# **Title:** The material-energy nexus in net-zero transition scenarios: exploring environmental trade-offs and uncertainties

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#### **Abstract:**

- As countries pursue net-zero energy systems, material demands intensify. This study integrates life cycle assessment with energy system modeling to quantify the environmental impacts and material needs of Switzerland's net-zero transition. Using global sensitivity analysis, we assess uncertainties in future material intensity, efficiency, and market share of energy technologies. Results reveal that 15 while life cycle greenhouse gas emissions decrease from over 40 megatons  $CO<sub>2</sub>$ -eq in 2020 to 4 by 2050, meeting domestic net-zero goals, demand for most potentially scarce materials rises substantially. For example, lithium demand expands from 250 tons in 2020 to 2,000 by 2050, driven by electric vehicles and large-scale battery storage, with estimates ranging from 800 to over 3,000 tons. The findings underscore the critical role of material resources in enabling the energy transition, environmental trade-offs, and the need to consider uncertainties in technology adoption and material use when planning for a sustainable energy future.
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- **Keywords:** Life Cycle Assessment (LCA); energy system modeling; energy system analysis; energy
- transition; critical raw materials; global sensitivity analysis

### 1. Introduction

 Climate change represents a global challenge that requires a profound shift towards low-carbon energy technologies (IEA, 2024). Moving away from combustion-based processes involves options like battery electric vehicles, electrification of heat demand in various sectors with technologies like high-temperature heat pumps, and the adoption of electric motors. This transition, along with expanded use of renewable energy sources (e.g., photovoltaic solar panels and wind turbines), offers wide-ranging benefits. These benefits span environmental (IPCC, 2023) and public-health (Shindell & Smith, 2019) areas, and provide economic (Pai et al., 2021) and social (Nature Editorial, 2023) opportunities.

 In parallel, the transition to a net-zero greenhouse gas (GHG) energy system is anticipated to drive a substantial rise in demand for critical raw materials (CRMs), positioning the energy sector as a key player in mineral markets (IEA, 2021). Low-carbon energy systems will necessitate greater quantities and diversity of minerals and metals compared to its fossil fuel-based predecessor (IEA, 2023). As 40 nations and economies strive to reduce emissions, the role of CRMs in enabling sustainable energy transitions draws increasing attention (Hund et al., 2020; IRENA, 2023; Noailly et al., 2024). This emphasizes exploring the material-energy nexus, highlighting the complex relationship between energy systems and material requirements and the need for robust modelling frameworks that help to understand and plan for these resource demands.

 Energy system models (ESMs) and integrated assessment models (IAMs) outline potential transformation pathways for the global energy transition toward future states achieving specific energy and climate targets (Chang et al., 2021; McLaren & Markusson, 2020). These models predominantly focus on cost- or utility-optimized future scenarios, highlighting, for example, the necessary changes in regional electricity mixes and means of transport to meet global warming mitigation objectives (Riahi et al., 2017). However, while initial efforts have been made to represent material demand within ESMs and IAMs, such frameworks do not yet endogenously incorporate this demand (Schulze et al., 2024). Additionally, their representation of broader environmental impacts, such as water use, ecotoxicity, and effects on human health, is limited. As a result, additional tools like life cycle assessment (LCA) are often soft-coupled with these models to provide a more detailed and comprehensive assessment of the different technologies (Vandepaer et al., 2020; Volkart et al., 2018).

 Environmental LCA is a complementary tool to comprehensively evaluate the environmental performance of energy technologies and systems. Applying LCA at the regional level in conjunction with ESMs provides a deeper understanding of potential supply chain-related impacts the energy system is responsible for. ESMs and IAMs scenarios can be used to project present-day life cycle inventories into future scenarios, using, for example, the IAM-LCA integration tool *premise* (Sacchi et al., 2022). Such inventories, temporally aligned with the energy system, allow for a comprehensive analysis of the sustainability of different energy system trajectories. This approach supports the creation and analysis of scenarios that address material demand, the interlinkage between energy and resources, and their associated environmental impacts (Harpprecht et al., 2021; van der Meide et al., 2022; C. Zhang et al., 2023).

 Conversely, numerous studies in the literature address the life cycle impacts of ESM scenarios. Some have integrated technology-specific LCA coefficients directly into ESMs, allowing for assessments that  reflect environmental impacts as scenarios are formulated (Addanki et al., 2024; Rauner & Budzinski, 2017; Vandepaer et al., 2020). Others have applied LCA post-scenario formulation to assess the environmental outcomes of specific model scenarios (Blanco et al., 2020; Gibon et al., 2015; Hertwich et al., 2015; Mellot et al., 2024; Volkart et al., 2018). Regardless of the approach — and despite the current lack of an established methodology or framework for applying LCA at the energy system scenario level (Hahn Menacho et al., 2024), supplementing ESM scenarios with LCA helps measure changes in material demand and the environmental impacts of sourcing these materials due to transitioning from fossil fuels, thereby helping to characterize the material-energy nexus and its broader environmental consequences.

 However, assessing energy systems' future material requirements relies on many uncertain input data, such as specific material intensities for each energy technology, technological developments, and market shares of sub-technologies (e.g., specific types of photovoltaic cells or specific battery cell chemistries) and their evolution over time (Schulze et al., 2024). Examples in the literature demonstrate that while some ESMs handle these uncertainties using methods like Monte Carlo simulations (Kalt et al., 2022; S. Wang et al., 2023) and stochastic approaches (Beylot et al., 2019), it 83 remains a challenge to consistently characterize the energy scenario and adjust the environmental impacts of sourcing the necessary resources based on varying material demands and market share and the technical evolution of different technologies.

86 This study uses LCA to characterize the case of a Swiss net-zero energy transition scenario, providing insights into a developed economy that has pledged to reach net-zero GHG emissions by 2050. By proposing a systematic approach and specific tools to calculate the life-cycle impacts of transition scenarios at a regional scale, we 1) estimate Switzerland's future demand for potentially critical raw materials, 2) evaluate the sensitivity of resource demand to the material intensity factors, future technological developments, and market shares assumed for emerging technologies, and 3) characterize the impacts of such material demand on various environmental impact categories variance. 4) Moreover, we develop a reproducible and replicable workflow that arranges prospective LCA databases along a time dimension to yield time series of environmental impacts for the energy system. This enables comprehensive, scenario-specific life-cycle impact assessments that can be extended beyond Switzerland to other national or regional contexts, offering a standardized approach for global energy analyses. Additionally, it allowsfor considering uncertainties in future material needs and their environmental impacts. Through this analysis, we demonstrate how changes in input data for various energy technologies influence their life cycle impacts. This provides a robust insight into the broader environmental consequences of material sourcing and the material-energy nexus.

 In the following sections, we outline our methodological approach, starting with the integration of ESM and LCA in section 2. Additionally, we detail the study's goal and scope, inventory analysis, impact 103 assessment, and sensitivity analysis. Section 3 presents results obtained from applying this framework to a Swiss net-zero energy transition scenario, highlighting key findings on CRM demand, environmental impacts, and trade-offs and co-benefits across various environmental categories. Section 4 provides a discussion on the implications of these findings, limitations of the current approach, and avenues for future research. Finally, section 5 concludes with insights for policy- and decision-making, underscoring the importance of comprehensive, resource-conscious planning for sustainable energy transitions.

# 2. Methods

111 In this section, we present the steps taken to systematically evaluate the energy system scenario's environmental performance and material demand using LCA. First, we detail the coupling between the ESM and the LCA framework. We then describe the different phases of the LCA, including (1) goal and scope definition, (2) inventory analysis, (3) impact assessment, and (4) interpretation. Within this last phase, we explain the global sensitivity analysis (GSA) conducted to evaluate how uncertainties in 116 the input data influence the results.

#### **2.1.Swiss TIMES energy model (STEM) and coupling with LCA**

 This study evaluates a long-term scenario to achieve net-zero territorial GHG emissions from Switzerland's fuel combustion and industrial processes by 2050. This scenario, called "*SPS1: Team Sprint. Focus on Sustainability*" (Panos et al., 2022) and referred to as "Net Zero" hereafter, has been developed within the SURE research project, supported by the Swiss Federal Office of Energy's SWEET program (SFOE, 2020) to help the country meet its net-zero emission target, which has become law 123 (SFOE, 2021). The scenario outlines the necessary steps and energy system configurations to meet this target. The Swiss TIMES energy model (STEM) (Panos et al., 2019), a comprehensive cost-optimization energy system model based on the TIMES framework, provides a solution that aligns with the scenario's objectives and constraints. The solution produced by STEM involves a portfolio of low- carbon power technologies, the electrification of passenger and freight transport and heating, the capture and storage of hard-to-abate fossil carbon emissions (e.g., from cement production), the use 129 of net negative carbon technologies, such as biomass-based power production with  $CO<sub>2</sub>$  capture and storage, and the use of synthetic liquid fuels for the few remaining processes relying on fuel combustion. The primary energy consumption and associated GHG emissions implied by the *Net Zero* scenario are illustrated in Figure 1. The detailed scenario outputs are available in the Supplementary Information material (SI1, S7). In-depth descriptions of the STEM model and the evaluated scenario can be found in (Panos et al., 2023) and (Panos et al., 2022), respectively.



Swiss Net Zero Scenario

 **Figure 1. Primary energy consumption and GHG emissions for Switzerland according to the** *Net Zero* **scenario evaluated.** 138 Primary energy consumption includes the total energy demand of all energy carriers, such as the energy used directly by<br>139 end-users and conversion losses in processes like thermal storage and electro-fuel synthesis. 139 end-users and conversion losses in processes like thermal storage and electro-fuel synthesis. The ambient heat retrieved by<br>140 heat pumps is counted as energy supply. The category "Other" includes the variables contri 140 heat pumps is counted as energy supply. The category "Other" includes the variables contributing less than 5% of the total.<br>141 Detailed information can be found in the supplemental data repository (SI1, S7). Detailed information can be found in the supplemental data repository (SI1, S7).

 Hahn Menacho et al. (2024) further developed the IAM/ESM-LCA soft-coupling tool *premise* (Sacchi et al., 2022) to integrate STEM results and adjust life-cycle inventories associated with Swiss processes and supply chains. In alignment with the projections of the STEM scenario, primary, secondary, and final energy carriers are modelled throughout the LCA database. Each variable representing energy conversion, transmission, distribution, and consumption within the STEM framework is linked to an LCA dataset, with detailed mapping in the SI document (SI1, S8). Altogether, 203 processes of STEM that produce or consume energy are mapped to the LCA database, encompassing final energy uses such as fossil fuels, electricity, and hydrogen used in transport, industrial and residential heat, and other industrial and service activities.

 Additionally, LCA datasets associated with STEM variables include the necessary infrastructure for energy use, such as the electricity network infrastructure for low-voltage consumers or batteries required for electric vehicles. The efficiencies of secondary energy conversion processes, such as heat and power plants, are also adjusted in the LCA database to align with those assumed in STEM. Processes located outside of Switzerland that directly and indirectly support the Swiss energy system (e.g., import of fuels, electricity, etc.) are also temporally adjusted using the global IAM scenario from REMIND (Luderer et al., 2015) under the SSP2-PkBudg1150 scenario. This scenario aims to limit global 158 warming to approximately 2 <sup>o</sup>C compared to pre-industrial levels, with a worldwide carbon budget of 159 1,150 Gton  $CO<sub>2</sub>$  for this century. Employing such a global scenario ensures consistency between the sectoral changes introduced by the Swiss *Net Zero* scenario domestically and those abroad, ensuring that processes producing material and energy commodities imported into Switzerland also undergo similar decarbonization efforts.

 Subsequently, the Python package *pathways* (Sacchi & Hahn-Menacho, n.d.) is used to systematically calculate the overall life cycle impacts of the scenario. The tool generates life-cycle environmental impacts for each final energy variable of the ESM scenario at each time step. Results are broken down by environmental indicator, product or service consumer, geographical location of the consumer, time step, geographical origin of impacts, and process category. As noted in Hahn Menacho et al. (2024), *pathways* addresses the issue of double-counting impacts in LCA supply chains by eliminating the contribution of final energy carriers within the supply chains of other final energy carriers. For example, the impact of diesel used in trucks is excluded from the electricity supply chain feeding into battery electric trucks, and vice versa. Access to the data package and the scripts used to produce the results in this study can be found in the Supplementary Information document (SI1, S5 and S8).

**2.2.Life cycle assessment**

#### *2.2.1. Goal and scope*

 This study defines the functional unit as the production, consumption and supply of final energy in Switzerland to satisfy the system energy demand from 2020 to 2050. This includes the necessary infrastructure for energy supply and usage. For example, the demand for a unit of energy stored in a stationary battery would be linked to the electricity grid demand, maintenance and losses, auxiliary components, and charging infrastructure.

 In the STEM model, final energy consumers fall into four economic sectors: transport, industry, service, and residential. Each subsector is further split by the type of energy carrier used and the technology employed (e.g., "Industry|Electricity|Electric boiler", "Industry|Electricity|Heat pump", etc.). The datasets used for each final energy consumer that constitute our functional unit are available in the Supplementary Information (SI1, S5 and S8).

#### *2.2.2. Life cycle inventory (LCI)*

 Life-cycle inventory (LCI) modeling requires comprehensive data collection, focusing extensively on the materials and energy consumed throughout the supply chain during the production, operation, and disposal of system components. The ecoinvent LCA database v3.10 (system model "allocation, cut-off by classification") is used as the main source of background data (Wernet et al., 2016), further modified by *premise* to align inventories and technology shares with the STEM scenario.

 Additionally, *premise* enhances the database by including inventories for emerging technologies relevant to the energy system and linked to important material requirements. These include, amongst others: perovskite (Roffeis et al., 2022) and gallium arsenide (Pallas et al., 2020) photovoltaic cells; sodium-ion (S. Zhang et al., 2024), lithium-sulfur (Wickerts et al., 2023), lithium-air (F. Wang et al., 2020), and vanadium redox-flow batteries (Weber et al., 2018); and, proton exchange membrane and alkaline electrolyzers (Gerloff, 2021).

 Regarding the co-production of metals in multifunctional mining processes, we modify the database to allocate according to physical mass balances: extraction of individual elements in the ore is fully attributed to the production of the respective metal; while other elementary and intermediate flows follow an economic allocation (SI1, S9), which is also the default option to deal with multi-functionality in ecoinvent (Wernet et al., 2016). As discussed in Berger et al. (2020), this approach ensures a correct mass balance.

#### *2.2.2.1. Material requirements and uncertainty*

 Current LCI databases inadequately represent potentially scarce raw materials, particularly those used in very small quantities, such as platinum group metals (PGMs) and rare earth oxides. To fill this gap, we build on the research by Schlichenmaier & Naegler (2022) and gather additional data on the 207 material requirements for various technologies. These technologies include wind turbines, electric and internal combustion engine vehicles, photovoltaic panels, concentrated solar power plants, nuclear plants, electric batteries (both mobile and stationary), fuel cells, and electrolyzers. We use the collected data to create probability distributions of each technology's current and future material needs. We define most of these probability distributions as triangular, using the median value found in the literature as the mode, with the lowest and highest values serving as the boundaries. The Supplementary Information (SI1, S2; and SI2) provides detailed data, distribution parameters, and references.

 Moreover, probability distributions are employed to represent the uncertainty surrounding future 216 technological efficiency, such as, among others, the lifespan and conversion efficiency of electrolyzers, the module efficiency of photovoltaic panels, and the energy density of battery cells—all of which significantly impact the demand for material resources. The distributions characterizing the uncertainty around the efficiency of technologies and the energy density of battery cells can be found in the Supplementary Information (SI1, S3-S5).

- 221 Finally, the uncertainty regarding the market shares of future technologies is also accounted for. An 222 algorithm generates pseudo-random market shares for each group of competing technologies from 223 2020 to 2050 (e.g., gearbox versus direct-drive wind turbines), ensuring that these shares fall within 224 anticipated intervals and collectively sum to 100%. The Supplementary Information (SI1, S1) details 225 the expected market share intervals.
- 226 The uncertainty in material requirements, combined with that of technological efficiency and market
- 227 shares, forms the basis of the input data used in the Monte Carlo simulations and GSA performed in
- 228 this study further detailed in section 2.2.4. Figure 2 illustrates the implementation of such probability
- 229 distributions along the electricity supply chain for battery-electric passenger cars.



#### 230

 **Figure 2.** System boundaries and uncertainties are considered along the supply of one megajoule of final energy to the final consumer (i.e., a battery electric passenger car). System boundaries include the production, supply and use of final energy, but also the infrastructure needed to use it (e.g., grid, battery, electric motor, etc.). Infrastructure that is not considered to change due to a change in the energy carrier is omitted (e.g., the car chassis, road, etc.). In this example, the capacity of the 235 onboard battery varies from 40 to 80 kWh (and is further normalized to one megajoule of electricity consumed by the vehicle). Several battery technologies compete to provide storage capacity, each associated with a probability distribution for the market share (specific to a year). Market share uncertainty values within the same market always sum to 100% for each Monte Carlo iteration. Each battery technology is associated with a probability distribution regarding the cell energy density, which also improves over time. At the electricity production level, within the scenario-defined technologies (e.g., 240 photovoltaic panels), sub-technologies compete to supply electricity based on market shares associated with probability 241 distributions. Each technology is also associated with probability distributions regarding material use. Efficiency and material 242 use boundary values usually change over time as well. In the case of photovoltaic panels, the module efficiency determines 243 the panel surface needed to reach the reference power output.

#### 244 *2.2.3. Life cycle impact assessment (LCIA)*

 We select eight key environmental impact categories to evaluate the environmental sustainability of the energy system scenario. These categories are chosen to capture the multidimensional aspects of environmental sustainability in the context of the energy-material nexus. We assess (1) climate change impacts, using the global warming potential (GWP) over a 100-year time horizon (Andreasi Bassi et al., 2023); (2) particulate matter formation potential, linked to human health impacts (Huijbregts et al.,

 2017); (3) acidification, to evaluate the impact of acidifying substances deposit (EPLCA, 2022); (4) freshwater ecotoxicity, evaluating emissions harmful to freshwater ecosystems (Huijbregts et al., 2017); (5) land use, quantifying total land area (all types) occupied over time; and, (6) net fresh water use, defined as the difference between freshwater abstraction and release. We also evaluate mineral resource depletion using (7) crustal scarcity, a scarcity-weighted minerals demand indicator that uses crustal concentrations as a proxy for long-term global elemental scarcity (Arvidsson et al., 2020); and (8) abiotic resource depletion for elements, where present production and reserves of individual elements are combined to measure the scarcity of the resources (van Oers et al., 2020). Finally, we report the physical annual demand for 64 metals classified as critical based on assessmentsfrom major international reports (Grohol & Veeh, 2023; Moreira & Laing, 2022) and scientific literature (Schlichenmaier & Naegler, 2022).

#### *2.2.4. Interpretation and global sensitivity analysis (GSA)*

 GSA assesses the contribution of each input parameter to the total variability in the model outputs. This method helps us understand how distinct sources of uncertainty can affect the various environmental and resource indicators, including metal demands. Our analysis specifically targets parameters related to material and metal requirements, technological advancements, and the market penetration of energy-related sub-technologies, as explained in earlier section 2.2.3. Other sources of uncertainty are deliberately excluded. For example, we do not consider uncertainty data included in the process inventories of the ecoinvent LCA database. We also omit uncertainty pertaining to the STEM scenario results.

 Uncertainty distributions are applied to three key areas: 1) 500 inventory exchanges related to the use of material resources within technologies, 2) 103 inventory exchanges reflecting variations in the lifespan, use, and efficiency of energy technologies, and 3) 36 inventory exchanges representing sub- technology market shares. These distributions are based on various model parameters detailed in the Supplementary Information (SI1, S1-5). All other exchange values in the LCA database are constant over time or modified according to the *Net Zero* scenario. The uncertainties are then propagated 276 through Monte Carlo simulations. We report the  $5<sup>th</sup>$ , 50<sup>th,</sup> and 95<sup>th</sup> percentile values of the resulting Monte Carlo distribution for each environmental and material indicator described in section 2.2.3.

 To identify which inputs have the most significant impact on the output distribution, we use the delta moment-independent method (DMIM). Originally introduced by (Borgonovo, 2007), this method is independent of the sampling generation technique (Plischke et al., 2013) and has been previously applied in LCA contexts (Kim, Mutel, & Froemelt, 2022; Kim, Mutel, Froemelt, et al., 2022). Delta indices range from 0 to 1, where higher values indicate a stronger influence on the output distribution. To ensure the robustness of our results, we conducted preliminary tests to determine the optimal number of Monte Carlo iterations, ultimately setting the iteration count to 2,000 to achieve convergence.

286 It is important to emphasize that the variability in the distribution of results presented in the following sections arises solely from uncertainties within the supply chain of technologies relevant to the demand for CRMs. The scenarios generated by STEM are exploratory in nature and thus inherently uncertain. Multiple technological pathways and strategies can achieve net-zero greenhouse gas (GHG) emissions, and the scenario used here represents just one possible approach, minimizing system costs based on a specific set of deterministic model input parameters. As a result, major sources of  uncertainty that could significantly impact GHG emissions and other environmental indicators are not accounted for in this analysis, to highlight the uncertainty that arises from CRM-demanding technologies.

## 3. Results

 The shift to a low-carbon energy system in Switzerland brings a marked increase in the demand for CRMs, driven largely by the adoption of electric vehicles (EVs) and renewable energy storage. For instance, as illustrated in Figure 3, the shift to EVs and large-scale battery storage, central to this transition, drives a substantial increase in lithium demand. The median annual lithium demand rises from 250 tons in 2020 to 2,000 tons by 2050. While the total demand continues to grow, the rate of increase slows over time due to expected improvements in battery energy density and material efficiency, which mitigate the need for even larger material inputs. These assumptions are built into the probability distributions applied to material intensities and technological advancements (SI1, S2- S5). This growth, however, is subject to considerable uncertainty, with estimates ranging from 800 to over 3,000 tons in 2050.

 This uncertainty is partly driven by potential shifts in market shares among battery chemistries, such as sodium-ion batteries, which do not require lithium. The exact trajectory of these shifts will depend on a range of factors, including technological advancements, cost reductions, and policy incentives, all of which influence the adoption rates of competing battery technologies. In our model, the projected shares of different battery chemistries are determined using probability distributions that reflect anticipated intervals for market shares (SI1, S1). The pink error bars in Figure 3, which represent uncertainties exclusively from projected market shares, show a variance for lithium demand in 2050 of -46% to +37%. However, the black error bars, representing the full uncertainty range, show a broader variance of -54% to +77%. This highlights that market share uncertainty alone does not account for the full variance in lithium demand. Other factors, such as material intensity and future technological advancements, also play critical roles in shaping these projections. As highlighted by the GSA (Figure 5 and SI1-S6), described in section 2.2.4, the electricity storage capacity of future batteries is identified as the main parameter influencing this variance.

 Similar dynamics are observed in other key metals for batteries, such as cobalt and vanadium, highlighting the complex balance between resource availability and technological development. Median vanadium demand, for example, is projected to rise sharply from 0.9 tons in 2020 to approximately 156 tons by 2050, with a wide range of uncertainty extending from 35 tons to 289 tons. This corresponds to a variance from the 2050 median demand of -77% to +85%, when accounting for all uncertainties. The adoption of low-lithium alternatives, such as vanadium redox-flow batteries for stationary energy storage, could reduce dependence on lithium but would simultaneously increase demand for vanadium. Beyond battery applications, vanadium plays an important role in producing high-strength steel alloys, which in our model are used in wind turbines, further contributing to increased vanadium demand. This illustrates how efforts to minimize reliance on one critical material may inadvertently increase dependency on another, underscoring the need for quantifying such consequences and a balanced approach to material management in the energy transition.

 In parallel with these shifts, the phase-out of internal combustion engines (ICEs) significantly affects the demand for PGMs, such as platinum and palladium. As the automotive industry transitions to battery electric vehicles (BEVs) and hydrogen-based technologies, the demand for platinum— commonly used in catalytic converters—declines, reaching approximately 540kg by 2040, only 30% of its 2020 demand. By 2050, platinum demand partially recovers to around 700kg, accounting for 42% of its 2020 level: despite advancements in catalyst efficiency, its use in electrolyzers becomes increasingly important. This underscores the complex interplay between declining uses and new emerging needs. This trend is also reflected in the surging demand for iridium – crucial for fuel cells and electrolyzers – which rises from negligible levels in 2020 to about 80kg by 2050. Similarly, silver, though not currently classified as CRM by entities such as the European Union, experiences a fourfold demand increase from 17 tons to 66 tons by 2050, largely due to its role in electrolyzers and PV panels.

 PV technologies further exemplify the link between technology choices and material demand. Gallium, a key component in certain PV sub-technologies such as copper indium gallium selenide (CIGS) and gallium arsenide (GaAs) solar cells, experiences a marked increase in demand, particularly from 2030 to 2050, as PV deployment accelerates. According to Figure 3, gallium demand could rise from 2.5 tons in 2020 to a median of nearly 40 tons by 2050. The variance in demand, ranging from as low as 20 tons to more than 50 tons, is largely driven by shifts in the market share of PV sub-technologies. At the lower end, increased deployment of cadmium telluride (CdTe) cells, which do not use gallium, drives demand down; while at the higher end, the widespread adoption of CIGS and GaAs significantly raises gallium demand. Crystalline silicon (c-Si) technologies also contribute to the gallium demand, although to a lesser extent than CIGS and GaAs. This underscores how the selection of specific PV sub- technologies may heavily influence the demand for certain CRMs, emphasizing the need for strategic decisions to ensure material availability for the successful upscaling of solar energy.

 Wind energy also illustrates the impact of different low-carbon electricity production technologies on CRMs demand. Wind turbines deployment significantly impacts the demand for rare earth elements like neodymium, dysprosium, and praseodymium. Neodymium, crucial for producing permanent magnets used in wind turbine generators, experiences a more than 300% increase in demand as wind energy capacity expands, rising from 5 tons in 2020 to an estimated 17 tons by 2050. The variance in neodymium demand is influenced by the material intensity of different wind turbine designs and the choice between direct-drive versus gearbox turbines, with the former requiring significantly more rare earth elements. According to our GSA (Figure 5 and SI1-S6), neodymium oxide requirements in onshore gearbox wind turbines, driven by their greater market share, emerge as our model's most influential uncertain parameter for neodymium extraction, which shows a variance of -26% to +28% by 2050.

 Finally, the mining sector presents a unique case of interconnectedness within the material-energy nexus. Sulfur, predominantly used in our model in upstream activities as sulfuric acid in refining various materials, more than doubles from 30 kton in 2020 to 70 kton by 2050. This increase reflects the rising need for refined metals to support the energy transition. Although sulfur is not scarce and does not currently face significant supply risks, it holds great economic importance, and its price has shown considerable volatility in recent decades (Blengini et al., 2020). Sulfur's supply is intricately 371 linked to the fossil fuel industry, as it is often produced as a byproduct of natural gas and petroleum refining, with few discretionary sources available (ecoinvent, 2023; Wagenfeld et al., 2019). Conversely, the demand for barium (SI1-S6, Fig. 8), mainly used in oil and gas drilling (ecoinvent, 2023;  USGS, 2023), is projected to decrease substantially, reaching only 14% of its initial demand, as a consequence of shifting away from fossil fuels. The interconnectedness between sulfur supply and fossil fuel production highlights potential resource availability and supply challenges as energy systems evolve. This aligns with the insights in (Månberger, 2021), which discusses the trade-offs associated with reduced fossil fuel use and its impact on the supply of critical resources, highlighting the importance of developing integrated models to anticipate potential barriers and ensure an effective transition to a sustainable energy future.

 As we shift focus to the overall environmental impacts, the analysis reveals a significant reduction in global warming potential for Switzerland's energy system, with life-cycle GHG emissions dropping from approximately 40 megatons in 2020 to 4 megatons per year by 2050, as illustrated in Figure 4. This reduction reflects the goal of domestic net-zero emissions, while the remaining 4 megatons represent GHG emissions occurring abroad. In 2020, the percentage change between the median and the 5th and 95th percentiles is within ±0.5%. By 2050, as varying parameters become more relevant, 387 this range expands to ±10%. The GSA identifies electricity storage capacity in electric vehicles as the most influential parameter driving uncertainty for this impact category.

 This reduction is associated with co-benefits such as decreased particulate matter formation and acidification. However, trade-offs emerge in other environmental categories, such as a rise in freshwater ecotoxicity by 40% (±9%). The same driver of variability —electricity storage capacity— plays a significant role in these categories, further highlighting its importance in shaping environmental outcomes in our model. Additionally, the analysis reveals increased land use impacts, measured as the total area occupied over time to meet the final energy demand of the system. This increase is primarily driven by the deployment of bioenergy with carbon capture and storage, which results in a growing need for managed forest land. However, uncertainties around land use impacts remain limited (±2%), since we only consider uncertainties mainly affecting metals and materials consumption rather than land-use management or shifts in afforestation rates.

 Resource depletion indicators are most influenced by the uncertainties considered in our analysis. The crustal scarcity indicator, a proxy for long-term global elemental scarcity based on crustal concentrations, decreases from 5 gigatons of silicon-equivalent in 2020 to 4.7 gigatons (±16) by 2050. This indicator, which heavily weighs the scarcity of PGMs, declines as demand for platinum and palladium in internal combustion engines and exhaust systems phases out. In contrast, the abiotic depletion indicator for elements, which focuses on minerals and metals and excludes fossil fuel resources, shows a significant increase from 255 to 601 (-17%, +20%) tons of antimony-equivalent between 2020 and 2050, underscoring the substantial impact of uncertainties surrounding material demand.



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410 **Figure 3.** Annual life-cycle material demand per final energy consumer category for Switzerland's *Net Zero* scenario. Pink 411 error bars indicate the range between the 5th and 95th percentiles, considering only variations in projected technology<br>412 market shares, with red dots marking the median (i.e., 50<sup>th</sup> percentile). Black error bars s market shares, with red dots marking the median (i.e., 50<sup>th</sup> percentile). Black error bars show the range between the 5<sup>th</sup> and<br>413 and 55<sup>th</sup> percentiles when all sources of uncertainty are considered, with black dots r 95<sup>th</sup> percentiles when all sources of uncertainty are considered, with black dots representing the median. Note that median<br>414 marks from both distributions do not necessarily align. Detailed results for 64 elements are 414 marks from both distributions do not necessarily align. Detailed results for 64 elements are available in the Supplementary<br>415 Information (SI2, S6). Pie charts show the contribution shares of the final energy process 115 Information (SI2, S6). Pie charts show the contribution shares of the final energy processes and sectors, respectively, to the 416 total demand for each material. Individual processes contributing less than 5% are aggr total demand for each material. Individual processes contributing less than 5% are aggregated under "Other".



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418 **Figure 4.** Annual environmental life cycle impacts per final energy consumer category for Switzerland's *Net Zero* scenario. 419 Pink error bars indicate the range between the 5th and 95th percentiles, considering only variations in projected technology 420 market shares, with red dots marking the median (i.e., 50<sup>th</sup> percentile). Black error b 420 market shares, with red dots marking the median (i.e., 50<sup>th</sup> percentile). Black error bars show the range between the 5<sup>th</sup> and<br>421 95<sup>th</sup> percentiles when all sources of uncertainty are considered, with black dots r 95<sup>th</sup> percentiles when all sources of uncertainty are considered, with black dots representing the median. Note that median<br>922 marks from both distributions do not necessarily align. Impact categories include (1) global 422 marks from both distributions do not necessarily align. Impact categories include (1) global warming potential, measured in<br>423 megatons of CO<sub>2</sub> equivalent; (2) particulate measure formation, in kilotons of PM<sub>2.5</sub> e 423 megatons of CO<sub>2</sub> equivalent; (2) particulate measure formation, in kilotons of PM<sub>2.5</sub> equivalent; (3) acidification, in million 424 mol H<sup>+</sup> equivalent; (4) ecotoxicity, in billion comparative toxic units; (5) land mol H+ equivalent; (4) ecotoxicity, in billion comparative toxic units; (5) land use, in square kilometer-year; (6) water use –<br>425 comprises the abstraction of freshwater – in cubic kilometers: (7) crustal scarcity, in gi 425 comprises the abstraction of freshwater – in cubic kilometers; (7) crustal scarcity, in gigatons of silicon equivalent; and (8)  $\overline{426}$  abiotic depletion, in tons of antimony equivalents. abiotic depletion, in tons of antimony equivalents.

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# 4. Discussion

#### **4.1.Key findings and implications**

 The findings of this study underscore the critical importance of adopting a holistic perspective when designing and implementing energy transition policies. Firstly, life-cycle impacts must be considered to ensure that transition scenarios effectively reduce environmental burdens. While decarbonization efforts focus on reducing GHG emissions, our results highlight the necessity of considering a broader array of environmental impacts, such as particulate matter formation, water use, and resource depletion, to evaluate the co-benefits and trade-offs associated with reducing climate impacts and the general feasibility of transition pathways.

 Secondly, the comprehensive evaluation of sub-technologies and material intensities within the energy-material nexus is crucial. Neglecting to account for the full spectrum of sub-technologies and material requirements could lead to unforeseen bottlenecks or hidden impacts, potentially compromising the feasibility and effectiveness of energy transition scenarios. While ESMs and IAMs project broad technology deployments, such as total PV or wind capacities, they often overlook the detailed differences in material needs and effects on different impact categories that LCA can provide. This level of detail is valuable, as our study suggests that while the specific selection of sub- technologies might not significantly impact the achievement of decarbonization targets, it substantially affects other environmental impacts and CRM demand.

 Furthermore, the GSA results highlight the factors in our model driving uncertainty in both material and environmental impacts, offering a valuable understanding for future research and mitigation efforts. As shown in Figure 5, electricity storage capacity in electric vehicles emerges in the evaluated Swiss scenario as the dominant factor affecting several environmental categories, including global warming potential, particulate matter formation, acidification and demand for CRMs. This reflects the strong influence that battery technologies have on shaping environmental outcomes. The impact of other specific products and processes is limited to single material demands, but in some cases even more pronounced: iridium demand is driven by its use in PEM electrolyzers, platinum demand by its use in ICEVs, and neodymium demand by its use in wind turbines. By revealing these critical sensitivities, the GSA pinpoints areas where technological advancements or material substitutions could have the greatest impact in reducing uncertainties and optimizing system sustainability. Ultimately, Figure 5 serves as a guide for identifying which parameters deserve the most attention and development to ensure the robustness of future energy transition strategies.



 **Figure 5.** Heatmap of Delta values from a moment-independent global sensitivity analysis, highlighting the most influential uncertain parameters across key life cycle environmental impact categories. Rows represent the parameters, and columns 465 represent the impact categories. For each category, only parameters with a normalized Delta value above 90% are shown,<br>466 and the exact Delta values are annotated within each cell. and the exact Delta values are annotated within each cell.

#### **4.2.Limitations and outlook**

 While this study provides valuable insights into the material-energy nexus, several limitations must be acknowledged. One such limitation concerns recycling rates and mining practices. The analysis assumes that current practices in material extraction and recycling will continue into the future, potentially overlooking advancements in these areas, and leading to an overestimation of material extraction and associated environmental burdens. Future work should incorporate scenarios that account for technological improvements in recycling and more sustainable mining practices, which could reduce the material demand and associated environmental impacts. However, as material demand exhibits substantial growth rates, recycling will in any case only provide limited shares of material demand and thus we consider this limitation in our work of minor importance.

 Additionally, the study lacks detailed regionalization of environmental impacts, particularly important for categories such as water use, biodiversity, and particulate matter formation—areas relevant to the mining sector (Cabernard & Pfister, 2022; Northey et al., 2018). For instance, water requirements previously driven by cooling in combustion-based processes may shift to mining regions to support mineral extraction for renewable technologies; while particulate matter pollution —formerly concentrated in urban areas from combustion vehicles— is expected to increasingly affect mining zones as electric vehicle production scales up (Hahn Menacho et al., 2024). Enhancing the spatial resolution of these impacts would provide a more accurate assessment of the environmental

 consequences of materials extraction and processing, allowing for more targeted and effective policy interventions.

 Finally, there is an opportunity to improve the granularity of material assessments in energy transition scenarios by integrating LCA with Material Flow Analysis (MFA). Currently, the demand for materials is linearized, i.e., evenly distributed over the entire lifetime of each infrastructure component, due to 490 the nature of LCA, smoothing out peaks and troughs. Although this approach preserves cumulative material demand, it does not accurately reflect the temporal dynamics caused by installation, operation, and decommissioning phases – information usually provided by ESMs and IAMs. For instance, demand for tungsten, primarily used in our model in nuclear energy as tungsten carbide, decreases gradually over time (SI1, S6-Figure 8). However, with no new nuclear power plants projected and the planned decommissioning of existing ones, tungsten demand is expected to drop sharply, rather than taper off gradually. Similarly, for emerging technologies like PV, the bulk of material demand occurs during installation, rather than being evenly distributed across the technology's operational lifetime. By coupling MFA and LCA, future studies could offer a more dynamic and detailed understanding of material flows, better capturing the complexities of the energy transition and its resource implications (Barkhausen et al., 2023).

 Furthermore, the study highlights the need for improved indicators to assess resource depletion in the context of prospective LCA. The crustal scarcity indicator, for example, very much emphasizes the scarcity of PGMs, which could be misleading when interpreting the overall resource demand as this indicator suggests a decreasing need for scarce materials in our case study. Similarly, the abiotic resource depletion indicator may not fully align with the goals of prospective LCA, since it relies on current production and reserve data to project future resource availability. To address these shortcomings, future research should explore the integration of emerging criticality indicators, such as SPOTTER (Berr et al., 2022) or GeoPolRisk (Santillán-Saldivar et al., 2021), into the prospective LCA framework. These indicators could provide more accurate insights into the potential risks and vulnerabilities associated with CRM supply chains, supporting more informed decision-making in the energy transition.

 Future research should focus on validating these findings through alternative scenarios and enhancing the integration of LCA with MFA. Alternative scenarios could reach the net-zero goal in other ways, for example, by employing more carbon dioxide removal or more low-carbon synthetic fuels instead of direct electrification. Extending the scenario space will allow for a more dynamic and nuanced understanding of material demands over time. Developing more robust resource depletion indicators, particularly those incorporating geopolitical risks, will also be crucial in assessing long-term resource supply.

# 5. Conclusion

 This study assesses Switzerland's material-energy nexus within a net-zero transition scenario, focusing on life-cycle environmental impacts and CRMs demand. By systematically combining LCA with ESM, we address key gaps in understanding how emerging energy technologies and sub-technology choices will shape future resource demand and environmental outcomes. Through this framework, we estimated Switzerland's future CRM demand, revealing substantial increases in materials like lithium  and vanadium, driven by EV and battery storage adoption, and highlighted the sensitivity of these projections to shifts in technology market shares and material intensities. Additionally, we identified drivers of uncertainty through global sensitivity analysis, such as electricity storage capacity in EVs, which significantly influences both material demand and environmental impacts. Furthermore, we developed an adaptable and reproducible workflow that allows for scenario-specific life-cycle impact assessments, which can be extended to different national context, providing a versatile tool for global

energy analyses that consider a broad range of environmental impacts and material demand.

 Several novel findings emerge from this analysis, particularly concerning the sensitivity of CRM demand to sub-technology selection within energy systems – a level of granularity often overlooked in ESMs and IAMs. Our study demonstrates that while specific choices, like battery chemistry or PV sub-technology, do not substantially affect decarbonization targets, they have a significant influence on CRM demand profiles and other environmental impact categories, underscoring the importance of these variables in planning for a sustainable energy future. Additionally, the detailed examination of co-benefits and trade-offs across environmental impact categories, such as particulate matter formation and freshwater use, provides actionable insights beyond conventional GHG-focused transition analyses.

 The Swiss case study offers valuable insights for other countries, particularly those that need to scale up renewable energy installations and electrify their energy systems. Such countries, especially those lacking significant hydropower capacity, may face even greater material demand increases and environmental trade-offs as they deploy more photovoltaic and wind power installations along with additional stationary battery storage. At the same time, they stand to benefit from more substantial environmental co-benefits than Switzerland. Diversifying technology options emerges as a key strategy to reduce dependency on specific CRMs, alleviate supply chain pressures, and enhance the resilience of energy systems.

 In conclusion, a holistic approach to energy transition planning is essential. This study's integrated workflow offers stakeholders a robust tool to assess both decarbonization goals and CRM needs, ensuring that the transition to low-carbon energy systems not only achieves emissions reductions but also considers long-term resource sustainability. These insights serve as a reference for policymakers and researchers aiming to navigate the complex landscape of energy transitions, with an emphasis on data-driven, resource-conscious planning.

# Glossary

**•** CRM: Critical Raw Material **· ESM: Energy System Model · GHG: GreenHouse Gas · GSA: Global Sensitivity Analysis · IAM: Integrated Assessment Model · LCA: Life Cycle Assessment · PGM: Platinum Group Metals •** STEM: Swiss TIMES Energy Model **· TIMES: The Integrated MARKAL-EFOM System** 

# Acknowledgements

 The authors thank Prof. Claudia R. Binder and Dr. Nino J. D. Jordan for the review work and time provided.

## Authors contributions

Conceptualization, A.J.H.M.; methodology, A.J.H.M., and R.S.; formal analysis, A.J.H.M.; software,

- A.J.H.M., and R.S.; validation, A.J.H.M., and R.S.; visualization, A.J.H.M; writing original draft,
- A.J.H.M; writing review and editing, C.B., E.P., P.B., R.M., and R.S.; funding acquisition, C.B. and P.B.

### Funding sources

 The authors gratefully acknowledge the financial support from the Swiss Federal Office of Energy (SFOE) via the SWEET program for the consortium SURE for developing the *premise* and *pathways* tools and thereby coupling the STEM model with the LCA framework. Additional funding is provided by the Swiss State Secretariat for Education, Research and Innovation (SERI) under the Horizon Europe project PRISMA (grant agreement no. 101081604) for supporting the work carried out in relation to the representation of material and metal consumption in net-zero scenarios. Christian Bauer is part of SPEED2ZERO, a Joint initiative co-financed by the ETH Board. We acknowledge the corresponding financial support.

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