D14.2 Materials properties suitable for Unit 1 (Final)

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Version	Issue Date	Changes
[1.0]	29.10.2024	Original draft
[2.0]	30.04.2025	Inclusion of survey feedback and sensitivity analysis. Radar Diagrams and plots attached.
[2.1]	27.07.2025	Added disclaimer text at the end of the deliverable

Table of Contents

1 Summary and scope

Work Package 14 (WP14) comprises of three key undertakings where the first involves the application of a Multi-Criteria Decision Analysis (MCDA) to aid in the selection of materials and configurations of Unit 1. An overview of the REFINE process recognises two key units with the first containing the photovoltaic and electrolytic devices. These have emerged as critical technologies within the renewable energy industry and are combined in the purposes of REFINE to deliver the input stream of green hydrogen for Unit 2.

Material selection is necessary to support decisions made by the technical teams associated with Unit 1 by comparing design options using detailed guidelines. Technical performance considers static and dynamic properties as well as the composition and scale of throughputs which ensures that the selected options can withstand operating (mechanical, chemical, electrical etc.) and external stresses. Additionally, this process adds another level of robustness by assessing further design metrics which do not necessarily impact material function, but should still be considered: including cost-effectiveness, safety (to humans and wildlife) and overall lifecycle performance.

In conducting this analysis, the principal aim is to identify optimal recommendations in the design of Unit 1 components consistent with sound technical performance and commitments to sustainability. Sustainability is examined from three perspectives: environmental, economic and social which evaluate the reasons outlined above driving the material selection process. We apply further consideration to other sustainability models including the Circular Economy framework to apply the sustainability domains to various stages of the materials' life cycle.

The completion of this report highlights the collaborative efforts of multiple REFINE members associated with the Unit 1 devices as well as WP14 with the employment of a survey to reach the wider REFINE members.

1.1 Objectives

As highlighted, the MCDA aims to provide a recommendation for the assessed Unit 1 components by using the following objectives which are expanded from the material selection process.

1. **Identify MCDA Application Areas:** Determine components and design elements involved with the PV module and electrolyser where an MCDA is required i.e. decisions where there is more than one option being considered.

2. **Develop Relevant Criteria:** Establish a comprehensive set of criteria within the technical, environmental, economic and social domains that address key challenges and performance targets outlined by the technical teams.

3. **Conceive Evidence-Based Recommendations:** Provide valid recommendations supported by a multi-criteria decision analysis using peer-reviewed literature, public records and reliable industry sources.

2 Multi-Criteria Decision Analysis (MCDA): Application and Method

Multi-Criteria Decision Analysis (MCDA) describes a category of methods for complex decision-making processes to assess options from a large set of guidelines [1]. Although there are various MCDA approaches, the Analytic Hierarchy Process (AHP) was employed in the material selection to provide simple and logical arguments for arriving at the recommendations detailed in the results [2]. This methodology is further benefitted by its versatility, which easily accommodates multileveled weightings from the domains and sub criteria as well as the range of quantitative and qualitative factors simultaneously. The general structure of the AHP uses the following the stages:

1. Describe the issue and determine the aim
2. Structure the hierarchy by assessing three stages:
   - ***Domain:*** e.g. Technical, Environmental, Economic and Social
   - ***Criteria:*** e.g. Tafel Slope, Recyclability, Capital Cost and Human Toxicity etc.
   - ***Alternatives (Materials/Configuration):*** *e.g.* Ni Mesh, STF, IBC Cells etc.
3. Apply weightings to the Domains and Criteria with considerations to the aim
4. Define a ratio scale for each criterion (0-5 etc.) and apply the scores
5. Calculate the overall scores using the weightings and identify the top scoring options

The overview of the stages display the ease of applying this method to our material selection process. Its versatility with criteria type, multileveled decision making (i.e. recommend options via overall, domain or criteria score) and application of a ratio scale for scoring makes this analysis easy to conduct and track results from.

2.1 Scope

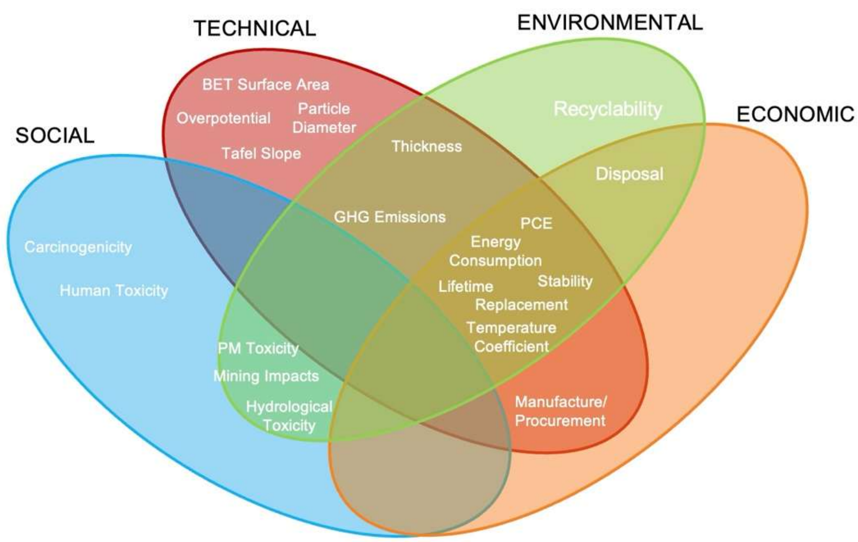


Figure 1: Overlapping MCDA Domains for Defining Sub-criteria

A critical component of the material selection process is with identifying the specific application requirements and performance needs of the design elements. These requirements shape the scope by mutually identifying what factors necessitate consideration (i.e. our domains: technical, environmental, economic and social) and therefore the criteria derived from these characteristics. Figure 1 illustrates the overlap between these influences and demonstrates how an individual criterion can constitute a combination of these and how criteria selection must have clarity within their definitions to ensure uniqueness.

Another area where we must define our scope is with the identification of the Unit 1 components which require material selection. From consultations with the technical teams, these were found to be the anode and cathode catalysts and substrates and the cell configuration of the PV module. Although Unit 1 comprises of numerous components which are suitable for material selection analysis, these design elements were prioritised due to their significant impact to the overall performance and output of the system.

Lastly, the scope defines at which lifecycle stage each criterion has been applied. While this study evaluates materials for equipment design rather than a final manufactured product, factoring this with the analysis is appropriate since:

1. The selected materials will eventually require replacement and disposal so manufacture and End-of-Life (EoL) stages should be considered
2. Many of the materials assessed for application within the electrolyser components are not commercial and have been specifically synthesised by REFINE members which offers the opportunity to further assess manufacture procedures or compositions from the outset
3. Early intervention in the material development stage allows for the integration of circular economy principles, including selection of sustainable raw materials or implementation of lower energy consumption synthesis routes

The tables in the next section define each of the assessment criteria and describe the lifecycle stage this was applied to. We see that there is a trend in applying the criteria to predominantly the raw material extraction and manufacturing phases which highlights the value of this consideration due to the additional support we can provide to the technical teams involved in the synthesis of these materials.

2.2 Domains and Criteria Selection

To create a more rigorous methodology and comply with the research purposes outlined in the objectives, consideration should be applied to non-technical standards as well. These are identified within a sustainability framework which refers to the environmental, economic and social aspects which scrutinise options outside of performance expectations. Within these domains, supplemental criteria have been derived to represent a mix of the key issues and concerns within that individual group. Below denotes the criteria we considered under this framework along with their definitions and explained applications within the MCDA for the PV cell and electrolyser. Technical criteria will be explored further ahead as these have been independently selected for each subunit and components.

Environmental

This domain addresses some of the key issues that are most commonly reported to impact the environment, including: resource depletion, pollution, greenhouse gas emissions, circular economy, impact to the ecosystem and waste generation. Although, there are other issues that require assessment, such as water consumption or biodiversity impact, reporting on these for our observed materials are fairly limited and difficult to derive reliable comparative scorings for so these have not been considered under this assessment. However, since a life-cycle assessment will be conducted as one of the tasks for WP14, these issues will be addressed then.

Table 1: Environmental Criteria Definitions and Scoring Metrics

Criterion	Definition	Life Cycle Scope	Unit	Scoring Method
Lifetime	The operational life of the material or configuration before reported degradation/reduction to efficiency where the impact of continued use produces an unsafe environment or impact to production is significant enough to require replacement.	Use	Years	0 – Option has a very short lifetime and requires replacement frequently within 10-year period i.e. 3 or more times. 1 – Option demonstrates moderate-low durability lasting between 4-7 years and requiring replacement at most twice within 10-year period. 2 – Option demonstrates moderate durability lasting 8-11 years (over 10 year period assessed for replacement requirement) 3 – Unreported information.

				4 – Option demonstrates moderate-high durability lasting 12-15 years (over 10 year period assessed for replacement requirement) 5 – Option demonstrates high durability lasting over 15 years without replacement requirement due to no detectable degradation to performance.
GHG Emissions	The GHG emissions associated with the manufacture of the materials or configurations. This considers the CO_2 equivalence of all greenhouse gases involved via its global warming potential (GWP).	Raw material extraction and Manufacturing for electrolyser Manufacturing for PV cell	kg CO2e	0 – Process for manufacture of option uses highest temperatures than other options and requires multiple processing steps i.e. >10 steps. 1 – Process for manufacture of option now uses high temperatures and requires a few more processing steps i.e. <10 steps. 2 – Process for manufacture of option now uses moderate temperatures but requires a few more processing steps i.e. <10 steps.

				3 – Unreported information. 4 – Process for manufacture of option still uses lower temperatures than other options but requires a few more processing steps i.e. <10 steps. 5 – Process for manufacture of option uses significantly lower temperatures than other options or much shorter processing steps i.e. <5 steps.
Air Pollution	Whether the materials involved in the composition or configuration are listed as monitored air pollutants in the UK and are considered toxic or adverse to human health.	Raw material extraction, manufacture and disposal/recycling	Fraction or count of identified pollutants in composition	0 – Contains at least 1 material that is reported to be over the EU limits or 4+ materials currently being monitored but under the EU limits. 1 – Contains 3 materials currently being monitored and are all reported in the UK as under the EU limits. 2 – Contains 2 materials currently being monitored and are all reported in the UK as under the EU limits. 3 – Unreported information.

				4 – Contains 1 material currently being monitored and is reported in the UK as under the EU limits. 5 – Materials in configuration are not monitored as they do not present as current concern.
Water Pollution	Whether the materials involved in the composition or configuration are listed as monitored heavy metals or metalloids contaminating soils in UK.	Raw material extraction, manufacture and disposal/recycling	Fraction or count of identified pollutants in composition.	0 – Contains at least 1 material that is reported to be over the EU limits or 3+ materials currently being monitored but under the EU limits. 1 – Contains 3 materials currently being monitored and are all reported in the UK as under the EU limits. 2 – Contains 2 materials currently being monitored and are all reported in the UK as under the EU limits. 3 – Unreported information. 4 – Contains 1 material currently being monitored and is reported in the UK as under the EU limits.

				5 – Materials in configuration are not monitored as they do not present as current concern.
Recyclability	This criterion considers the material the electrolyser components, but overall configurations for the PV cell. This explores whether material/s can be recycled for initial purpose, alternative purpose or must be disposed of altogether.	Disposal/recycling	Number of Cycles, Examples of final recycled product.	0 – Option is single use and must be disposed after / cannot be recycled or repurposed. 1 – Option contains mostly materials which can be repurposed for a lower value use. 2 – Option contains a proportional or slightly greater composition of non-100% recyclable materials. 3 – Unreported information. 4 – Option is 100% recyclable or contains mostly 100% recyclable materials but is less easy/widely recycled. 5 – Option is 100% recyclable and reported to be easily or widely recycled.

Economic

Some of the concerns highlighted below touch on the issues addressed in the environmental domain which include stability (i.e. lifetime) and raw resources. We consider cost at four tiers of the life cycle: extraction, manufacture, use and disposal. Although, this covers the full life cycle; this does not consider alternative economic factors which may relate to some of the current options; these include transportation/logistical or other maintenance associated costs. Due to the novelty of some materials and difficulty in finding clear costs in other options, only a few economic issues have been considered at this time, but this will be further developed during the techno-economic analysis (TEA).

Table 2: Economic Criteria Definitions and Scoring Metrics

Criterion	Definition	Scope	Unit	Scoring Method
Cost/ Module Construction	Relating to the electrolyser, this considers the cost of the metal precursors needed to manufacture 1 kg of product via sol-gel method i.e. no consideration of synthesis method. Concerning the PV cell, this considers the cost of manufacturing a module as a function of the output power produced.	Raw material extraction for electrolyser Raw material extraction and manufacture for PV cell	EUR/kg USD/W	0 – Option uses all high-cost resources and a complex and high-energy extensive processing procedure leading to overall cost greater than EUR10^5. 1 – Option uses mostly high-cost resources and a complex or high-energy extensive processing procedure leading to overall cost within EUR10^5. 2 – Option uses a mix of low-cost and high-cost resources paired with a moderately complex or mid-energy extensive processing procedure leading to overall cost within EUR10^4.

				3 – Unreported information. 4 – Option uses mostly low-cost resources or a somewhat simple or low-energy extensive processing procedure leading to overall cost (e.g. within EUR10^3) 5 – Option uses abundant and very low-cost resources or a simple and low-energy extensive processing procedure leading to overall cost (e.g. within EUR10^2)
Replacements	The cost of maintaining the material or configuration within a 10 year period considering only replacements instead of the potential for repairs. This criterion ties in with the lifetime found for each option and is associated alongside the costs found for the criterion above	Up to use	EUR/10-Years USD/10-Years	0 – Option is a mix of very low cost and lifetime. 1 – Option is a mix of low cost and lifetime. 2 – Option is a mix of moderate cost and moderate lifetime. 3 – Unreported information. 4 – Option is low cost, and high lifetime i.e. may score 4 or 5s for each category.

				5 – Option is very low cost, and very high lifetime i.e. scores top in each category.
Disposal/Recycling Treatment	The cost of the disposal or recycling process associated with the material. The ratio of non-hazardous to hazardous contaminants is observed and higher costs are associated with options containing more hazardous elements.	Disposal and recycling	Fraction or count of hazardous material.	0 – Option contains mostly or all hazardous waste and is difficult to recycle or dispose/requires specialised treatment centres. 1 – Option contains mostly hazardous waste and is difficult to recycle or dispose. 2 – Option contains proportional amounts of hazardous and non-hazardous waste and is moderately difficult to recycle or dispose. 3 – Unreported information. 4 – Option contains mostly non-hazardous waste and is recycled or disposed of widely. 5 – Option does not contain any hazardous waste and is recycled or disposed of widely.

Social

Considering the social implications of the recommendations from the study are critical in understanding the impact to people and communities. Likewise, with economic factors, social criteria are also interlinked with some key environmental issues particularly with harm to wildlife either due to direct hazards with the material or of land-use. This domain expands on key social issues expanding across the materials' life cycle which include ethics, human rights and community welfare.

Table 3: Social Criteria Definition and Scoring Metrics

Criterion	Definition	Scope	Unit	Scoring Method
Human Toxicity	Explores the potential of a metal, chemical or substance to cause harm to human health through any exposure route leading to mild or severe effects occurring immediately or over a longer period.	Manufacture	Fraction or count of toxic contaminants	0 – Contains or involves 4+ materials/metals which are known to be harmful. 1 – Contains or involves 3 materials/metals which are known to be harmful. 2 – Contains or involves 2 materials/metals which are known to be harmful. 3 – Unreported information. 4 –Contains or involves 1 material/metal which is known to be harmful. 5 – Does not contain or involve any materials/metals which are known to be harmful.

Carcinogenicity	Considers the ability of any involved materials to cause cancer in humans from a range of exposure times. Distinguishes scores based on known, probable and possible carcinogens from each step of the life cycle which involves exposure to the material.	Manufacture	Fraction or count and degree of carcinogenicity	0 – Contains or involves at least 1 known carcinogen and >2 probable/possible carcinogens 1 – Contains or involves at least 1 known carcinogen. 2 – Contains or involves up to materials/metals which are probable carcinogens. 3 – Unreported information. 4 –Contains or involves material/metal which are possibly carcinogenic. 5 – Does not contain or involve any materials/metals which are known to be carcinogenic.
Mining Implication	This explores ethical issues associated with the extraction of the raw materials used to construct each of the considered alternatives. The issues explored include Economy, Income and Security; Employment and Education; Demography; Land Use and Territorial Aspects; and Human Rights. Consideration to these sub-parameters were used since these were identified in	Raw material extraction	See table below	0 – Contains 6+ materials/metals which are involved in any of the mining issues in Table 4. 1 – Contains 5-6 materials/metals which are involved in any of the mining issues in Table 4.

	the report as these are recognised as the key ethical offences in industrial materials [3]. The method of scoring involves breaking down the raw materials involved in the composition or configuration of each option and matching this to the list of materials reported in the study. These materials were assessed to find which of the ethical offences they violate. An example is seen in Table 4. Scores have been applied from the value of the fraction or summed offences.		2 – Contains 3-4 materials/metals which are involved in any of the mining issues in Table 4. 3 – Unreported information. 4 – Contains 1-2 materials/metals which are involved in any of the mining issues in Table 4. 5 – Does not contain any materials/metals which are involved in any of the mining issues in Table 4.

Table 4: Example Tally for Mining Impact Assessment

Option	Economy, Income and Security	Employment and Education	Demography	Land Use and Territorial Aspects	Human Rights	Fraction / Sum
1	2	3	1	1	2	9/n
2	1	2	1	2	4	10/n
n	x	y	z	1	2	x+y+z/n

Technical: Electrolyser

The scores for the technical criteria are less specific to those described for the previous domains. These are more standard and general where 0 – Very Poor, 1 – Poor, 2 – Moderate, 3 – Unreported Information, 4 – Good and 5 – Very Good.

Table 5: Electrolyser Catalyst Technical Criteria

Criterion	Definition	Unit	Relevance
Overpotential	Overpotential is the difference in the theoretical vs applied potential (voltage) required to drive a half-cell reaction at an electrode to achieve a certain rate.	m^2/g	• Low overpotential indicates high electrochemical efficiency as less excess energy is required alongside the theoretical potential • This also indicates faster reaction kinetics where higher reaction rates can be achieved
Mass Activity	Mass activity refers to the current generated from a certain mass of catalyst.	A/g	• Higher mass activity indicates a better catalyst due to its ability to achieve higher current density despite loading amount
ECSA	ECSA refers to the electrochemically active surface area of an electrocatalyst to determine its contact and interaction with the electrolyte. Here we use Cdl (double layer capacitance) as a proxy measurement for ECSA	Cm^2 Cdl = mF	• High ECSA is associated with a high Cdl, this indicates a larger surface area catalyst enabling this to have more contact with the electrolyte
Tafel Slope	The Tafel slope indicates how the overpotential changes with significance to the current density.	mV/dec	• Low Tafel slopes indicate fast reaction kinetics and higher rates of electron transfer • This indicates good catalytic performance since faster rate of reaction are achieved

Electrical Conductivity	Electrical conductivity measures the ability of the material to conduct electric current.	S/cm	• High electrical conductivity indicates good electron transfer which is required to drive electrochemical reactions • This also indicates lower power losses from reduced electrical resistance

Technical: PV Cell

The scores for the PV module match those used for the electrolyser elements where 0 – Very Poor, 1 – Poor, 2 – Moderate, 3 – Unreported Information, 4 – Good and 5 – Very Good.

Table 6: PV Module Technical Criteria

Criterion	Definition	Unit	Relevance
Power Conversion Efficiency (PCE)	PCE is the percentage of light energy that can be converted into electrical energy by a PV cell.	%	• A high PCE indicates increased efficiency and productivity of the output power produced • Less energy is wasted via heat or other forms as a higher proportion of the input energy is converted to the desired output
Stability	Stability refers to the ability of the PV cell to maintain its performance over time under various operating conditions.	Hours/ Qualitative	• Long-term stability indicates better performance over time where a high PCE can be maintained • This indicates reliable power output and is more economically beneficial as less replacements are required
Energy Consumption	This normalises the energy consumed during the manufacturing stage of a PV cell to create one unit of power.	kWh/kW	• Lower energy consumption is desired as it can lead to a higher net energy output (when

			considering energy consumption from manufacture) • This also leads to a smaller environmental impact as less resources are required
Temperature Coefficient	In our application, the temperature coefficient quantifies the impact of the temperature to the PCE.	%/ºC	• A lower temperature coefficient indicates better performance stability across a higher range of environmental conditions • Energy production is more consistent and reliable

2.3 Domain and Criteria Weightings

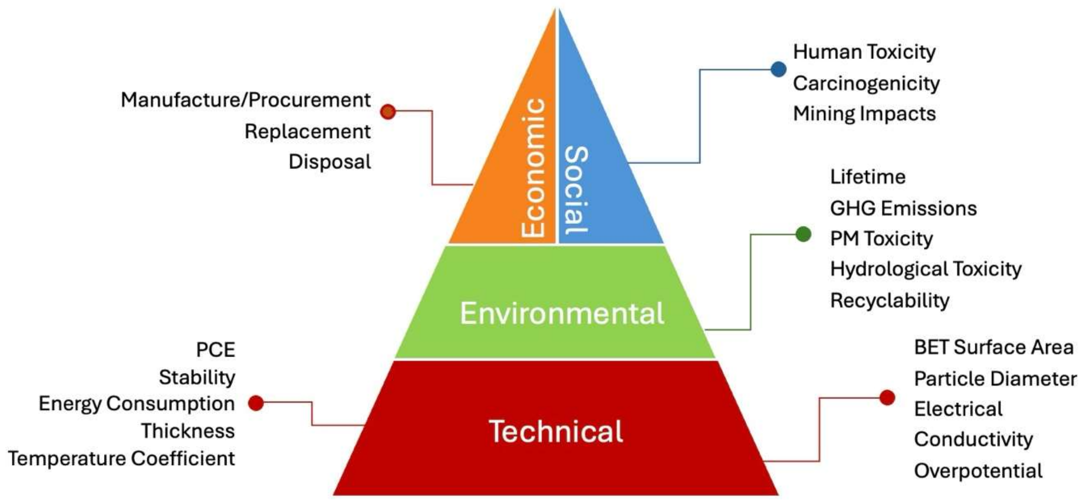


Figure 2: Hierarchy of Domains Associated with their Weightings

Table 7: Justifications of Domain Weightings

Domain	Weighting (%)	Explanation
Technical	35 for Electrode 30 for PV Cells	The primary function of the materials and configurations is to perform effectively in its intended role. The technical parameters reflect this the most and is therefore weighted the highest. Additionally, the criteria representing this domain, has been devised with other REFINE members outside of WP14 so this validates their importance to the overall objectives.
Environmental	25 for Electrode 30 for PV Cells	Environmental concerns have a growing importance in the larger context outside of REFINE but is also one of the key driving forces for the emergence of WP14. This domain is ranked the second highest since it encompasses some key objectives between REFINE and WP14 which are heavily focused on green and environmentally driven purposes, goals and choices. This is ranked higher than the last two only marginally since it has more direct relevance to WP14.
Economic	20 for Electrode 25 for PV Cells	Economic and Social criteria have been weighted the lowest and equal to each other at 20%. Although these are important factors that deserve consideration, they are secondary to the purposes of REFINE and WP14 in that their impacts are less

Social	20 for Electrode 15 for PV Cells	direct to the performance of Unit 1. Additionally, much of the scorings applied with these criteria are more qualitative in nature and cannot be accurately measured without more comprehensive analysis methods i.e. expert surveys, TEA etc.

2.4 Inter-domain Weightings

The tables show individual criterion weightings used for each domain. These have been developed from feedback from REFINE members.

Overpotential	Mass Activity	ECSA	Tafel Slope	Electrical Conductivity
mV	A/g	Cdl = mF	mV/dec	S/cm
40%	20%	15%	15%	10%

Corrosion Resistance	Compressive Strength	Electrical Conductivity	Hardness	Yield Strength
Rating	MPa	S/cm	MPa	MPa
30%	30%	20%	10%	10%

Power Conversion Efficiency	Stability	Energy Consumption	Temperature Coefficient
%	Description	kWh/MW	%/^{O}C
50%	25%	15%	10%

Lifetime	GHG Emissions	Recyclability	Air Pollution	Water Pollution
Years	kgCO2eq	Cycles	Fraction/Count	Fraction/Count
30%	25%	25%	10%	10%

Cost/Module Construction	Replacement	Disposal
EUR/kg or USD/W	EUR/kg or USD/W	Fraction/Count
50%	30%	20%

Toxicity	Carcinogenicity	Mining Impacts
Fraction/Count	Fraction/Count	Fraction/Count
30%	20%	50%

2.5 Assumptions and Limitations

Table 8: Methodology Assumptions, Limitations and Improvements

Assumption	Limitations	Advised Improvements
A limited number (3-5) criterions chosen for each domain.	1. Disregard of more relevant or necessary criteria leading to misrepresentation or incomplete picture of the full domain.	Addition of more criteria to each of the domains. Consult technical teams to include updated parameters required to be studied.
	2. Oversimplification may have led to missing more complex or new/emerging sustainability concerns.	Review the criteria periodically before the final draft and include any new considerations from similar literature.
	3. Inviting personal or disciplinary biases with considering concerns most relevant to their work package objectives/interests.	Establish a diverse review panel to validate the work before the final submission. Create questionnaires/surveys to add/update criteria as advised by technical teams.
	4. Insufficient granularity between criteria which overlap in covering similar issues.	Reassess definitions to ensure detailed distinction between similar criteria. If any overlapping criteria is found, resolve this by eliminating one or applying distinct definitions to each.
	5. Reduced sensitivity to significant differences between material or configuration options due to missed considerations.	Develop detailed scoring metrics with current criteria and if scores or applied definition drift from what is presented in the methodology, consider this as a new

		parameter.
Scores are explained for each criterion however 3 is defined for all as ‘Unreported’ regardless of whether all values for the options within the criteria are reported and known.	1. Falsely devalues some options where these have very minute differences to others	Consult with other members to uncover if this will have a significant impact to the final scores if maintained. Ensure that all criteria have detailed guidelines for the scores and any instances where this differs has been described and justified i.e. assumptions and limitations.
	2. Falsely inflates the overall scores of some materials more than others due to unreported information.	Compare with other missing data protocols used in other material selection analyses and validate applicability to this study.

Table 9: Domain Assumptions, Justifications and Limitations

Domain	Assumption	Justifications and Limitations
Environmental	Lifetime criteria scored for anodic catalyst options were estimated from the assessment of the stability of the A-site elements.	Lifetime is a difficult criterion to analyse as most testing is done under lab conditions so applicability to a larger scale is difficult to justify. A-site elements maintain the structure of a perovskite and act as a support for the B-site cations to migrate, so the assumed stability of the structure is derived mainly from the durability of the A-site. This does not consider the interactions between all the elements within the composition since the majority of the perovskites we analyse are complex which can lead to less stable structures and lower lifetime.
	Lifetime scoring method is based on arbitrarily selected 10 year assessment period.	It was simpler to consider replacements or degradation of performance within decades instead of other time periods. For the PV cell configurations, this did not distinguish between the options as most were found to have a lifetime longer than 20+ years.
	GHG emissions scored for anodic catalysts are assumed from synthesis route however all compositions can be made from the lowest GHG emission synthesis route.	Due to the novelty of the catalysts, this information is not reported on, so some basis had to be found. Since these materials are made by the WP2 teams, synthesis routes were known and could be used for distinguishing the scores. This negatively impacts compositions which were made from higher GHG emission synthesis routes as this is more dependent on the choice of synthesis made by the lab user and does not inherently reflect the composition.
	Air pollution and water pollution measurements have been extrapolated	This assumption was made to make a more comprehensive scoring process

	from UK reports despite locations of REFINE plants are not defined yet.	for these two criterions, so this location was selected as the reports were easily accessible to the researcher. This does not accurately reflect the situation in other potential REFINE sites so this can be omitted from consideration when scoring within the final draft.
	Recyclability scores for PV cells were assumed more from qualitative reports. This also does not follow the definition of recyclability attached to the methodology since these are full configurations instead of individual materials.	To find the number of cycles of recyclability in each of the materials involved in each PV cells configuration would be time consuming and difficult. Additionally, applying this logic to the scoring assumes the recyclability of the separated pure material. The scoring for each option may be more open to dispute as there could be author biases from the literature used to describe the recyclability of the configurations.
	Some scores for the anodic substrate do not follow the criteria definitions listed in the methodology and instead more of a comparative analysis was employed. i.e. Lifetime scored Ti mesh higher due to this material generally being stronger than Ni.	Since there are less alternatives considered for this electrolyser component, these assumptions were made to ensure more distinguishability between the two options. This complicates the justification of the scores as readers are unable to attribute these to the described meanings and must rely on the discretion of the author.
Economic	Capital costs calculated from electrolyser components do not consider operational or logistical costs i.e. labour, heat, transport etc.	At this stage of WP14, these considerations are difficult to estimate so have been omitted to avoid incorrect calculation. This simplifies the definition and does not capture the full significance of this criterion. However, over the course of the REFINE timeline, the costs of these materials can potentially be more accurately estimated from TEA.
	Maintenance costs have not been considered apart from cost of replacements.	Maintenance information was not found to be widely reported so this was

	omitted to avoid inaccurate estimations. Scores can potentially be higher than estimated as some options may only require cheaper maintenance treatments rather than complete replacement.
Replacement cost scores use an arbitrarily selected 10 year time period.	As with the Lifetime criterion, this time period was used to simplify calculation as the scores for this were derived from this criterion. This may visualise an incomplete lifecycle for some of the options which have a lifetime longer than 10 years. Additionally, this misleads comparisons as this does not distinguish between material options which require replacement more than this time period e.g. a material which requires replacement every 11 years is scored equal to that of a material which can last 20+ years.
Replacement costs use an average score extrapolated from the scores given for capital cost and lifetime.	This was performed to simplify the scores made for this criterion as information on future changes to costs would be difficult to consider at this stage of WP14. This assumption disregards cost changes attributed to the advancement of these technologies i.e. options may require less frequent replacement or may be more affordable due to market demands.
Disposal/treatment costs are assumed from the waste hazard classification reported by the UK government.	These reports were most accessible to the author, and it is assumed that this will have close likeness to waste classifications from EU countries. Significant differences to other nations' waste hazard classifications can lead to alternative scores however once REFINE locations have been decided, these scores can be adjusted.

	Disposal/treatment costs are scored qualitatively i.e. based on hazardous content requiring more specialised treatment hence elevated costs.	Specific costs associated with the disposal or treatment of the options were difficult to find so an estimate was used from this definition. Non-hazardous materials can still accrue high disposal/treatment costs, and this assumption generalises potential fees from complex handling procedures. Alternatively, hazardous materials do not necessarily result in high costs as facilities may already be in place to manage these.
Social	Human toxicity scores for the electrolyser also do not consider other substances, solvents or chemicals which can also pose harm to human health.	The assumption to attribute toxicity concerns to only the metals present in the composition is to simplify the analysis as well as to ensure level comparison between all compositions i.e. avoids non-material based toxicity from different synthesis routes/manufacturing processes. This is not a full representation of the hazards associated with the materials lifecycle and those with more dangerous manufacturing procedures are generalised with materials which use a safer process.
	Carcinogenicity for the electrolyser assumes only harm from the metals in the final composition instead of other materials used during synthesis/manufacture.	Again, this assumption is used to simplify the analysis as listing all of the substances and chemicals used for each material and finding carcinogenic information is tedious and can be inaccurate since it may not be representative of actual lab work. Likewise, this misrepresents potential carcinogens involved in the synthesis/manufacture of these materials.
	Mining implications only consider a limited group of ethical aspects.	The report used to formulate the scores for this criterion only describes these ethical violations, so this was maintained to simplify the analysis.

		Again, this may misrepresent some materials/configurations where other violations may apply.

3 MCDA Electrolyser: Considerations

Applying the MCDA methodology to material considerations with the electrolyser revolved around the electrode components to support the work being conducted by WP2 and WP5 members. The options were provided by these teams and these represented materials for the catalyst and substrates for the anode and cathode.

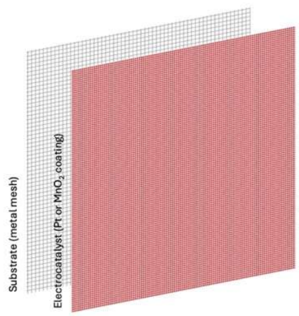


Figure 3: Diagram of Cathode Layers

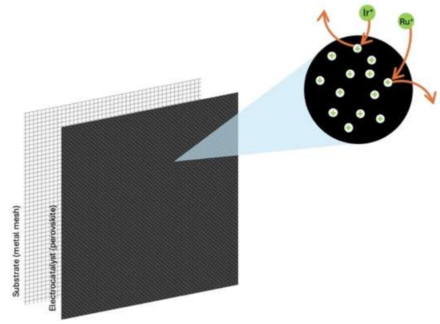


Figure 4: Diagram of Anode Layers with Schematic of Galvanic Replacement

The decision for the materials used in the design of these components is paramount for ensuring fast kinetics and improved efficiency with the entire electrolytic system. From Figures 3 and 4, it can be observed that the substrate serves as a carrier for the catalyst to provide structural support as well as facilitate with electron transfer. The catalyst, however, provides the active sites to accelerate the electrochemical reactions which occur at the electrode surface. Therefore, it is justified that the application of MCDA is required here to consider non-technical parameters which can provide alternative recommendations to work package teams assessing these materials experimentally.

For the anode, the substrate and catalyst are considered separately due to the novelty with some of the materials considered for the latter. Substrate options have been advised as **Titanium mesh and Nickel mesh** which are more common materials for this purpose. In the analysis of catalysts, these proved to be more diverse, but options remained with perovskite oxide structures with the general formula of ABO_3 due to their inherent electric and catalytic activities as well as established ability to combat high overpotentials caused by the Oxygen Evolution Reaction (OER). We analyse ten perovskite structures including:

- **STF** (Sr, Ti, Fe)
- **STFC** (Sr, Ti, Fe, Cu)
- **STFN** (Sr, Ti, Fe, Ni)
- **LSTN** (La, Sr, Ti, Ni)
- **BSCF** (Ba, Sr, Co, Fe)
- **BSCFN** (Ba, Sr, Co, Fe, Ni)
- **BGLC** (Ba, Gd, La, Co)
- **BGLCF** (Ba, Gd, La, Co, Fe)
- **BGLCN** (Ba, Gd, La, Co, Ni)
- **BGLCFN** (Ba, Gd, La, Co, Fe, Ni)

Concerning the cathode, there are fewer options being considered with most of these commonly observed in literature and practice. The novelty with these materials lie within their construction but due to more commonly examined materials options of the full electrode system can be analysed together. The substrate options are the same with what is considered with the anode. However, the catalysts options are split between Pt and MnO_2 where the electrode compositions being analysed are listed as:

- Pt/Ni Mesh
- MnO_2/Ni Mesh

3.1 Literature and Data

3.1.1 Technical

Material	Electrolyte	Overpotential	Mass Activity	ECSA	Tafel Slope	Electrical Conductivity	Reference
		mV (@ 10 mA/cm^2)	A/g (@ 450 mV)	Via Cdl (mF)	mV/dec	S/cm	
STF	0.1M KOH	490	10	0.272	58	0.08 [4]	Wang et al. [5]
STFC	X	X	X	X	X	X	X
STFN	0.1M KOH	412	40	X	103	23.9 [6]	Xu et al. [7]
LSTN	1M KOH	474	4	X	140	X	Khan et al. [8]
BSCF	1M KOH	394	28	X	74	28 [9]	Gol et al. [10]
BSCFN	1M KOH	300	25	X	51	43 [11]	Dong et al. [12]
BGLC	1M KOH	500	14	59	85	X	Petlund et al. [13]
BGLCF	1M KOH	420	68	51	68	X	
BGLCN	1M KOH	511	13	49	80	X	
BGLCFN	1M KOH	495	18	32	77	X	
Pt/Ni	1M KOH	75	200	X	120	9.4*10^4	Fiameni et al. [14]
MnO_2/ Ni	1M KOH	230	X	X	38	10^{-5}	Saha et al. [15]

Material	Corrosion Resistance	Compressive Strength	Electrical Conductivity	Hardness	Yield Strength	Reference
	a.u.	MPa	S/cm	MPa	MPa	
Ti	4	130-170	0.0180	1150-1250	275	AZO Materials, Apex Engineered Products [16]
Ni	5	70-935	0.1044	800-3000	110	AZO Materials, Apex Engineered Products [16]

3.1.2 Environmental

Material	Lifetime	GHG Emissions [17]	Recyclability	Air Pollution [18]	Water Pollution [19]
	Years	Via GWP (kg/CO2-eqkg)	Cycles	Fraction/Count	Fraction/Count
STF	X	6.52	X	0	Fe 0.33
STFC	X	6.65	X	Cu 0.25	Fe, Cu 0.50
STFN	X	7.02	X	Ni 0.25	Fe, Ni 0.50
LSTN	X	13.7	X	Ni 0.25	Ni 0.25
BSCF	X	8.64	X	0	Co, Fe 0.50
BSCFN	X	8.46	X	Ni 0.20	Co, Fe, Ni 0.60
BGLC	X	61.68	X	0	Co 0.25
BGLCF	X	54.88	X	0	Co, Fe 0.40
BGLCN	X	59.88	X	Ni 0.20	Co, Ni 0.40
BGLCFN	X	56.88	X	Ni 0.17	Co, Fe, Ni 0.50
Pt/Ni	X	$1.25*10^4$	Electrode [20]	0	0
MnO_2/ Ni	X	1	Battery [21]	1	1

Material	Lifetime	GHG Emissions [17]	Recyclability [22]	Air Pollution [18]	Water Pollution [19]
	Years	Via GWP kg/CO2-eqkg	Via OSR (Old Scrap Ratio) %	Fraction/Count	Fraction/Count
Ti	>10	8.1	10-25	0	0
Ni	50+	6.5	> 50	1	1

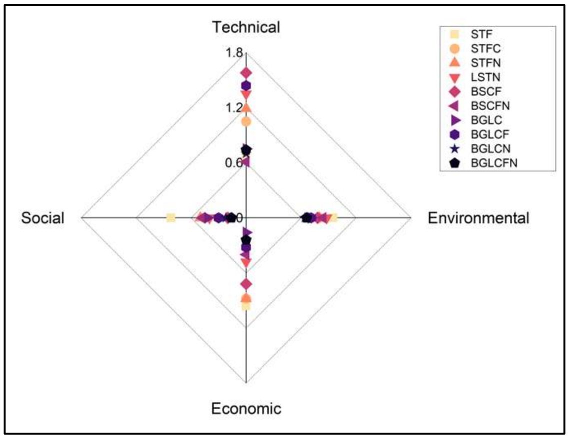
3.1.3 Economic and Social

Material	Cost	Disposal [23]	Toxicity [24]	Carcinogenicity [25]	Mining Impacts [26]
	Euro/kg	Via Hazardous Compounds Fraction/Count	Fraction/Count	Group/ Compound	Via Sanctions Fraction/Count
STF	547	Ti, Fe 0.67	Fe 0.33	0	0
STFC	541	Ti, Fe, Cu 1	Fe, Cu 0.50	0	Cu 3.50
STFN	532	Ti, Fe, Ni 1	Fe, Ni 0.50	Ni compound 1, Ni metallic 2B	Ni 1.00
LSTN	1134	Ti, Ni 0.75	Ni 0.25	Ni compound 1, Ni metallic 2B	La, Ni 2.75
BSCF	915	Co, Fe 0.50	Co, Fe 0.50	Soluble Co Salts 2A, Co Oxide 2B	Co 2.50
BSCFN	842	Co, Fe, Ni 0.80	Co, Fe, Ni 0.60	Soluble Co Salts 2A, Co Oxide 2B, Ni compound 1, Ni metallic 2B	Co, Ni 2.80
BGLC	2298	Co 0.25	Co 0.25	Soluble Co Salts 2A, Co Oxide 2B	Gd, La, Co 6.00
BGLCF	2047	Co, Fe 0.40	Co, Fe 0.40	Soluble Co Salts 2A, Co Oxide 2B	Gd, La, Co 4.80
BGLCN	1996	Co, Ni 0.60	Co, Ni 0.40	Soluble Co Salts 2A, Co Oxide 2B, Ni compound 1, Ni metallic 2B	Gd, La, Co, Ni 5.60
BGLCFN	2021	Co, Fe, Ni 0.67	Co, Fe, Ni 0.50	Soluble Co Salts 2A, Co Oxide 2B, Ni compound 1, Ni metallic 2B	Gd, La, Co, Ni 4.67
Pt/Ni	57522	0	1	0	8
MnO_2/ Ni	110	1	1	0	4

Material	Cost	Disposal [23]	Toxicity [24]	Carcinogenicity [25]	Mining Impacts [26]
	Euro/kg	Via Hazardous Compounds Fraction/Count	Fraction/Count	Group/ Compound	Via Sanctions Fraction/Count
Ti	547	0.67	0	0	0
Ni	541	1	1	Ni compound 1, Ni metallic 2B	4

3.2 Results and Discussion

3.2.1 Anode



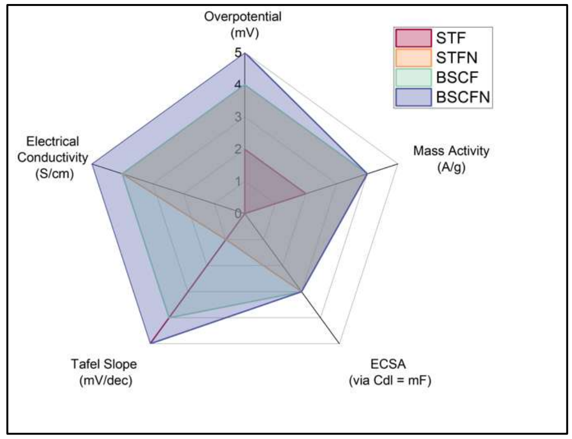


Figure 6: Domain Performance of Anode Catalyst **Figure 5:** Technical Scoring of Anode Catalyst

Figure 6 only looks at the top scoring half of the materials with STFC omitted due to unavailable technical data. STF performs best in all sustainable categories (environmental, economic and social), but is in the bottom half for technical KPIs. Despite this, section 3.3 shows that this remains as the overall recommendation. The STF subset of perovskites significantly outperform the other materials with regards to economic feasibility. However, in the other sustainable domains the performance of all materials show to be consistent with each other demonstrated by the minimal spread of scores. Ni-doped and pristine BSCF stand out as the best performing in terms of technical KPIs with top scores in three categories. The sensitivity analysis in S3.3 will identify BSCFN as a potential recommendation if the priority on technical performance is further weighted.

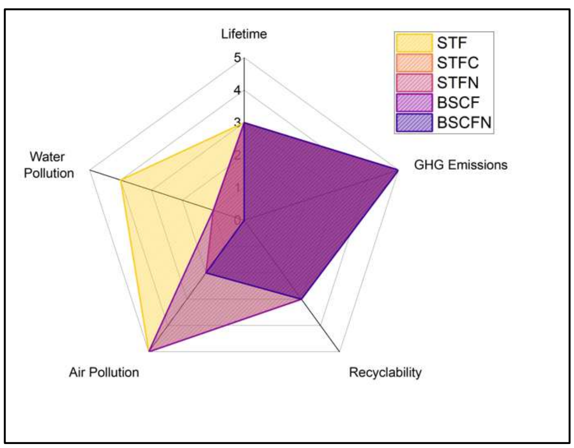


Figure 8: Environmental Scoring of Top Anodic Catalysts

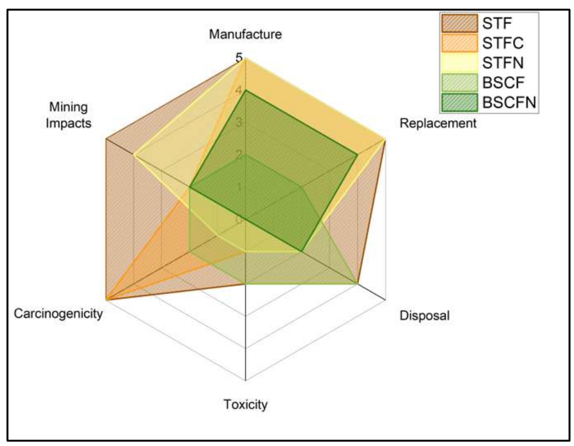


Figure 7: Economic and Social Scoring of Top Anodic Catalysts

Figures 7 and 8 further demonstrate the superior performance of STF, where we see this ranked the highest in half of the criterions considered across the economic and social domains. On the other end of this, BSCFN ranks the lowest (from this half of the catalysts) despites its ideal technical performance. This scores 0 in ‘Carcinogenicity’ and Toxicity due to its Co, Fe and Ni content, where Ni compounds are group 1 carcinogens i.e. known carcinogen.

3.2.2 Cathode

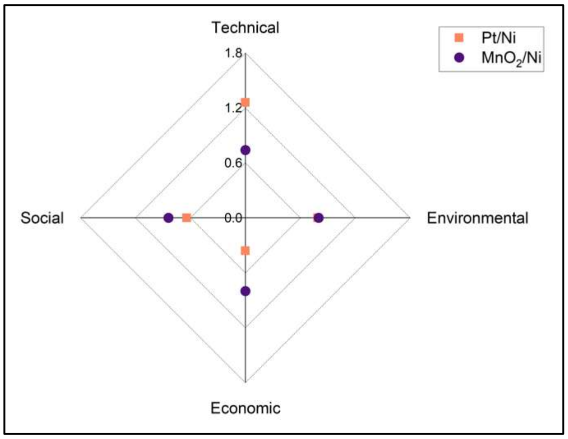


Figure 10: Domain Performance of Cathode Catalyst

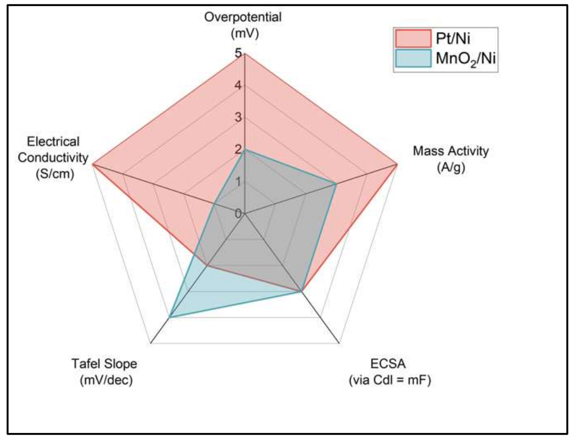


Figure 9: Technical Scoring of Top Cathodic Catalysts

MnO_2 has consistent performance in all the categories ranking better or similar to Pt in all sustainable specifications. The sensitivity analysis further shows how this material emerges as the recommendation when each of these domains are weighted higher. Pt outperforms in technical aspects with perfect scores in three out of five parameters; however, this comes at a significant expense with S3.1.3 showing the vast difference in price with MnO_2 costing more than a factor of 100 less than Pt. The trade-offs between technical and economic aspects are clearly observed in Figure 6 which show almost an equal difference in scoring at these two domains.

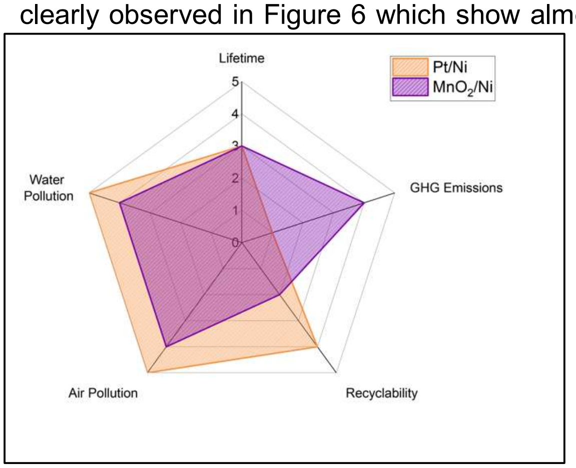


Figure 12: Environmental Scoring of Cathodic Catalysts

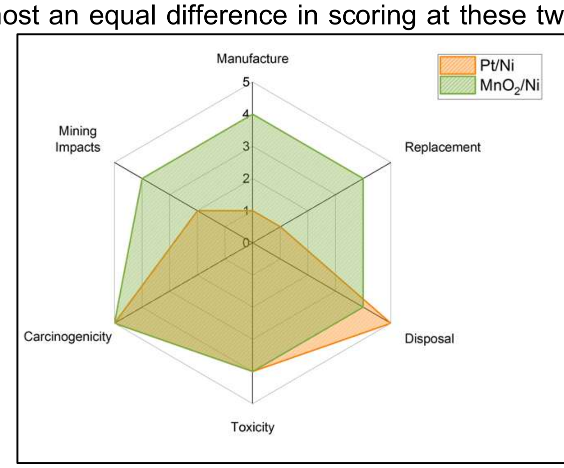


Figure 11: Economic and Social Scoring of Cathodic Catalysts

MnO_2 again shows consistent performance across all criterions considered in the economic and social domain. Alongside Pt, both of these metals have perfect scores in carcinogenicity. Pt has further perfect scores in Water and Air Pollution as well as Disposal as this is not considered as an environmental pollutant across the literature. However, as discussed previously, this is significantly more expensive in Manufacture and Replacements which is indicated by the low score in these categories. Pt also performs poorly in GHG emissions as the GWP of this is found to be 10^5 greater than MnO_2 potentially due to its rarity and the difficulty in its extraction and refining. This is further supported by its relatively lower score in Mining Impacts where South African mines are found to damage the local environment by consuming significant volumes of water and producing significant levels of air pollution when mining. This low score is also due to the poor working conditions local miners are subjected to, including low wages and poor health and safety protection.

3.2.3 Substrate

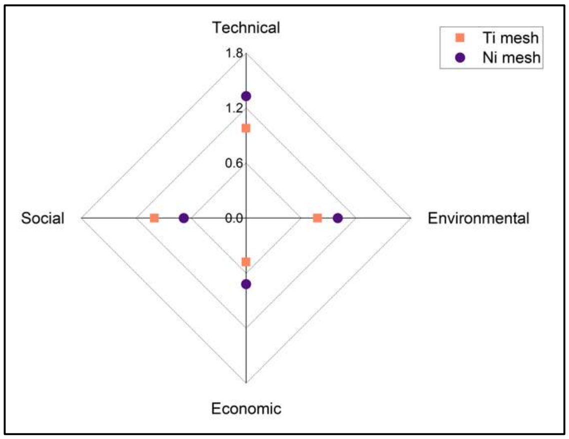


Figure 13: Domain Performance of Substrates

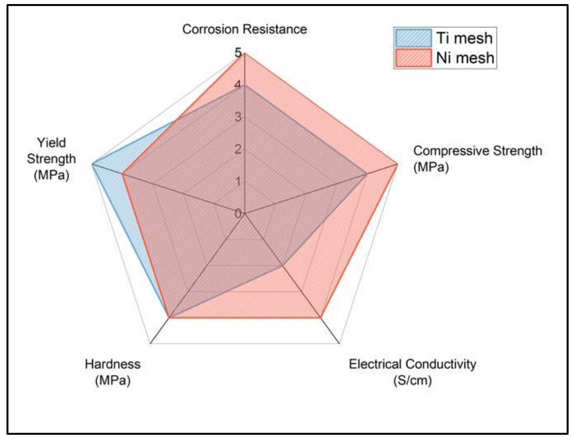


Figure 14: Technical Scoring of Substrates

Ni mesh performs better than Ti mesh in technical, environmental and economic criterions. This is further seen in Figure 14 where this substrate has the lowest score of 4 and top scores in Corrosion Resistance and Compressive Strength. Nickel is an essential metal for alloys due to these qualities and its high temperature resistance. Titanium also performs well across the technical KPIs and best in Yield Strength. This metal is known for its strength and durability which is demonstrated by its high scores in these categories. The main difference in technical performances are observed within each metal's electrical conductivity. S3.1.1 shows the specific values for each of this; however, Nickel is found to be a relatively good conductor

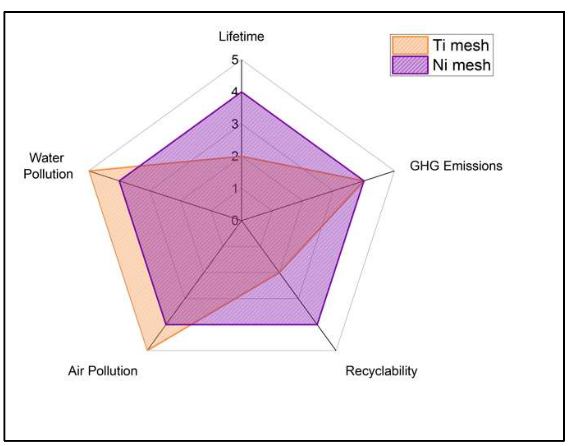


Figure 15: Environmental Scoring of Substrates

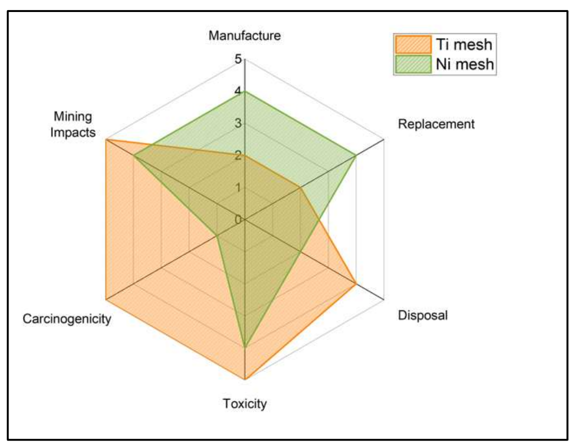


Figure 16: Economic and Social Scoring of Cathodic Catalysts

scoring around 20% against the International Annealed Copper Standard (IACS) outperforming Titanium with an IACS conductivity of 3.1%.

Titanium ranks top in many of the criterions assessed for sustainability, including Water and Air Pollution, Mining Impacts, Carcinogenicity and Toxicity. Titanium is not a heavy metal unlike Nickel meaning that it is not monitored or considered as a pollutant. Furthermore, literature does not show any case studies or examples of the mining of Ti ore to breach any human right laws or cause any social injustices. Nickel, on the other hand, has caused harm to its mining countries. An example of this is in Greece, where mining companies were found dumping their waste in the waters, polluting the sea and destroying marine life. Due to this, protests were held to demand for more stringent commercial waste management laws prohibiting companies from dumping their waste in the seas.

3.3 Sensitivity Analysis

Sensitivity analysis was conducted by individually intensifying the weightings of each of the domains by an additional 10%. The 10% gained by the prioritised domain was forfeited equally by the remaining parameters. For example, the applied weightings to each of the domains follow as: Technical 35%; Environmental 25%; Economic 20% and Social 20%. An additional 10% weighting to the technical parameter would lead to weightings of: Technical 45%; Environmental 21%; Economic 17% and Social 17%. This methodology was used for each of the categories to compare and assess top scoring materials at different applied weightings

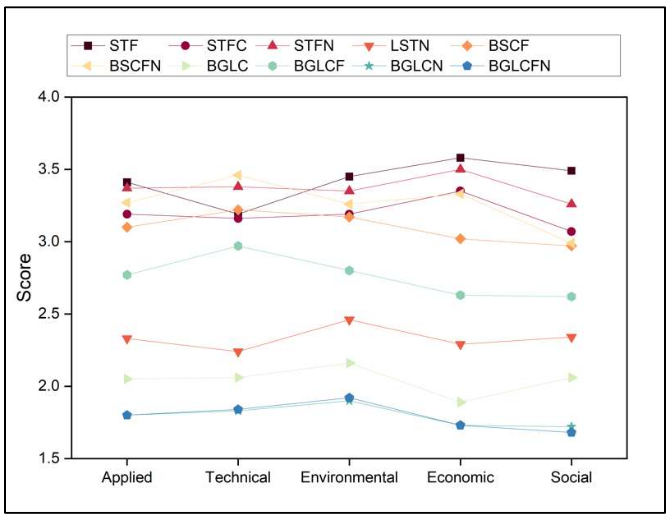


Figure 17: Sensitivity Analysis on Anodic Catalysts

and prioritisations.

Figure 17 shows that STF performs consistently at the top for all sustainable parameters which

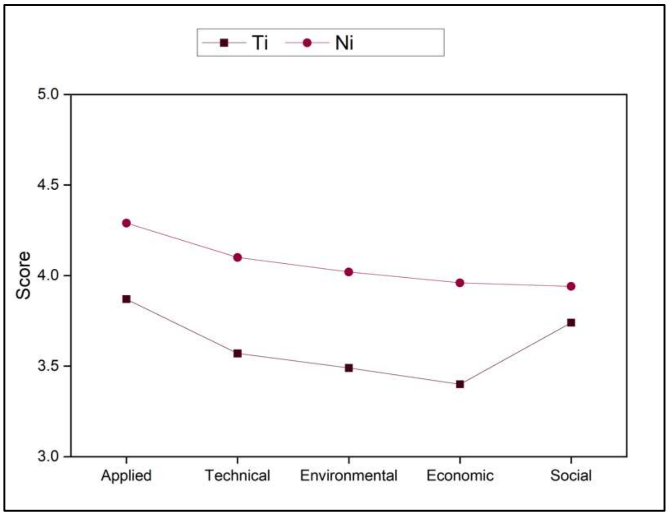


Figure 19: Sensitivity Analysis on Cathodic Catalysts

is expected as this scores the highest in each of these categories at the regular applied weightings. With higher weighting applied to technical, BSCFN is shown to be the top which is also expected due to its superior performance in this category. STFN is shown to perform second-best at each emphasised weighting indicating that this has the most consistent

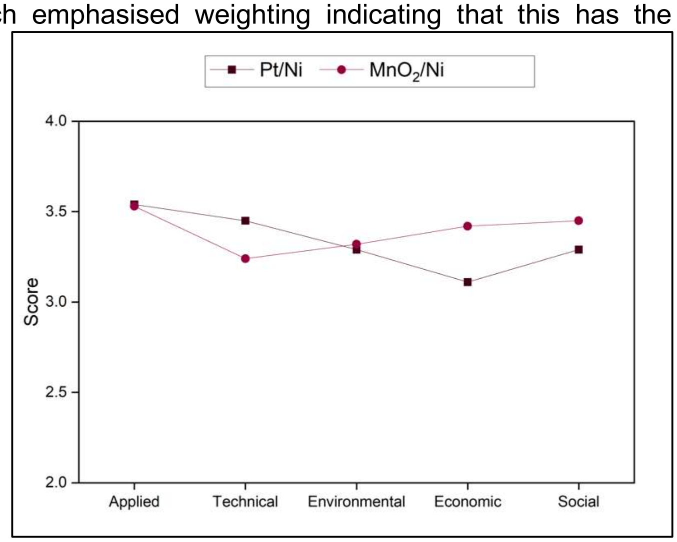


Figure 18: Sensitivity Analysis on Substrates

performance across the parameters.

Pt and MnO_2 follow the same pattern observed in the original applied weightings where Pt has better technical performance, but MnO_2 is more sustainable. This is highlighted in Figure 18 alongside the similar overall scores of each of these at the original and enhanced environmental weightings.

Figure 19 shows that Ni mesh is superior to Ti mesh at each category. The difference in scores for each are significant with an enhanced Social weighting demonstrating potentially more similar performance. The most significant difference in scores is seen with Economic due to Ti mesh costing more than double that of Ni mesh.

3.4 Recommendations from results

From the radar diagrams we can list the primary recommendations for the anode as STF on Ni mesh and for the cathode as Pt on Ni mesh (Pt/Ni) as these have attained the highest overall score across the domains and criteria. The plots as well as sensitivity analysis also indicate the materials which perform optimally in each of the explored categories so we can further evaluate how this may influence the overall selection if alternative weightings had been applied. STFN appears to be a good secondary recommendation due to its consistent performance in each of the categories.

4 MCDA PV Cell: Considerations

The structure of a PV module contains seven layers: frame, glass, front and back encapsulants, PV cell, back sheet and junction The application of the methodology for the PV module diverges from the electrolyser as this is used to evaluate complete technologies instead of individual materials and components. This approach aligns with the strategies of the PV technical team in sourcing commercial options.

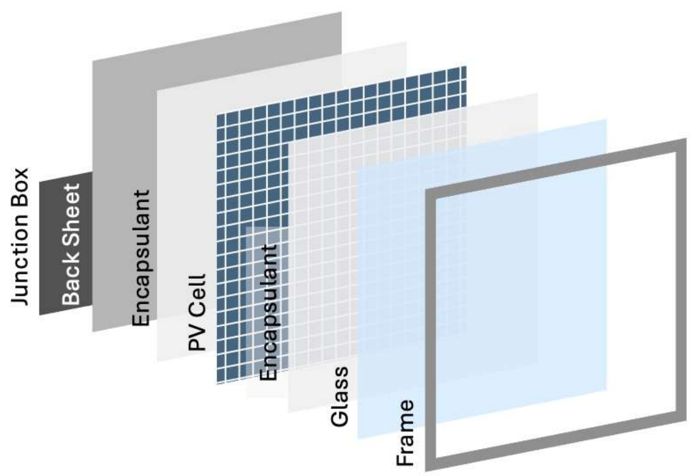


Figure 20: PV Module Configuration

The structure of a PV module comprises of seven layers: frame, glass, front and back encapsulants, PV cell, back sheet and junction box in the order presented in Figure 5. The methodology focuses on the PV cell layer as this controls the solar-to-electrical energy conversion and determines the performance of the module in conversion efficiency as well as stability over time and against environmental stresses i.e. temperature fluctuations, weather exposure etc.

As advised by the WP6 team, five PV cell configurations were examined of the monocrystalline structure as these boast reliably high efficiencies. From this cell category, the following technologies have been examined:

- **IBC** – Interdigitated Back Contact
- **SHJ** – Heterojunction/Silicon Heterojunction
- **TOPCon** – Tunnel Oxide Passivated Contact
- **PERC** – Mono Passivated Emitter & Rear Cell
- **Perovskite/Silicon Tandem**

These technologies represent varying degrees of commercial maturity, with PERC and IBC options having well-established positions in the industry. This is followed by SHJ and TOPCon which are relatively recent commercially available options. The Perovskite/Si Tandem cell is an emerging technology, with performance metrics currently limited to laboratory scale testing so far.

4.1 PV Cell Literature and Data

Cell Structure	PCE	Stability	Energy Consumption	Temperature Coefficient	Reference
	%	Description	kWh/MW	%/°C	
IBC	26.3	UV light and temperature Instability [27]	62000	0.26-0.3	CPIA, Clean Energy [28]
SHJ	25.9	UV light instability [29]	43000	0.25-0.27	
PERC	23.5	Good thermal stability [30]	42000	0.35-0.40	
TOPCon	25.7	UV light and temperature Instability [29]	51000	0.29-0.32	
PK/Si	>30% [31]	Challenges with structure, material processing and general stability [29]	>5% than SHJ [32]	0.26 [33]	-

Cell Structure	Lifetime	GHG Emissions	Recyclability	Air Pollution [18]	Water Pollution [19]
	Years	Via GWP (kg/CO2-eqkg)	Cycles	Fraction/Count	Fraction/Count
IBC	25	X	X	Sn	Ag, Sn
SHJ	25	X	X	Sn	Ag, Sn
PERC	25	X	X	X	Ag, Al
TOPCon	25	X	X	X	Ag, Al
PK/Si	X	47.46 [34]	X	Ag, Sn, Pb	Ag, Sn, Pb

Material	Module Construction Cost	Disposal [23]	Toxicity [24]	Carcinogenicity [25]	Mining Impacts [26]
	USD/W	Via Hazardous Compounds Fraction/Count	Fraction/Count	Group/ Compound	Via Sanctions Fraction/Count
IBC	0.26 [35]	Sn	Ag, Sn	ITO 2B	Ag, Sn 15
SHJ	0.24 [35]	Sn	Ag, Sn	ITO 2B	Ag, Sn 15
PERC	0.26	X	Ag	X	Ag, Al 10
TOPCon	0.27	X	Ag	X	Ag, Al 10
PK/Si	X	Sn, Pb	Ag, Sn, Pb	ITO 2B, Pb Inorganic Compounds 2A, Pb 2B	Ag, Sn, Pb 20

4.2 Results and Discussion

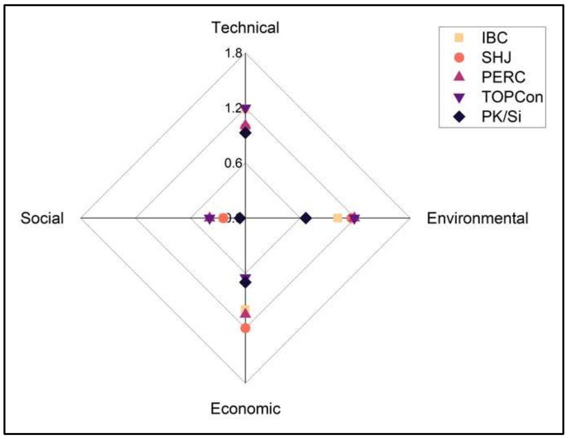


Figure 21: Domain Performance of PV Cells

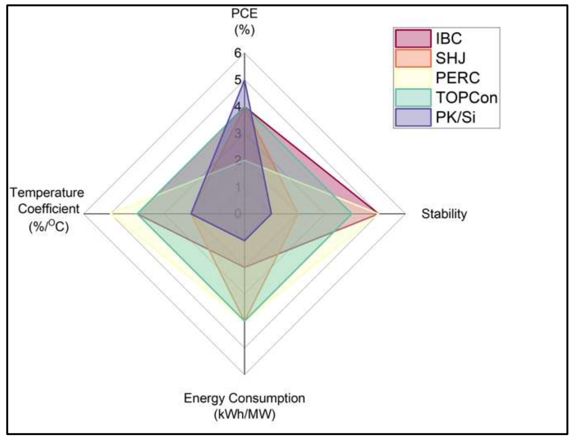


Figure 22: Technical Scoring of PV Cells

The TOPCon and PERC cell structures perform better than the others for each domain whereas PK/Si is seen at the lower end consistently, potentially due to its low technical readiness. This cell structure is not commercially available and much of the data found for its performance were sourced from scientific journals instead of published industry data. In Figure 23, its poor performance can be seen clearly across the technical criterions except in PCE where this is found to score the highest due to lab testing achieving efficiencies higher than 30%. TOPCon has consistently high scores across the KPIs due to a high PCE of 25.7%, temperature coefficient between 0.29-0.32 5/°C and good stability. IBC and PERC also have high technical performance, where these options are found to be in the top in the sensitivity

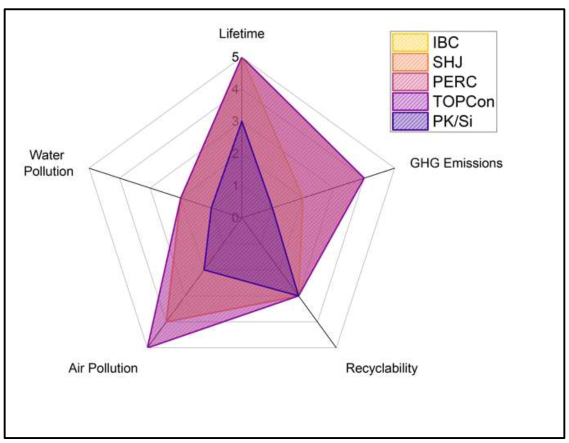


Figure 24: Environmental Scoring of PV

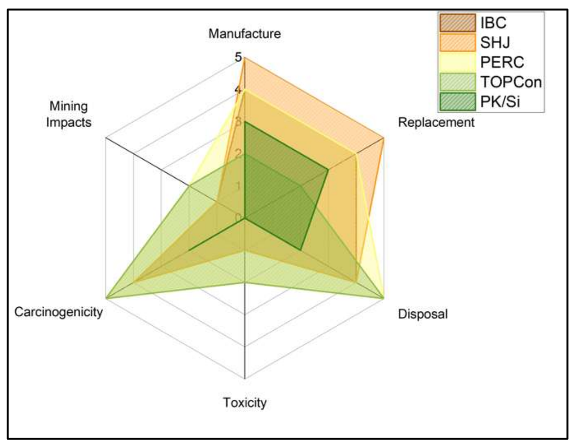


Figure 23: Economic and Social Scoring of PV Cells

analysis.

PERC and TOPCon score the same in each of the criterions for the environmental category where these have perfect scores in air pollution due to the absence of tin used in ITO. Due to the commercial availability of IBC, SHJ, TOPCon and PERC, expected lifetimes of these are well documented and found to be averagely 25 years. This information is unavailable for PK/Si again due to its low technical readiness. All cell structures score poorly in toxicity attributing to the silver, tin, aluminium and lead content in each of these which is also reflected in the scores for water pollution and mining impacts. The silver paste used in each of the cell structures comes with many social implications. Bolivia has experienced many of the repercussions of silver mining including impacts to their demography. Silver mines in Bolivia are found to use child labour and fail to provide safe working conditions for miners, leading to fatalities. This causes demographic changes as many of the women frequently become widowed.

4.3 Sensitivity Analysis

Sensitivity analysis for the PV Cells were conducted similarly to the electrode materials however due to some differences in the original applied weightings for each of the categories, the weightings used to perform the analysis are different. For example, the applied weightings to each of the domains follow as: Technical 30%; Environmental 30%; Economic 25% and Social 15%. An additional 10% weighting to the technical parameter would lead to weightings of: Technical 40%; Environmental 26%; Economic 22% and Social 12%. This methodology was used for each of the categories to compare and assess top scoring materials at different applied weightings and prioritisations.

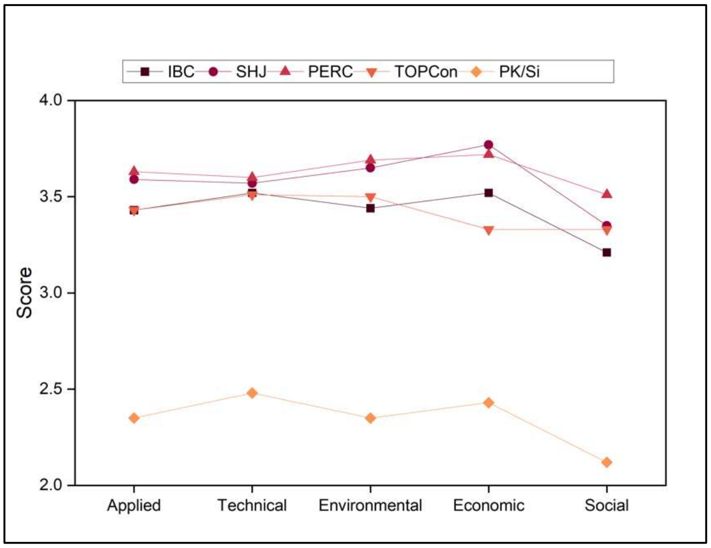


Figure 25: Sensitivity Analysis on PV Cells

Figure 25 demonstrates the strong similarity in the technical performances of each of the full silicon cell structures. PK/Si remains consistently poor across each category despite having the highest PCE. PERC is found to be top in three parameters including technical, environmental and social with SHJ overtaking this in economic viability. SHJ also maintains a top consistent performance where this could be given as a secondary recommendation. TOPCon and IBC appear to have very similar overall performances, where they overtake each other in half of the categories. This further supports the original applied weightings which show that these have almost identical performance.

4.4 Recommendations from Results

The primary recommendation for the PV cell structure is PERC. Although, in the original weightings this cell only demonstrated top performance in the environmental category, the overall scores with the original weightings and in the sensitivity analysis show that this was consistently superior across all categories except economic viability where SHJ emerges on top. SHJ ranks consistently well across all categories and emerges as a good secondary recommendation.

5 Summary of Findings and Recommendation

This study conducted a comprehensive meta-analysis to determine optimal material design choices for the components involved in the construction of Unit 1. In alignment with the objectives, recommendations were developed through a holistic approach combining sustainability metrics alongside traditional performance indicators. This methodology is not only in fulfilment with the purposes of WP14 in bridging these concerns but establishes a preliminary framework to support the technical teams in comparative analysis.

The scope identifies three design elements in the electrolyser which required the application of this methodology: anode catalyst, electrode substrate and cathode catalyst/substrate. We evaluate ten perovskite compositions for the electrode catalyst; two metal meshes with the electrode substrate, and two configurations with the cathode. Additionally, analysis of the PV module comprised of five configurations of PV cells. Through evaluation of technical, environmental, economic and social criteria, we were able to conduct our assessment to find the following primary recommendations:

- Anode catalyst: STF
- Anode substrate: Ni mesh
- Cathode: Pt/Ni mesh
- PV cell: PERC

The study employed an MCDA, supported by an extensive literature review to enable the identification of both primary and secondary recommendations. The procedure also allowed for the recognition of optimal materials within the assessed domains, permitting an alternative recommendation based on priorities. A sensitivity analysis was also conducted to identify alternative material recommendations dependent on the enhanced weighting of a category. Alongside these methods of data collection and analysis, a survey was employed to collect larger stakeholder input and was used to design a methodology more consistent with expert opinion.

While the methodology incorporated detailed criteria definitions and scoring metrics, this also highlights the assumptions made during the course of the study. Many of these assumptions can be attributed to the novelty and low technical readiness of the materials assessed, leading to gaps in literature. Due to the employment of a survey to collect feedback from REFINE members, many of the initial limitations relating to the restriction of larger input on the weightings and non-technical parameters, the most significant assumptions have been reduced to the following:

- Scores determination was primarily conducted by the author

This still poses some potential limitations, particularly regarding the accuracy of the scores and the identification of optimal candidates. However, subjectivity and bias has been controlled as much as possible through sensitivity analysis and actioning of stakeholder input. Overall, despite some methodological oversights, the study successfully achieves its primary aim in identifying evidence-based material recommendations.

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Appendix

A.1 Electrolyser Matrix and Calculations

Anode Catalyst	Technical					Environmental				
	Overpotential	Mass Activity	ECSA	Tafel Slope	Electrical Conductivity	Lifetime	GHG Emissions	Recyclability	Air Pollution	Water Pollution
STF	2	2	0	5	0	3	5	3	5	4
STFC	3	3	3	3	3	3	5	3	2	1
STFN	4	4	3	1	4	3	5	3	2	1
LSTN	2	1	3	0	3	3	4	3	2	5
BSCF	4	4	3	4	4	3	5	3	5	1
BSCFN	5	4	3	5	5	3	5	3	2	0
BGLC	1	2	5	2	3	3	2	3	5	5
BGLCF	4	5	4	4	3	3	2	3	5	2
BGLCN	1	2	4	2	3	3	2	3	2	2
BGLCFN	2	2	2	2	3	3	2	3	4	1

Anode Catalyst	Economic			Social		
	Manufacture	**Replacement**	**Disposal**	**Toxicity**	**Carcinogenicity**	**Mining Impacts**
STF	5	5	4	2	5	5
STFC	5	5	2	1	5	2
STFN	5	5	2	1	1	4
LSTN	2	2	2	4	1	2
BSCF	2	2	4	2	2	2
BSCFN	4	4	2	0	0	2
BGLC	0	0	4	4	2	1
BGLCF	1	1	4	2	2	1
BGLFN	1	1	2	2	0	1
BGLCFN	1	1	2	1	0	1

	Technical					Environmental				
	Overpotential	Mass Activity	ECSA	Tafel Slope	Electrical Conductivity	Lifetime	GHG Emissions	Recyclability	Air Pollution	Water Pollution
STF	0.28	0.14	0.00	0.26	0.00	0.23	0.31	0.19	0.13	0.10
STFC	0.42	0.21	0.16	0.16	0.11	0.23	0.31	0.19	0.05	0.03
STFN	0.56	0.28	0.16	0.05	0.14	0.23	0.31	0.19	0.05	0.03
LSTN	0.28	0.07	0.16	0.00	0.11	0.23	0.25	0.19	0.05	0.13
BSCF	0.56	0.28	0.16	0.21	0.14	0.23	0.31	0.19	0.13	0.03
BSCFN	0.70	0.28	0.16	0.26	0.18	0.23	0.31	0.19	0.05	0.00
BGLC	0.14	0.14	0.26	0.11	0.11	0.23	0.13	0.19	0.13	0.13
BGLCF	0.56	0.35	0.21	0.21	0.11	0.23	0.13	0.19	0.13	0.05
BGLCN	0.14	0.14	0.21	0.11	0.11	0.23	0.13	0.19	0.05	0.05
BGLCFN	0.28	0.14	0.11	0.11	0.11	0.23	0.13	0.19	0.10	0.03

	Economic			Social		
	Manufacture	Replacement	Disposal	Toxicity	Carcinogenicity	Mining Impacts
STF	0.50	0.30	0.16	0.12	0.20	0.50
STFC	0.50	0.30	0.08	0.06	0.20	0.20
STFN	0.50	0.30	0.08	0.06	0.04	0.40
LSTN	0.20	0.12	0.08	0.24	0.04	0.20
BSCF	0.20	0.12	0.16	0.12	0.08	0.20
BSCFN	0.40	0.24	0.08	0.00	0.00	0.20
BGLC	0.00	0.00	0.16	0.24	0.08	0.10
BGLCF	0.10	0.06	0.16	0.12	0.08	0.10
BGLFN	0.10	0.06	0.08	0.12	0.00	0.10
BGLCFN	0.10	0.06	0.08	0.06	0.00	0.10

	Technical	Environmental	Economic	Social	Total
STF	0.68	0.95	0.96	0.82	3.41
STFC	1.05	0.80	0.88	0.46	3.19
STFN	1.19	0.80	0.88	0.50	3.37
LSTN	0.61	0.84	0.40	0.48	2.33
BSCF	1.35	0.88	0.48	0.40	3.10
BSCFN	1.58	0.78	0.72	0.20	3.27
BGLC	0.75	0.79	0.16	0.42	2.12
BGLCF	1.44	0.71	0.32	0.30	2.77
BGLCN	0.70	0.64	0.24	0.22	1.80
BGLCFN	0.74	0.66	0.24	0.16	1.80

Cathode Catalyst	Technical					Environmental				
	Overpotential	Mass Activity	ECSA	Tafel Slope	Electrical Conductivity	Lifetime	GHG Emissions	Recyclability	Air Pollution	Water Pollution
Pt/Ni Mesh	5	5	3	2	5	3	1	4	5	5
MnO2/Ni Mesh	2	3	3	4	1	3	4	2	4	4

Cathode Catalyst	Economic			Social		
	Manufacture	Replacement	Disposal	Toxicity	Carcinogenicity	Mining Impacts
Pt/Ni Mesh	1	1	5	4	5	2
MnO2/Ni Mesh	4	4	4	4	5	4

	Technical					Environmental				
	Overpotential	Mass Activity	ECSA	Tafel Slope	Electrical Conductivity	Lifetime	GHG Emissions	Recyclability	Air Pollution	Water Pollution
Pt/Ni Mesh	0.53	0.53	0.21	0.14	0.35	0.23	0.06	0.25	0.13	0.13
MnO2/Ni Mesh	0.21	0.32	0.21	0.28	0.07	0.23	0.25	0.13	0.10	0.10

	Economic			Social		
	Manufacture	Replacement	Disposal	Toxicity	Carcinogenicity	Mining Impacts
Pt/Ni Mesh	0.10	0.06	0.20	0.24	0.20	0.20
MnO2/Ni Mesh	0.40	0.24	0.16	0.24	0.20	0.40

	Technical	Environmental	Economic	Social	Total
Pt/Ni Mesh	1.75	0.79	0.36	0.64	3.54
MnO2/Ni Mesh	1.09	0.80	0.80	0.84	3.53

Electrode Substrate	Technical: Corrosion Resistance	Technical: Compressive Strength	Technical: Electrical Conductivity	Technical: Hardness	Technical: Yield Strength	Environmental: Lifetime	Environmental: GHG Emissions	Environmental: Recyclability	Environmental: Air Pollution	Environmental: Water Pollution
Ti	4	4	2	4	5	2	4	2	5	5
Ni	5	5	4	4	4	4	4	4	4	4

Electrode Substrate	Economic: Manufacture	Economic: Replacement	Economic: Disposal	Social: Toxicity	Social: Carcinogenicity	Social: Mining Impacts
Ti	2	2	4	5	5	5
Ni	4	4	2	4	1	4

	Technical					Environmental				
	Overpotential	Mass Activity	ECSA	Tafel Slope	Electrical Conductivity	Lifetime	GHG Emissions	Recyclability	Air Pollution	Water Pollution
Ti	0.42	0.42	0.14	0.28	0.35	0.15	0.25	0.13	0.13	0.13
Ni	0.53	0.53	0.28	0.28	0.28	0.30	0.25	0.25	0.10	0.10

	Economic			Social		
	Manufacture	Replacement	Disposal	Toxicity	Carcinogenicity	Mining Impacts
Ti	0.20	0.12	0.16	0.30	0.20	0.50
Ni	0.40	0.24	0.08	0.24	0.04	0.40

	Technical	Environmental	Economic	Social	Total
Ti	1.61	0.78	0.48	1.00	3.87
Ni	1.89	1.00	0.72	0.68	4.29

A.2 PV Cell Matrix and Calculations

	Technical				Environmental				
	PCE	Stability	Energy Consumption	Temperature Coefficient	Lifetime	GHG Emissions	Recyclability	Air Pollution	Water Pollution
IBC	4	5	2	4	5	2	4	2	3
SHJ	4	2	4	2	5	4	4	2	3
TOPCon	2	5	4	5	5	4	5	2	3
PERC	4	4	4	4	5	4	5	2	3
Perovskite/Si	5	1	1	2	3	1	2	1	3

	Economic			Social		
	Manufacture	Replacement	Disposal	Toxicity	Carcinogenicity	Mining Impacts
IBC	2	2	4	1	1	0
SHJ	2	2	4	1	1	1
TOPCon	4	4	4	1	1	0
PERC	4	4	4	1	1	0
Perovskite/Si	1	1	3	0	0	0

	Technical				Environmental				
	PCE	Stability	Energy Consumption	Temperature Coefficient	Lifetime	GHG Emissions	Recyclability	Air Pollution	Water Pollution
IBC	0.60	0.38	0.09	0.12	0.45	0.15	0.12	0.06	0.23
SHJ	0.60	0.15	0.18	0.06	0.45	0.30	0.12	0.06	0.23
PERC	0.30	0.38	0.18	0.15	0.45	0.30	0.15	0.06	0.23
TOPCon	0.60	0.30	0.18	0.12	0.45	0.30	0.15	0.06	0.23
Perovskite/ Si	0.75	0.08	0.05	0.06	0.27	0.08	0.06	0.03	0.23

	Economic			Social		
	Manufacture	Replacement	Disposal	Toxicity	Carcinogenicity	Mining Impacts
IBC	0.50	0.30	0.20	0.05	0.12	0.08
SHJ	0.63	0.38	0.20	0.05	0.12	0.08
PERC	0.50	0.30	0.25	0.09	0.15	0.15
TOPCon	0.25	0.15	0.25	0.09	0.15	0.15
Perovskite/Si	0.38	0.23	0.10	0.00	0.06	0.00

	Technical	Environmental	Economic	Social	Total
IBC	1.19	1.01	1.00	0.24	3.43
SHJ	0.99	1.16	1.20	0.24	3.59
PERC	1.01	1.19	1.05	0.39	3.63
TOPCon	1.20	1.19	0.65	0.39	3.43
Perovskite/Si	0.93	0.66	0.70	0.06	2.35

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