Supplementary Information

All primary data sources, calculation methods, and assumptions used in this study are detailed below. Raw data from proprietary databases (GREET, Ecoinvent) are subject to respective licensing agreements. Derived datasets and calculation spreadsheets developed for this study are available from the corresponding author upon reasonable request.

Section S1. AEM Electrolysis Technology Development

AEM electrolysis is not yet represented in established LCA databases; the technology context and motivation are summarized in the main text, in the section titled "Water Electrolysis Technologies and LCA Framework."[1] Accordingly, we constructed a literature–synthesized life cycle inventory for AEM components. Table S1 summarizes the baseline AEM component inventory compiled from recent peer–reviewed sources.[2]

Table S1. Material inventory and substitution strategy for AEM electrolyzer components

Components	**Materials**	**Substitute Materials**	**Mass (kg)**
Membrane	Quaternary Ammonium Polysulfone	Polysulfone	0.0042–0.0048
Substrate (HER)	Carbon cloth	Ni	0.0051–0.0059
Catalyst (HER)	NiMo	NiAlMo	0.0021–0.0025
Substrate (OER)	Ni foam	Ni	0.0132–0.0153
Catalyst (OER)	NiFe	NiCrFe	0.0013–0.0015
Bipolar plates	Ni-coated stainless	Stainless steel	1.1304–1.3112

	steel		
End plates	Ni-coated stainless steel	Stainless steel	1.1304–1.3120
Sealant material	Synthetic rubber	Polyolefin	0.0016–0.0019
Fixing elements	Stainless steel	Stainless steel	0.0767–0.0890

For entries not available in GREET, we applied functional substitution using three criteria: (1) physicochemical similarity, (2) comparable manufacturing energy, and (3) equivalent electrochemical function. For example, quaternary ammonium polysulfone was substituted with polysulfone owing to identical polymer backbones and comparable synthesis energy. The complete substitution mapping and supporting evidence are provided in Tables S1–S2.[3]

To validate these material substitutions, we conducted targeted sensitivity analyses; the design and results are described in the Supplementary Information under the section titled ″Electrolyzer System Data Sources and Material Inventories.″ For balance of plant (BOP) components in AEM electrolyzers (e.g., power supplies and control systems), we used PEM electrolyzer data in GREET as a surrogate, given the architectural similarity between these technologies. This approach is consistent with methods employed in their process development LCA case studies when dealing with emerging technologies.[4]

Section S2. Electrolyzer System Data Sources and Material Inventories

To evaluate the environmental performance of four water electrolysis technologies—Alkaline, PEM, SOEC, and AEM—across their full supply chains, we developed four life cycle models using GREET and SimaPro. For Alkaline, PEM, and SOEC systems, stack and BOP inventories were obtained directly from the GREET database.[5] For AEM electrolysis, which is not yet included in GREET, we constructed a representative model by benchmarking recent peer–reviewed literature and adapting inputs to conform to GREET's methodological framework.[1]

For AEM electrolysis, sensitivity analyses were performed to validate the material substitutions, demonstrating that the use of proxy materials caused less than a 5% deviation in overall environmental impact results, consistent with established LCA uncertainty thresholds. The complete material composition and mass requirements for electrolyzer stacks across all four technologies are provided in Table S2

Table S2. Material composition and mass requirements for electrolyzer stack components across four water electrolysis technologies. Data for Alkaline, PEM, and SOEC systems are sourced from the GREET database; AEM system data are derived from literature synthesis and validated through sensitivity analysis.

Water Electrolysis stack	Material	Mass (kg)
Alkaline stack	Nickel	11,995
	Steel	2,159
	Ethylene Propylene Diene Monomer	1,618
	PolyEther Ether ketone	1,207
	AGFA Zirfon Perl UTP 500	138.8
	Polypropylene	90.06
	Ni-Al-Mo alloy	75.45
	Copper Wire	71.75
	Polytetrafluoroethylene (PTFE)	4.660
	Cobalt Nitrate	2.603
	Nickel Nitrate	1.564
	Ruthenium Nitrate	0.863
PEM stack	Titanium Sponge Metal	107.9
	Steel	71.96
	Titanium Powder	56.72

	Polyethylene Terephthalate	20.31
	High-Density Polyethylene	14.93
	Nafion Dry Polymer	12.38
	Polypropylene	8.047
	Copper Wire	5.380
	SGL Carbon: GDL 34 BA (Non-Woven)	2.178
	Polytetrafluoroethylene (PTFE)	1.319
	Polyolefin Elastomer	1.284
	Iridium powder	0.550
	Vulcan XC-72	0.365
	Pt/C powder	0.300
	Zinc Stearate Lubricant Powder	0.290
	Polyurethane Adhesive Powder	0.260
	Platinum - PGM	0.127
	CeO_2 additive	0.022
	Gold PGM	0.013
SOEC stack	Iron-Chromium Alloy	27.26
	Ni-Cr-Fe alloy	12.94
	Nickel Oxide	7.221
	Steel	5.794
	3% Yttria-Stabilized Zirconia	3.982
	Gadolinia-doped Ceria	1.265
	Aluminum Silicate Fiber	0.762
	Lanthanum Strontium Cobalt Ferrite	0.540
	8% Yttria-Stabilized Zirconia	0.468
	Glass powder	0.406
	Aluminum Oxide	0.200
	Cobalt Carbonate	0.104
	Manganese Carbonate	0.094
AEM stack	Steel	5,105

	Nickel	47.70
	Polysulfone	13.31
	Ni-Al-Mo alloy	5.550
	Polyolefin Elastomer	4.260
	Ni-Cr-Fe alloy	3.330

BOP materials for Alkaline, PEM, and SOEC systems were obtained from internal documentation within the GREET model.[5] For the AEM system, where technology–specific data remain limited, the BOP configuration was approximated by scaling the PEM BOP inventory in GREET. The complete material composition and mass requirements for all BOP components are reported in Table S3.[6] Materials with total mass< 0.001 kg were excluded from the analysis to maintain data relevance and computational efficiency.

Table S3. BOP material composition and mass requirements for water electrolysis systems by technology and capacity. Materials with total mass <0.001 kg were excluded from analysis to maintain data relevance and computational efficiency.

Water Electrolysis BOP	Material	Mass (kg)
Alkaline BOP	Concrete	255,455
	Steel	69,492
	Reinforced concrete	40,420
	Copper Wire	9,215
	Iron	4,374
	Sodium Hydroxide	2,723
	Potassium Hydroxide	1,726
	Silicon	1,262
	Aluminum	580.9
	Pt/Al_2O_3 catalyst	285.6
	Polystyrene-Divinylbenzene	111.3
	Rubber heat resistance water resistance	110.9
	Activated carbon	91.82
	Hydrochloric Acid	45.30
	Aluminum Oxide	43.31

	Glass Fiber-Reinforced Plastic	14.02
	High-Density Polyethylene	7.958
	Poly Ether Ether Ketone	6.515
	Cu-Cr alloy	5.145
	Porcelain	5.018
	Mo-Mn-Ni Plated Alumina	2.714
	Nickel	0.786
	Polyurethane Flexible Foam	0.646
	Polytetrafluoroethylene (PTFE)	0.563
	Styrene-butadiene Rubber	0.347
	Bronze	0.069
	Elastomer	0.061
	Sand	0.024
	SiC/C	0.014
	Chlorosulfonated Polyethylene	0.007
	Silicon Carbide	0.001
	Tin	0.001
PEM/AEM BOP	Concrete	22,311
	Steel	4,654
	Reinforced concrete	3,808
	Copper Wire	2,351
	Ni-Cr-Fe Alloy	1,500
	Silicon	343.3
	Polystyrene-Divinylbenzene	255.8
	Activated carbon	167.9
	Aluminum	116.5
	Iron	112.2
	Polyvinyl Chloride	65.03
	Glass-Fiber-Reinforced Plastic	31.37
	Rubber heat resistance water resistance	19.61
	Sodium hydroxide	14.71

	Hydrochloric Acid	11.79
	Aluminum Oxide	7.959
	Poly Ether Ether Ketone	1.498
	Cu-Cr alloy	1.335
	Porcelain	1.300
	Polyurethane Flexible Foam	1.184
	Mo-Mn-Ni Plated Alumina	0.704
	Nickel	0.552
	High-Density Polyethylene	0.170
	Bronze	0.127
	Elastomer	0.113
	Styrene-butadiene Rubber	0.079
	SiC/C	0.025
	Sand	0.006
	Silicon Carbide	0.003
SOEC BOP	Concrete	1,159
	Steel	359.6
	Ni-Cr-Fe Alloy	167.3
	Copper Wire	125.4
	Polyvinyl Chloride	77.50
	Nickel	33.06
	Silicon	16.13
	Iron	19.74
	Rubber heat resistance water resistance	2.713
	Aluminum Oxide	2.494
	Manganese Greensand	1.851
	Polystyrene-Divinylbenzene	1.722
	Poly Ether Ether Ketone	1.164
	Sodium Thiosulfate	0.658
	Hydrochloric Acid	0.591
	Sodium Oxychloride	0.570
	Aluminum	0.563

	Aqueous organophosphates and surfactants	0.479
	Reinforced Concrete	0.432
	Sand	0.327
	Glass Fiber-Reinforced Plastic	0.297
	Cu-Cr alloy	0.100
	Porcelain	0.098
	Mo-Mn-Ni Plated Alumina	0.053
	Mylar	0.029
	High-Density Polyethylene	0.021
	Low-Density Polyethylene	0.014
	Tricot	0.014
	Styrene-butadiene Rubber	0.012
	Polyurethane Flexible Foam	0.007
	Glass Fiber	0.005
	Polysulfone	0.005
	Aromatic polyamide	0.003
	Nylon 6	0.002
	Polytetrafluoroethylene (PTFE)	0.001
	Elastomer Bronze	Less than 0.001

Table S4 summarizes the standardized system capacities, defined according to GREET model specifications to ensure comparability across technologies: Alkaline (3,836 kW), PEM (998 kW), and SOEC (50 kW).[5] For AEM electrolysis, which is not represented in GREET, the system capacity was derived through a three-step procedure: 1) Calculations were based on a reference AEM system designed to produce 1,000 kgH_2/day as reported in the literature; 2) The established efficiency range (53.19–61.73%) and the theoretical energy requirement for H_2 production were applied to determine the corresponding power input; and 3) Operational parameters and component specifications were incorporated to yield an estimated AEM system capacity of 2,247−2,608 kW. Accordingly, all inventories (Tables S1−S4) are based on the same functional unit (1 kg H_2) but use technology-specific system capacities consistent with GREET defaults or literature sources.

Table S4. Component Utilization for Different Water Electrolysis Technologies. System capacities and operational parameters for green H_2 production via Alkaline (3,836 kW), PEM (998 kW), SOEC (50 kW), and AEM (2,247–2,608 kW) electrolysis, detailing stack and BOP utilization (item/kg H_2) and water input (kg/kg H_2). Data for Alkaline, PEM, and SOEC are sourced from the GREET model, with electricity input (kWh/kg H_2) determined from efficiency ranges in Table 1; AEM parameters are predicted using GREET methodology adapted to literature-derived efficiency ranges.

Electrolysis Type	System capacity (kW)	Stack utilization (item/kg H_2)	BOP utilization (item/kg H_2)	Water input (kg water/kg H_2)	Electricity input (kWh/kg H_2)
Alkaline	3,836	1.9937e-7– 2.7564e-7	9.9648e-8– 1.3782e-7	10.9777	45.8867– 63.4407
PEM	998	5.3965e-7– 1.2961e-6	1.8794e-7– 4.5362e-7	10.9777	44.6560– 64.6728
SOEC	50	3.6680e-5– 7.4622e-5	7.3360e-6– 1.4924e-5	7.9987	36.6801– 46.6387
AEM	2,247–2,608	7.3846e-7– 1.0667e-6	2.5847e-7– 3.7334e-7	10.9777	53.9428– 62.6058

The utilization factors (item/kgH_2) represent the fraction of a complete electrolyzer system required to produce 1 kg of H_2. These values were calculated according to Eq. S1, where the capacity factor was fixed at 0.9 for all technologies, consistent with GREET model assumptions for industrial-scale operation.

$$Utilization\ factor = \frac{1}{System\ capacity\ \times (Operational\ lifetime/Electricity\ input)\ \times\ C} \quad \text{Eq.S1}$$

Section S3. Scope 3 Categories: Upstream

Scope 3 emissions, as defined by the GHG Protocol, encompass 15 categories of indirect emissions occurring throughout a company's value chain.[7] Our analysis focused on upstream Scope 3 emissions directly relevant to H_2 production via water electrolysis, consistent with methodological frameworks established for energy technology assessment. We excluded organizational-specific categories to maintain focus on process-specific emissions. Capital goods (Category 2) were excluded to avoid double-counting, as our analysis accounts for manufacturing processes within Category 1 (Purchased goods and services), following approaches used in comparable H_2 production assessments. Similarly, we excluded upstream and downstream leased assets, franchises, and investments as they related to business structure rather than production technology. Downstream categories (Categories 9-15) were excluded because this study applies a cradle-to-gate system boundary, which considers emissions up to the point of H_2 generation rather than during its end use. While H_2 utilization does not generate CO_2 during combustion or electrochemical conversion, recent work has shown that H_2 leakage in the use-phase can contribute to indirect radiative forcing through atmospheric chemistry interactions. For example, Sand et al. (2023) report that H_2 has a non-zero Global Warming Potential when leakage is considered.[8] These indirect climate effects occur during the use-phase and therefore fall outside the system boundary adopted in this assessment. Consistent with this boundary definition, our analysis focuses on three upstream Scope 3 categories (Categories 1, 3, and 4) that contribute most significantly to the environmental impacts of water electrolysis H_2 production.

For each category, we developed technology-specific calculation methodologies based on material composition, manufacturing processes, and supply chain characteristics. We used SimaPro software with the Ecoinvent database to calculate emissions factors for material extraction, processing, and transportation activities. These emissions factors were then integrated with technology-specific inventory data to calculate the complete Scope 3 emissions profile for each water electrolysis technology.

For purchased goods and services (Category 1), we developed detailed life cycle inventories for each technology, accounting for material composition, manufacturing processes, and associated emissions, including the extraction and refining of raw materials, as well as the fabrication of stack and BOP components.

For Category 3 (Fuel and Energy related activities not included in Scope 1 & 2), We estimated GHG emissions related to electricity consumption during stack production by referencing data from the GREET model. However, due to limited information for the AEM electrolyzer, it was not possible to determine the amount of electricity used in manufacturing its stack. Therefore, leveraging the similarities between PEM and AEM electrolyzers, we estimated the electricity required for producing a 1 kW AEM stack based on the electricity consumption for producing a 1 kW PEM stack.

To comprehensively assess supply chain emissions from critical raw materials (CRM), we identified one representative CRM for each electrolysis technology based on material criticality, quantitative significance in the electrolyzer composition, and functional importance of electrolyzer. We selected nickel for alkaline and AEM electrolysis (representing >30% by weight of alkaline and AEM electrodes, catalysts, and structural components), platinum for PEM electrolysis (despite low weight percentage, accounting for up to 50% of stack manufacturing costs), and yttrium for SOEC electrolysis (essential for high-temperature operation, 700-850°C).[9-11]

For Category 4 (Upstream transportation and distribution), we developed transportation scenarios based on actual global supply chains for the selected CRMs, as illustrated in Figure S1. These scenarios were constructed using region-specific supply chain data for key CRMs, including nickel sourced from Indonesia, platinum from South Africa, and yttrium from China, reflecting the dominant global production regions for these materials.

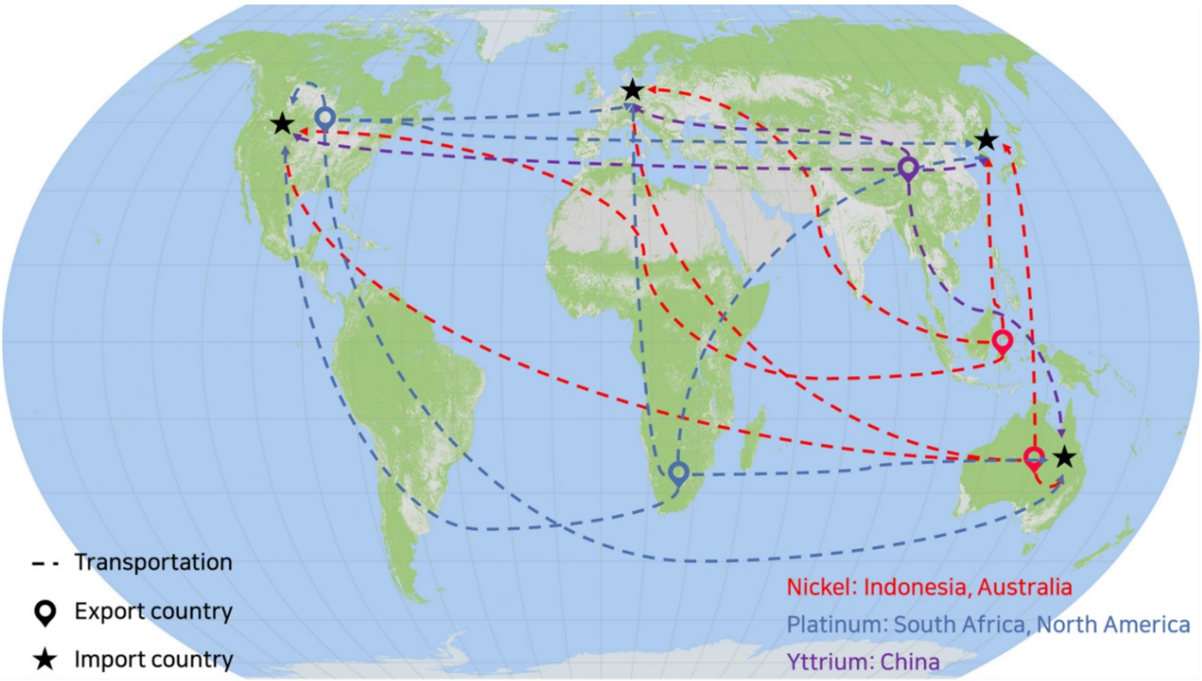

Figure S1. Visualization of international transportation routes for CRMs required in water electrolysis technologies. The map depicts shipping pathways for nickel (from Indonesia), platinum (from South Africa), and yttrium (from China) to four H_2-producing countries (South Korea, U.S.A, Australia, and Germany). Transportation distances range from 911.2 km (China-South Korea) to 22,920.3 km (South Africa-U.S.A), illustrating how geographic factors influence Category 4 emissions.

Transportation distances were calculated using a commercial maritime distance calculator that accounts for shipping lanes and canal passages.[12] We selected port pairs based on two criteria: (1) proximity to major CRM extraction/processing facilities and (2) container throughput volumes at destination ports. For extraction origins, we identified: Tanjung Priok (Indonesia) for nickel, reflecting Indonesia's position as the world's largest nickel producer (40.2% of global production), Durban (South Africa) for platinum, which handles exports from the Bushveld Complex that produces approximately 75% of global platinum, and Shanghai (China) for yttrium, as China produces over 95% of global rare earth elements, including yttrium.[13, 14]

For destination ports, we selected major industrial hubs with established or developing H_2 production capabilities: Busan (South Korea): Asia's second-largest container port and a hub for Korea's H_2 strategy, Los Angeles (U.S.A): Primary Pacific gateway for U.S. imports and key to California's H_2 infrastructure, Melbourne (Australia): Major industrial port in a country with significant renewable H_2 potential, and Hamburg (Germany): Europe's third-largest container port and central to Germany's H_2 import strategy.

Transportation-related Scope 3 emissions were modeled using a combination of actual shipping route data and Ecoinvent database market datasets. Because detailed CRM-specific shipping data were limited, conservative assumptions based on established maritime transport patterns were applied and validated against industry transport reports.

Ecoinvent datasets, which embed assumptions on loading weights and transport distances, were used to approximate marine shipping emissions for CRMs used in stacks and BOPs. The specific datasets employed for nickel, platinum, and yttrium are summarized in Table S5. These datasets provide embedded transportation assumptions, including average loading weights and transport distances, which were used to approximate the emissions associated with marine shipping.

Table S5. Ecoinvent datasets used within SimaPro to model maritime transport scenarios for CRMs.

Nickel	Nickel, class 1 [GLO] market for nickel, class 1 | Cut-off, U
Platinum	Platinum market [GLO] for platinum | Cut-off, U
Yttrium	Yttrium oxide market for [GLO] yttrium oxide | Cut-off, U

Major producing countries (Indonesia for nickel, South Africa for platinum, and China for yttrium) and representative destination ports (Busan–South Korea, Los Angeles–U.S.A, Melbourne–Australia, and Hamburg–Germany) were selected to reflect established or emerging H_2 production hubs.[15] Transportation scenarios were then constructed, yielding geographically explicit estimates of upstream emissions.

This approach provides a comprehensive assessment of Category 4 emissions, highlighting supply-chain hotspots and opportunities for environmental improvement that are often overlooked in conventional hydrogen production assessments.

Section S4. Software and Tools

- **Life cycle assessment**: SimaPro 9.6 with Ecoinvent 3.8 database

- **GREET model**: Version 2023 (Argonne National Laboratory)
- **Maritime distance calculations**: Sea-distances.org commercial calculator
- **Data processing**: Microsoft Excel with specialized LCA calculation templates

References

1. E. Schropp, F. Campos-Carriedo, D. Iribarren, G. Naumann, C. Bernäcker, M. Gaderer and J. Dufour, *Applied Energy*, 2024, **356**, 122247.
2. C. Simari, M. U. Rehman, A. Caprì, I. Gatto, V. Baglio and I. Nicotera, *Materials today sustainability*, 2023, **21**, 100297.
3. D. Koch, A. Friedl and B. Mihalyi, *Environment, Development and Sustainability*, 2023, **25**, 6269-6293.
4. E. M. Taibi, R.; Carmo, M.; Blanco, H., *Green Hydrogen Cost Reduction: Driving down the cost of electrolyzers*, International Renewable Energy Agency (IRENA), 2020.
5. R. K. Iyer, J. C. Kelly and A. Elgowainy, *Electrolyzers for Hydrogen Production: Solid Oxide, Alkaline, and Proton Exchange Membrane*, Argonne National Lab.(ANL), Argonne, IL (United States), 2022.
6. P. V. R.K. Iyer, J.C. Kelly, and A. Elgowainy, *Electrolyzer Manufacturing Updates in GREET 2023*, 2023.
7. G. P. Team, *Corporate Value Chain (Scope 3) Accounting and Reporting Standard*, 2011.
8. M. Sand, R. B. Skeie, M. Sandstad, S. Krishnan, G. Myhre, H. Bryant, R. Derwent, D. Hauglustaine, F. Paulot and M. Prather, *Communications Earth & Environment*, 2023, **4**, 203.
9. S. Grigoriev, V. Fateev, D. Bessarabov and P. Millet, *International Journal of Hydrogen Energy*, 2020, **45**, 26036-26058.
10. R. J. Ouimet, J. R. Glenn, D. De Porcellinis, A. R. Motz, M. Carmo and K. E. Ayers, *ACS catalysis*, 2022, **12**, 6159-6171.
11. J. Schefold, A. Brisse and M. Zahid, *Journal of The Electrochemical Society*, 2009, **156**, B897.
12. Sea-distances.org, https://sea-distances.org).
13. E. Warburton, *The Extractive Industries and Society*, 2024, **20**, 101564.
14. R. G. Cawthorn, *Platinum Metals Review*, 2010, **54**, 205-215.
15. U. N. C. o. T. a. Development, *Review of Maritime Transport 2024: Navigating Maritime Chokepoints*, 2024.