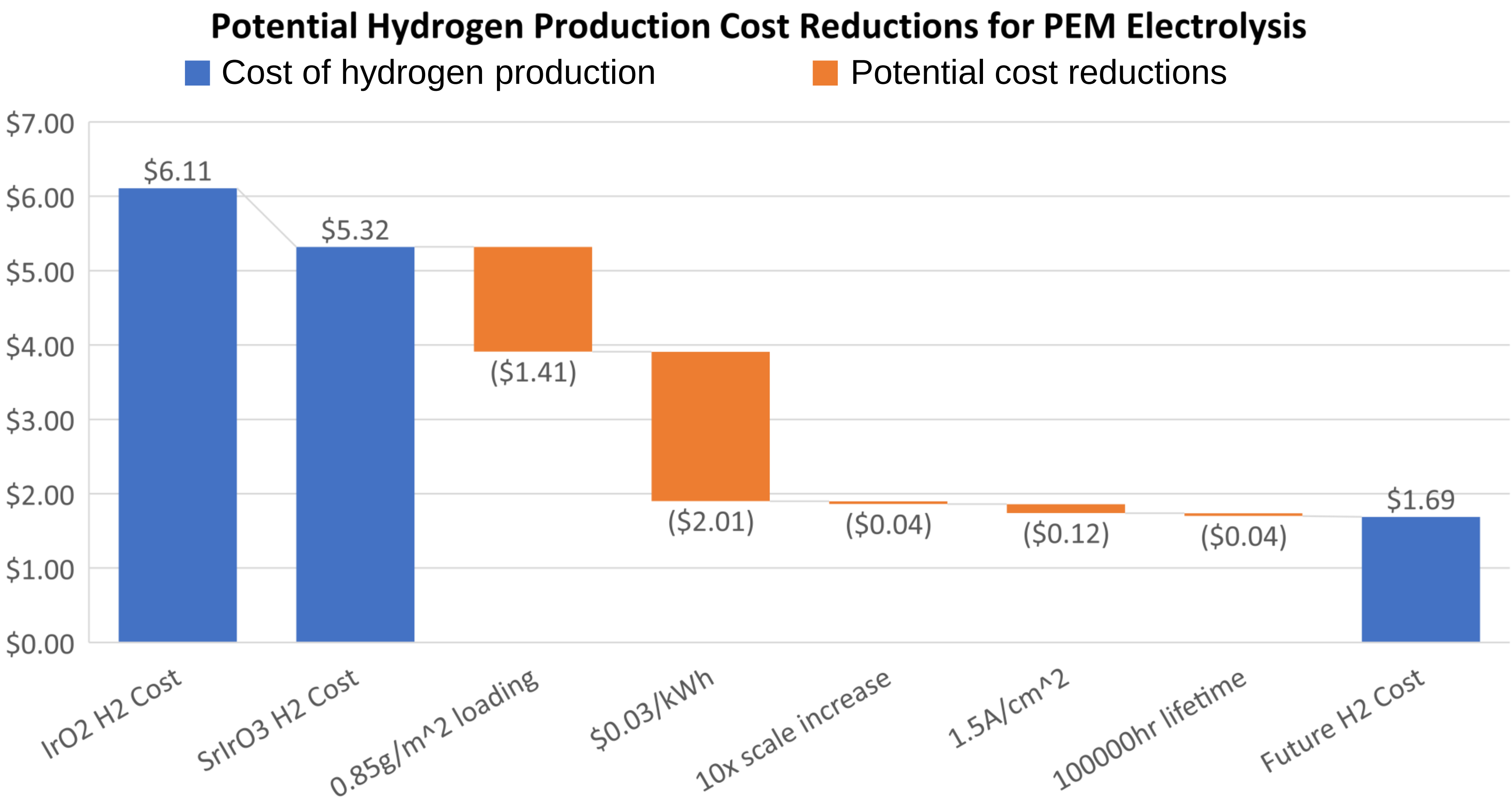
Using renewable energy & thin-film loading, $SrIrO_3$ is able to meet the DOE 2025 target of $2/kg

Parameter	IrO_2	$SrIrO_3$
Voltage (V)	1.68	1.57
Catalyst Loading (g/m^2)	3	0.85
Catalyst Cost ($/g)	200	146

Future Improvements

- Overpotential reductions
- Use of thin-film $SrIrO_3$/decrease in catalyst loading (100nm, 0.85g/m^2)
- Decreased electricity cost (<0.03$/kWh)
- Increase in current density to 1.5A/cm^2
- Increase in catalyst lifetime to 100000 hrs
- Capital costs decrease 10% every 10x increase in scale (includes balance of power costs)

Roadmap to DOE Targets Using $SrIrO_3$



To reach $1/kg:

- Catalyst efficiency
- Electricity cost (<$0.03/kWh)

Conclusion

- PEM electrolysis with the $SrIrO_3$ catalyst can supersede current IrO_2 electrolyzers for cheaper & more sustainable H_2 production
- The main improvement needed for the $SrIrO_3$ catalyst is its loading density
- Electricity cost will be the largest cost factor, and if decreased, can make PEM electrolysis meet the DOE goal of $2/kg H_2 by 2025