Supply risk considerations for photoelectrochemical water splitting materials

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Appendix A: Supplementary Material

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Summary

This supplementary Material A includes an explanation of the eleven indicators (S1-S5) and the interpretation and calculation of the aggregation methods (S6). The complete input data, instructions, Python scripts, and model results are publicly available via an OSF registration: https://doi.org/10.17605/OSF.IO/D9E8X. The data plotted in the figures in the paper are available in spreadsheet form (Supplementary data), as well as the article itself, via: https://doi.org/10.1039/D3EE04369J.

1. Short explanation of the eleven indicators

Table S1: Explanation of supply risk indicators for the criteria "risk of supply reduction".

ID	Indicator	Indicator Description	Dimension	Calculation	Data & Calculation Description	Sources	Perspective
S1	Scarcity, based on reserves	The Scarcity, based on reserves, is an indication of the market pressure for further exploration and for the development of new extraction capabilities, possibly leading to higher price levels. The scarcity, based on reserves, is sometimes also called static reach reserves or depletion time of reserves.	years	$S1 = 100 - a_1 T - b_1 T^2$ $S1 = 100 - 0.2T - 0.008T^2$ $T = \frac{Reserves}{Annual\ Production}$	The scarcity, based on reserves, of a raw material is given by the ratio of annual primary production to the estimated global reserves. Reserves are the ores currently technically and economically extractable from known deposits. The parameters a_1 and b_1 are defined as normalization factors to get a common scale from 0 (lowest supply risk) to 100 (highest supply risk). A risk value of 100 is obtained by a T of 0 years, a value of 70 by a T of 50 years and 0 by a T of 100 years.	1,2	Present
S2	Scarcity, based on resources	The Scarcity, based on resources. is an indication of the long-term market pressure for further exploration and for the development of new extraction capabilities, possibly leading to higher price levels. The scarcity, based on resources, is sometimes also called static reach resources or depletion time of resources.	years	$S2 = 100 - a_2 T - b_2 T^2$ $S2 = 100 - 0.1T - 0.002T^2$ $T = \frac{Resources}{Annual\ Production}$	The scarcity, based on resources, of a raw material is given by the ratio of annual primary production to the estimated global resources. Resources are the ores contained in deposits that are economically and technically extractable now or in the future. The parameters a_2 and b_2 are defined as normalization factors to get a common scale from 0 (lowest supply risk) to 100 (highest supply risk). A risk value of 100 is obtained by a T of 0 years, a value of 70 by a T of 100 years and 0 by a T of 200 years.). In contrast to the S1 indicator, the reserves are used for the calculation and not production, as the reserves serve as approximate values for potential future production.	1,2	Future
S3	Dependence on primary production	The dependence on the primary production is an estimate of the amount of available secondary material that is independent of mining and primary refining activities and can thus smooth out supply disruptions or price peaks.	%	$S3 = 100 \cdot (1 - EoLRIR)$	The dependence on the primary production of a raw material is given by the ratio of the current annual recycled material flow to the annual discard rate of the raw material, also named End-of-Life Recycling Input Rate (EoLRIR). The EoLRIR is calculated by multiplying the old scrape ratio (OSR) with the recycled content ratio (RCR). A EoLRIR of 100% results on a supply risk value of 0 while a EoLRIR of 0% results in a score of 100.	1,3,4	Present, Future

Table S2: Explanation of supply risk indicators for the criteria "risk of demand increase".

ID	Indicator	Indicator Description	Dimension	Calculation	Data & Calculation Description	Sources	Perspective
D1	Demand growth	Demand growth gives an indication of the market pressure for an increase in global extraction due to future technologies. The demand growth is sometimes also called future technology demand.	%	$D1 = 1{,}000 \cdot DG$ $DG = \left(1 + \frac{FTD_{2040} - FTD_{2018}}{Production_{2018}}\right)^{\frac{1}{years}} - 1$ $years = 22$	Demand growth (DG) is given by the ratio of expected additional demand in a future year from new, future technologies ($FTD_{2040} - FTD_{2018}$) to global production in a past year ($Production_{2018}$).	[1,5]	Present, Future
D2	By-product dependence	The by-product dependence is the amount of an element mined as a by-product given as a percentage of the global production of the host element(s). Extraction as a by-product occurs when mining solely for the raw material itself is not economically feasible. The figure is a measure of the possible inability to increase primary production in response to an increase in demand. The by-product dependence is sometimes also called companion metal fraction.	%	$D2 = Percentage\ of\ global\ production\ obtained\ as\ companion$	The percentage of global production obtained as companion is collected from [6].	[1,6]	Present, Future
D3	Sector Competition	The Sector Competition Index (SCI) measures the risk of competing demands for raw materials among industries, particularly those willing to pay premium prices.	qualitative	$D3 = SCI$	The Sector Competition Index (SCI) calculates the average added value per unit of material consumed, weighted using these materials across major industry sectors, highlighting the economic impact of material inputs.	[1,7]	Present
D4	Lack of substitution options	Lack of substitution options is an estimate of the extent to which a raw material can be replaced by another raw material without there being too great a loss of essential properties. The value gives an estimate of the extent to which demand can be shifted to other materials in the case of supply shortage and, thus, of the potential to smooth out supply disruptions or price peaks.	qualitative	$D4 = Substitute\ Performance$	The substitute performance is assessed by experts and collected from [8].	[1,8]	Present, Future

Table S3: Explanation of supply risk indicators for the criteria "concentration risk".

ID	Indicator	Indicator Description	Dimension	Calculation	Data & Calculation Description	Sources	Perspective
C1	Country Concentration, based on production	The concentration of the annual production of a raw material in one, or in only a few, countries is measured by the Herfindahl-Hirschman Index. The value directly indicates market concentration and thus the possibility of strategic exploitation of a monopolistic position at times of international crisis or dispute.	HHI	$C1 = c_1 \ln(HHI) - d_1$ $C1 = 21.64 \ln(HHI) - 99.31$ $HHI = 10{,}000 \sum production_i^2$ i: Countries	The Herfindahl-Hirschman Index (HHI) is the sum over the squares of the production shares of the countries in percent. The parameters c_1 and d_1 are defined as normalization factors to get a common scale from 0 (lowest supply risk) to 100 (highest supply risk). A supply risk value of 100 is obtained by a HHI of 10,000, a value of 70 by a HHI of 2,500 and 0 by a HHI of 100.	[1,2]	Present
C2	Country Concentration, based on reserve	The concentration of the estimated global reserves of a raw material in one, or in only a few, countries is measured by the Herfindahl-Hirschman Index. The value directly indicates long-term market concentration and thus the possibility of strategic long-term exploitation of a monopolistic position at times of international crisis or dispute.	HHI	$C2 = c_1 \ln(HHI) - d_1$ $C2 = 21.64 \ln(HHI) - 99.31$ $HHI = 10{,}000 \sum reserves_i^2$ i: Countries	The Herfindahl-Hirschman Index (HHI) is the sum over the squares of the reserve shares of the countries in percent. The parameters c_1 and d_1 are defined as normalization factors to get a common scale from 0 (lowest supply risk) to 100 (highest supply risk). A supply risk value of 100 is obtained by a HHI of 10,000, a value of 70 by a HHI of 2,500 and 0 by a HHI of 100.). In contrast to the C1 indicator, the reserves are used to calculate the HHI and not production, as the reserves serve as approximate values for potential future production.	[1,2,9]	Future

Table S4: Explanation of supply risk indicators for the criteria "political risk" in the present scenario.

ID	Indicator	Indicator Description	Dimension	Calculation	Data & Calculation Description	Sources	Perspective
P1	Political instability (WGI-PV)	The risk of Political Instability (WGI-PV) is an indication of the likelihood of disruption in production and export in the countries concerned due to unrest, coups d'état, terrorism or other situations involving violence.	qualitative	$P1 = 20 \cdot (2.5 - WGI)$ $WGI = \sum_i wgi_i \cdot production_i$ i: Countries	The risk of political instability in producing countries is measured by the Worldwide Governance Indicator for Political Stability and Absence of Violence/Terrorism (WGI-PV), published by the World Bank. It is weighted by the production share in each producing country.	1,2,10	Present
P2	Regulation (PPI)	The Regulation (PPI) is a measure of the ability of the market to continue to function and/or of primary production to continue to increase based on the functioning of the rule of law and governance procedures in producing countries.	qualitative	$P2 = (100 - PPI)$ $PPI = \sum_i ppi_i \cdot production_i$ i: Countries	The policy perception indicator (PPI) is an assessment of the ability of producing countries to implement new mining projects, weighted by the production share in each producing country. It is evaluated by mining industry experts and summarized by the Fraser Institute as the policy perception index (PPI).	1,2,11	Present
P3	Regulation (HDI)	The Regulation (HDI) attempts to measure the likelihood of producing countries to implement restrictions on mining, refining and trade, as indicated by their level of societal development. The value assesses the likelihood that further mineral extraction and refining activities are prevented due to regulations, taxes, tariffs, or taxes in producing countries.	qualitative	$P3 = 100 \cdot \frac{HDI - e_1}{f_1 - e_1}$ $P3 = 100 \cdot \frac{HDI - 0.352}{0.949 - 0.352}$ $HDI = \sum_i hdi_i \cdot production_i$ i: Countries	The HDI value is calculated by the Human Development Index for each producing country, as presented by the United Nations Development Programme, and weighted by the production share in each producing country. HDI scores are rescaled according to the minimum (e_1) and maximum (f_1) value of all countries.	1,2,12	Present

Table S5: Explanation of supply risk indicators for the criteria "political risk" in the future scenario.

ID	Indicator	Indicator Description	Dimension	Calculation	Data & Calculation Description	Sources	Perspective
P4	Political instability (WGI-PV), based on reserves	The risk of Political Instability (WGI-PV) is an indication of the likelihood of disruption in potential future production and export in the countries concerned due to unrest, coups d'état, terrorism or other situations involving violence.	qualitative	$P4 = 20 \cdot (2.5 - WGI)$ $WGI = \sum_i wgi_i \cdot reserves_i$ i: Countries	The risk of political instability in potential future producing countries is measured by the Worldwide Governance Indicator for Political Stability and Absence of Violence/Terrorism (WGI PV), published by the World Bank. It is weighted by the reserve share in each potential future producing country. In contrast to the P1 indicator, the reserves are used for weighting and not production, as the reserves serve as approximate values for potential future production.	1,2,9,10	Future
P5	Regulation (PPI), based on reserves	The Regulation (PPI) is a measure of the ability of the market to continue to function and/or of primary production to continue to increase based on the functioning of the rule of law and governance procedures in potential future producing countries.	qualitative	$P5 = (100 - PPI)$ $PPI = \sum_i ppi_i \cdot reserves_i$ i: Countries	The policy perception indicator (PPI) is an assessment of the ability of producing countries to implement new mining projects, weighted by the reserve share in each potential future producing country. It is evaluated by mining industry experts and summarized by the Fraser Institute as the policy perception index (PPI). In contrast to the P2 indicator, the reserves are used for weighting and not production, as the reserves serve as approximate values for potential future production.	1,2,9,11	Future
P6	Regulation (HDI), based on reserves	The Regulation (HDI) attempts to measure the likelihood of potential future producing countries to implement restrictions on mining, refining and trade, as indicated by their level of societal development. The value assesses the likelihood that further potential future mineral extraction and refining activities are prevented due to regulations, taxes, tariffs, or taxes in producing countries.	qualitative	$P6 = 100 \cdot \frac{HDI - e_1}{f_1 - g_1}$ $P6 = 100 \cdot \frac{HDI - 0.352}{0.949 - 0.352}$ $HDI = \sum_i hdi_i \cdot reserves_i$ i: Countries	The HDI value is calculated by the Human Development Index for each potential future producing country, as presented by the United Nations Development Programme, and weighted by the reserve share in each potential future producing country. In contrast to the P3 indicator, the reserves are used for weighting and not production, as the reserves serve as approximate values for potential future production. HDI scores are rescaled according to the minimum (e_1) and maximum (f_1) value of all countries.	1,2,9,12	Future

2. Calculation of aggregation methods

Table S6: Explanation of supply risk indicator aggregation for PEC absorber materials.

Aggregation approach	Description	Calculation	Source
Equal weighting	The equal weighting approach calculates the supply risk values of the materials (SR_{mean}) as arithmetic mean of the supply risk values of the individual elements (SR_i) of all elements contained within the material.	$SR_{mean} = \frac{\sum_{i \in Material} SR_i}{\sum_{i \in Material} 1}$	[1]
Mass-based weighting	The mass-based weighting approach calculates the supply risk values of the materials (SR_{mass}) as weighted average of the supply risk value of the elements (SR_i), where the weighting score is the share of each element's mass (m_i) relative to the total mass of all elements.	$SR_{mass} = \frac{\sum_i m_i SR_i}{\sum_i m_i}$	[1]
Cost-based weighting	The cost-based weighting method calculates the supply risk values of the materials (SR_{cost}) as weighted average of the supply risk value of the elements (SR_i), where the weighting score is the share of each element's mass (m_i) multiplied by its price (p_i) relative to the total costs of all elements.	$SR_{cost} = \frac{\sum_i p_i m_i SR_i}{\sum_i p_i m_i}$	[1]
Maximum approach	The maximum aggregation approach considers only the element with the highest supply risk score within each material.	$SR_{max} = \max_{i \in Material} SR_i$	[1]

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