Methodology development for upscaling in prospective LCA: The case of perovskite solar cells as emerging functional material-based energy technology

Entwicklung einer Methodik für das Upscaling in der prospektiven Ökobilanz am Beispiel von Perowskit-Solarzellen als neuartige Energietechnologie auf der Basis von Funktionsmaterialien

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Abstract

This cumulative dissertation developed a novel upscaling methodology for prospective life cycle assessment (LCA) to project environmental performances of emerging technologies from a current to future development stage using perovskite solar cells (PSC) as a case study for an emerging functional material (FunMat)-based energy technology. Beyond the case study, upscaling in LCA is essential to assist research groups, technology developers, planners, and policymakers prioritize responsible research activities proactively and prevent unintended consequences early in innovations.

This methodology development was carried out in three publications and consisted of four steps: First, a **meta-analysis** was conducted to understand and define the upscaling challenges in LCAs of PSC and further emerging photovoltaic technologies (PVs) (Publication 1). Second, an **upscaling scheme called UpFunMatLCA** was developed for generating upscaling scenarios in prospective LCA. The upscaling scenarios were modeled qualitatively and quantitatively using upscaling mechanisms and modules as predefined development pathways (Publication 2). Third, a **PSC-LCI-database** evolved from applying and validating UpFunMatLCA in the case study of evaluating the environmental sustainability of PSCs upscaled from lab samples to commercial deployment as PV modules. Last, the **environmental break-even time (e-BET)** was introduced as a novel indicator for interpreting when the upscaled PSC's environmental performance achieves benefits over current commercial benchmarks (Publication 3).

The results highlight that the PSC's environmental performance cannot be adequately demonstrated from previous LCA studies compared to other emerging PVs and commercial benchmarks. The PSC's high environmental impacts were attributed to high processing energies of inefficient laboratory (lab) equipment resulting from a low technology maturity. Upscaling scenarios provide a method to integrate technology development into prospective LCA by projecting potential development pathways. PSC's development pathways include combinations of the three technological mechanisms during upscaling: A) process learning, B) material learning, and C) external developments. Process learning is the key mechanism for upscaling processing energies from lab to fabrication in industrial manufacturing factories (fab) as the main contributor to energy-related impacts like global warming. Material-related impacts like resource use require including additional material learning in the assessment.

Upscaling in prospective LCA does not provide definitive environmental impacts but strives to generate realistic scenarios based on current knowledge to drive the future environmental sustainability of emerging technologies. **The developed methodology pioneers upscaling in prospective LCA by combining a specific technology group's theoretical and practical methods.** It represents, thus, an essential template for other technology groups to transfer similar upscaling methods for increasing and supporting the comprehensiveness of the LCA results on emerging technologies compared to commercial benchmarks.

Kurzfassung

In dieser kumulativen Dissertation wurde eine neuartige Methodik für das Upscaling in der prospektiven Ökobilanzierung (LCA) anhand eines Fallbeispiels entwickelt, um die Umweltverträglichkeit innovativer Technologien vom aktuellen auf ein zukünftiges Entwicklungsstadium abzuschätzen. Als Fallbeispiel wurden Perowskit-Solarzellen (PSC) als innovative Energietechnologie auf der Basis von Funktionsmaterialien (FunMat) untersucht. Das Upscaling in der Ökobilanz soll Forschungsgruppen, Technologieentwicklern, Planern und politischen Entscheidungsträgern dabei unterstützen, verantwortungsvolle Forschungsaktivitäten zu priorisieren und proaktiv voranzutreiben, um unbeabsichtigte Folgen bei Innovationen frühzeitig zu erkennen und zu vermeiden.

Die Methodenentwicklung erfolgte in drei Publikationen und anhand der vier folgenden Schritte: Erstens wurde eine Meta-Analyse durchgeführt, um die Herausforderungen des Upscalings von Ökobilanzen für PSC und weiterer innovativer Photovoltaik-Technologien zu verstehen und zu definieren (Publikation 1). Zweitens wurde ein Upscaling-Schema namens UpFunMatLCA entwickelt, um Upscaling-Szenarien für prospektive Ökobilanzen zu erstellen. Die Upscaling-Szenarien wurden qualitativ und quantitativ mittels sogenannter Upscaling-Mechanismen und -Module modelliert (Publikation 2). Drittens wurde für das Fallbeispiel eine Sachbilanz-Datenbank (PSC-LCI-Datenbank) entwickelt. Diese ermöglicht die Anwendung und Validierung von UpFunMatLCA zur Hochskalierung der Umweltverträglichkeit von PSCs von Laborsamples zum kommerziellen Einsatz als PV-Module. Zuletzt wurde die ökologische Break-Even-Zeit (e-BET) als neuer Indikator zur Interpretation von Ökobilanzergebnissen eingeführt. E-BET legt einen Schwellenwert fest, ab wann die Umweltleistung der innovativen Technologie, hier der PSCs, Vorteile gegenüber den derzeitigen kommerziellen Benchmarks erzielt (Publikation 3).

Die Ergebnisse zeigen, dass die Umweltleistung von PSC im Vergleich zu anderen innovativen PVs und kommerziellen Benchmarks nicht ausreichend durch bisherige LCA-Studien untersucht wurde. Die hohen Umweltauswirkungen der PSC wurden auf die hohe Verarbeitungsenergie ineffizienter Laborgeräte zurückgeführt, die aus einem geringen Technologiereifegrad der PSC resultiert. Upscaling-Szenarien bieten eine Methode zur Integration der Technologieentwicklung in prospektive LCA durch Projektion möglicher Entwicklungspfade. Die Entwicklungspfade von PSC umfassen Kombinationen der drei technologischen Mechanismen während des Upscalings: A) Prozesslernen, B) Materiallernen und C) externe Entwicklungen. Prozesslernen ist der Schlüsselmechanismus für die Hochskalierung von Verarbeitungsenergien vom Labor bis zur Fertigung in industriellen Produktionsfabriken (from lab to fab), die am meisten zu energiebezogenen Umweltauswirkungen wie der globalen Erwärmung beitragen. Materialbezogene Umweltauswirkungen wie die Ressourcennutzung erfordern die Einbeziehung von zusätzlichem Materiallernen in die Bewertung.

Das Upscaling in der prospektiven Ökobilanz liefert keine endgültigen Ergebnisse, sondern zielt darauf ab, realistische Szenarien auf der Grundlage des aktuellen Wissensstandes zu erstellen, um die künftige Umweltverträglichkeit innovativer Technologien zu fördern. Die entwickelte Methodik leistet Pionierarbeit beim Upscaling in der prospektiven Ökobilanzierung, indem sie die theoretischen und praktischen Methoden einer bestimmten Technologiegruppe kombiniert. Sie stellt somit eine wesentliche Vorlage für andere Technologiegruppen dar, um ähnliche Methoden zur Verbesserung und Unterstützung der Ökobilanzergebnisse neuer Technologien im Vergleich zu kommerziellen Benchmarks abzuleiten.

Publications

I) Weyand S, Wittich C, Schebek L. (2019): Environmental Performance of Emerging Photovoltaic Technologies: Assessment of the Status Quo and Future Prospects Based on a Meta-Analysis of Life-Cycle Assessment Studies. Energies; 12(22): 4228, DOI: 10.3390/en12224228.

II) Weyand S, Kawajiri, K., Mortan, C., Schebek L. (2023): Scheme for Generating Upscaling Scenarios of Emerging Functional Materials Based Energy Technologies in Prospective LCA (UpFunMatLCA). Journal of Industrial Ecology, DOI: 10.1111/jiec.13394.

III) Weyand S, Kawajiri, K., Mortan, C., Zeller, V., Schebek L. (2023): Are perovskite solar cells an environmentally sustainable emerging energy technology? Upscaling from lab to fab in life cycle assessment. ACS Sustainable Chemistry & Engineering, DOI: 10.1021/acssuschemeng.3c03019.

IV) Glogic, E., Weyand, S., Tsang, M. P., Young, S. B., Schebek, L., Sonnemann, G. (2019): Life cycle assessment of organic photovoltaic charger use in Europe: the role of product use intensity and irradiation. Journal of Cleaner Production 233, 1088-1096, DOI: 10.1016/j.jclepro.2019.06.155.

Contents

List of Abbreviations

ABL	Absorber layer
ACT	Active layer (also referred to as ABL)
ADP-fossil	Abiotic resource depletion – fossil fuels (see also RDPf)
ADPm	Abiotic resource depletion ultimate reserves (see also RDPm)
ALCA	Attributional LCA
a-Si	Amorphous silicon
BE	back electrode
BOS	Balance-of-system
CdTe	Cadmium-telluride solar cells
CED	Cumulative energy demand
CIGS	Copper-indium-gallium-diselenide solar cells
CLCA	Consequential LCA
CO_2	Carbon dioxide
DSC	Dye-sensitized solar cells
e-BET	Environmental break-even time
EBL	Electron blocking layer (also referred to as ETL)
ETL	Electron transport layer
ETPf	Ecotoxicity potential for freshwater
Fab	fabricated in industrial manufacturing factories
FunMat	functional material
GHG	Greenhouse gas
GWP	Global warming potential
HTL	Hole transport layer
HTPc	Human toxicity, cancer effects
I	Irradiation
KEYAs	key modeling assumptions
KEYIs	key indicators
KEYPs	key performance parameters
Lab	manufactured in laboratory surroundings
LCA	Life cycle assessment
LCI	Life cycle inventory
LCIA	Life cycle impact assessment
mono-Si	Monocrystalline silicon
MPL	Market penetration level
MRL	Manufacturing readiness level
multi-Si	Multicrystalline silicon

NREL	National Renewable Energy Laboratory
OPV	Organic Photovoltaics
PCE	Power conversion efficiency
PR	Performance ratio
PSC	Perovskite solar cell
PV	Photovoltaic technology
QDPV	Quantum-dot photovoltaic
RDPf	Resource use, fossils; abiotic resource depletion – fossil fuels (see also RDPf)
RDPm	Resource use, minerals and metals; abiotic resource depletion ultimate reserves
SDG	Sustainable Development Goal
SFE	Substrate with front electrode
STC	Standard test conditions
TRL	Technology readiness level
UNDP	United Nations Development Programme
UpFunMatLCA	Scheme for generating upscaling scenarios in prospective LCA
Wp	Watt-peak

1 Introduction

Access to energy is an essential driver for sustainable development. It promotes economic growth and social progress. Ensuring access to a sustainable - affordable, reliable, and environmentally friendly - energy supply for the world population and future generations is one of the 17 United Nations' Sustainable Development Goals (SDG) (United Nations 2015). Today, the energy sector still requires large amounts of fossil raw materials and is responsible for around 70-75% of global and European greenhouse gas (GHG) emissions (Gütschow & Pflüger 2022). Renewable energy technologies like wind and solar are a cornerstone of transitioning to a climate-neutral circular economy (European Commission 2019). Their performance depends highly on functional materials (FunMat) (Kuznetsov & Edwards 2010, Schebek et al. 2019). FunMats often are based on specific elements, notably metals, such as rare earths, in wind turbine permanent magnets or semiconductors in photovoltaic technologies (Kuznetsov & Edwards 2010, Schebek et al. 2019). They possess a distinct electronic structure and physical-chemical properties responding to electrical, magnetic, optical, or chemical influences (Chung 2021). However, while FunMats enable a climate-neutral energy conversion in the use phase, their manufacturing requires a high amount of energy. Above this, many of the specific elements yielding the desired material properties are so-called critical elements, for which supply risks are feared for economic and geopolitical reasons. Therefore, research continuously targets the development of even more energy- and material-efficient FunMat-based energy technologies built on abundant and non-critical raw materials.

For the earliest orientation on energy and material efficiency and mitigation of environmental impacts, sustainability assessment is more and more integrated into technology development. Specifically, the life cycle assessment (LCA), standardized in the ISO 14040/14044 (ISO 14040 2006, ISO 14044 2006), is a supportive methodology that introduces a system-wide understanding of supply chains, life cycles, and resulting impacts, such as global warming and resource use, into developing emerging technologies (Villares et al. 2017). LCA enables the evaluation of a full range of environmental impacts to identify opportunities for improving environmental performance. However, LCA was initially developed for commercial products and technologies. For commercial energy technologies, the life cycle stages in terms of the product system and benefits per functional unit are already known and necessary primary data for the life cycle inventory (LCI) is available. Furthermore, many studies reported the environmental impacts and discussed implications (Dolan & Heath 2012, Hsu et al. 2012, Kim et al. 2012). However, this knowledge is missing for emerging technologies, currently developed as ideas or concepts, manufactured in laboratories (lab) or pilot plants (Cucurachi et al. 2018). Therefore, performing LCA is challenging for emerging technologies to evaluate environmental impacts, leading to contentious findings due to different methodological procedures and factual assumptions.

This challenge is not new and known as the Collingridge Dilemma in literature. As illustrated in Figure 1.1, the problem is “when the change is easy” due to high design freedom, “the need for it cannot be foreseen” as the knowledge is too low; when the technology is matured and “the need for change is apparent, change has become [. . .] difficult” due to low design freedom (Collingridge 1980). However, this challenge is topical and acknowledged in the LCA community under the terms ex ante and prospective LCA. This terminology distinguishes traditional ex-post or conventional LCAs, which assess mature commercial technologies at a current development stage (status quo) with real-world data, and prospective or ex-ante LCAs. However, the terms ex-ante and prospective are used inconsistently in the literature.

First, ex-ante and prospective LCA was used in a similar way, modeling and assessing an

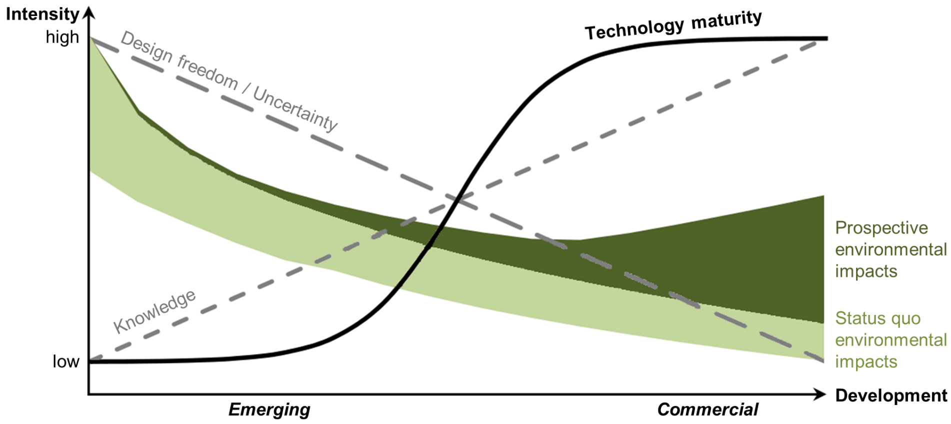

Figure 1.1: Illustration of the knowledge level versus design freedom during technology development from emerging to commercial technology. In addition, the progress of the environmental impacts is illustrated for two cases. Case 1: Status quo impacts (light green): The range of potential environmental impacts narrows as knowledge increases and uncertainty decreases. Case 2: Ex-ante or prospective impacts (ligtht +dark green): The range remains broad and uncertain at the commercial development stage when considering data from an emerging development stage (composed diagram derived from Arvidsson et al. (2017), Hübschmann et al. (2009), Villares et al. (2017)

emerging technology at a higher development stage aiming to guide technology development sustainably (Arvidsson et al. 2017, Cucurachi et al. 2018). The difference was that ex-ante LCAs focus on the assessment before market introduction (van der Giesen et al. 2020), whereas “an LCA is prospective when the (emerging) technology studied is in an early phase of development (. . .), but (. . .) is modeled at a future, more-developed phase” using the definition of Arvidsson et al. (2017). Consequently, prospective LCA is not limited to the pre-market phase (van der Giesen et al. 2020). Then, Arvidsson (2023) updated the definition recently to “an LCA is prospective when the technology is modeled at a future” and generalized it to such an extent that it is no longer exclusively related to emerging technologies. Nonetheless, this thesis uses the term prospective LCA as a synonym for LCA of emerging technologies instead of ex-ante LCA, as prospective LCA also covers trends after a market introduction, including future developments of commercial technologies, and it is still commonly used in the LCA community.

1.1 Problem definition

Returning to the Collingridge dilemma, early awareness of environmental impacts is essential in addressing and avoiding them in technology development before commercialization. As shown in Figure 1.1, the range of potential environmental impacts of the status quo narrows as knowledge increases and uncertainty decreases (light green). However, rectifying environmental impacts becomes difficult once the technology is on the market. In addition, the range of prospective environmental impacts remains broad and uncertain at the commercial development stage when using data from an emerging development stage in LCAs (dark green). Therefore, improving the ability to anticipate, detect recurring trends, and take proactive measures, even when knowledge is scarce, is crucial.

The ability to anticipate from current emerging to prospective commercial development stages is described as upscaling. However, there is no clear definition of upscaling in the literature on prospective LCA (Bergerson et al. 2020). The terms "upscaling" or "scale-up" originally came from another discipline. In chemical engineering, the terms meant a size scaling, an increase of physical dimensions of process from the laboratory (lab) to the fabrication in industrial manufacturing factories (fab) at a commercial scale, using scaling relationships (Sotudeh-Gharebagh & Chaouki 2022). In the first LCA context, upscaling was used similarly, focusing solely on the size scaling of the physical dimensions of facilities or equipment (Schebek L. et al. 2012, Viebahn et al. 2008) and was implemented using scaling factors (Caduff et al. 2011, Kawajiri et al. 2020).

Nowadays, a recent review defined upscaling for prospective LCA "as a transforming function applied to a studied system or a study boundary, and taking it from one state to another" and subsumed size scaling, industrialization, massification, technology diffusion, up- and down-zooming and down-limiting under upscaling (Riondet et al. 2022). Another review only defines the term upscaling methods as the "procedure that projects how (...) [an emerging] technology currently available (...) may look and function at a higher [technology scale]" (Tsoy et al. 2020). In addition, it presents a three-step upscaling framework as a recommendation for estimating prospective data. Other frameworks recommend how to model technology development in prospective LCAs but don't use the term upscaling (Thonemann & Schulte 2019, van der Hulst et al. 2020). These reviews and frameworks help structure prospective LCAs regarding upscaling. However, they have conflicting definitions and are too general for providing guidance on concrete case studies, e.g., for the particular application for FunMats. Consequently, there is still a gap regarding a clear upscaling definition and practicable upscaling methodology in prospective LCA case studies.

1.2 Overall research goal

This thesis aims to develop a **structured methodology to clearly, transparently, and comprehensively implement a case study's upscaling into prospective LCA**. The novel methods strive to evaluate and harmonize the environmental performance from an emerging to a projected commercial technology scale for comparison with commercial benchmarks. The methodology is developed with a specific focus on FunMat-based energy technologies, using a concrete case study of FunMat development.

In this context, the prospective LCA attempts to shed light on emerging technologies before market introduction to guide environmental-friendly technology development benefitting from high design freedoms and early signaling of unintended consequences.

As aforementioned, there is no clear definition of the term upscaling. Therefore, **upscaling is defined in this thesis as transferring the functionality and characterization of an emerging technology to a possible target stage, considering development pathways from a current stage within the course of research and development to this future stage.** The upscaling focuses on the **manufacturing phase as this is where the specific processes of technology development take place**. The use- and end-of-life-phase are also essential but out of the scope of this thesis. However, methods used there, like user behavior (Glogic et al. 2019) or scenario techniques (Saavedra del Oso et al. 2023), can be combined with the intended methodology development of this thesis.

The environmental performance contains a set of various environmental impacts based on attributional modeling, meaning that the environmental impacts of the upscaled technology are attributed to the prospective function or functional unit when the technology enters the market. Consequently, the commercial benchmark is the technology delivering the same function as the upscaled technology. In contrast, consequential modeling would evaluate the potential implications of the decision to release the technology to the market and the substituted technology as commercial benchmark. However, the intended upscaling methodology will be compatible with the methods developed there (Glogic et al. 2019, Maes et al. 2023) as described in the discussion.

1.3 Case selection and description: Perovskite solar cells

For developing a novel upscaling methodology, a specific case of emerging FunMat-based energy technology is selected to deduce upscaling requirements and prove the novel methods. Three prerequisites are defined for selection: 1) The technology is still at an early stage of technology development. 2) The technology must show promise for future commercialization. 3) Direct cooperation with technology developers is desirable.

Perovskite solar cells (PSC) applied as photovoltaic (PV) modules are selected as they fulfill all three defined prerequisites. PSCs are currently the most promising emerging PV materials. This is notably evidenced by their outstanding evolution in power conversion efficiency (PCE) achieved in the lab from 3.8 % in 2009 (Kojima et al. 2009) to 25.8 % in 2023 (NREL 2023) and their possibility to form high-efficient (29.8 %) and low-cost PSC-silicon or PSC-PSC tandems (Li & Zhang 2020, Werner et al. 2018) but so far only on small-scale lab samples. Additionally, their novel thin-film material structure with simple bulk chemicals is expected to considerably reduce upstream environmental impacts and make the PSC a more climate-friendly and resource-efficient PV technology. Research on the PSC is being carried out at the Technical University of Darmstadt to make direct cooperation with technology developers feasible.

1.4 Structure of the thesis

This thesis is a cumulative dissertation based on three publications. It is divided into six chapters.
Chapter 1 so far has introduced the motivation and problem definition, presented the overall research goal of this thesis, and selected PSC as a case study for an emerging FunMat-based energy technology.

In Chapter 2, the meta-analysis of LCAs of emerging PVs compared with commercial benchmarks provides the state of the art for assessing PSC as an emerging FunMat-based energy technology in **Publication 1, Weyand et al. (2019)**, first published 6 November 2019: **Weyand S, Wittich C, Schebek L.: Environmental Performance of Emerging Photovoltaic Technologies: Assessment of the Status Quo and Future Prospects Based on a Meta-Analysis of Life-Cycle Assessment Studies. Energies; 12(22): 4228, DOI: 10.3390/en12224228**.

Chapter 3 contains the newly developed methodology as the core of this thesis in **Publication 2, Weyand et al. (2023a)**, first published 24 April 2023: **Weyand S, Kawajiri, K., Mortan, C., Schebek L.: Scheme for Generating Upscaling Scenarios of Emerging Functional Materials Based Energy Technologies in Prospective LCA (UpFunMatLCA). Journal of Industrial Ecology, DOI: 10.1111/jiec.13394**.

Chapter 4 presents the case study application of the developed methodology in **Publication 3, Weyand et al. (2023b)**, first published 11 September 2023: **Weyand S, Kawajiri, K., Mortan, C., Zeller, V., Schebek L.: Are perovskite solar cells an environmentally sustainable emerging energy technology? Upscaling from lab to fab in life cycle assessment. ACS Sustainable Chemistry & Engineering, DOI: 10.1021/acssuschemeng.3c03019**.

In **Chapter 5**, the key findings, contributions, recommendations, implications for decision-makers, and limitations are synthesized and discussed for the three publications. This thesis ends with concluding remarks and an outlook in **Chapter 6**.

2 Environmental Performance of Emerging Photovoltaic Technologies: Assessment of the Status Quo and Future Prospects Based on a Meta-Analysis of Life-Cycle Assessment Studies

This chapter contains Publication 1, Weyand et al. 2019:

> Weyand S, Wittich C, Schebek L. Environmental Performance of Emerging Photovoltaic Technologies: Assessment of the Status Quo and Future Prospects Based on a Meta-Analysis of Life-Cycle Assessment Studies. Energies 2019; 12(22): 4228, DOI: 10.3390/en12224228.

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Review

Environmental Performance of Emerging Photovoltaic Technologies: Assessment of the Status Quo and Future Prospects Based on a Meta-Analysis of Life-Cycle Assessment Studies

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Abstract: Emerging photovoltaic technologies are expected to have lower environmental impacts during their life cycle due to their extremely thin-film technology and resulting material savings. The environmental impacts of four emerging photovoltaics were investigated based on a meta-analysis of life-cycle assessment (LCA) studies, comprising a systematic review and harmonization approach of five key indicators to describe the environmental status quo and future prospects. The status quo was analyzed based on a material-related functional unit of 1 watt-peak of the photovoltaic cell. For future prospects, the functional unit of 1 kWh of generated electricity was used, including assumptions on the use phase, notably on the lifetime. The results of the status quo show that organic photovoltaic technology is the most mature emerging photovoltaic technology with a competitive environmental performance, while perovskites have a low performance, attributed to the early stage of development and inefficient manufacturing on the laboratory scale. The results of future prospects identified improvements of efficiency, lifetime, and manufacturing with regard to environmental performance based on sensitivity and scenario analyses. The developed harmonization approach supports the use of LCA in the early stages of technology development in a structured way to reduce uncertainty and extract significant information during development.

Keywords: Meta-analysis; harmonization; life-cycle assessment; perovskite solar cell; organic photovoltaic; emerging technology

1. Introduction

Renewable electricity generation technologies—wind, solar, and water—induce very low greenhouse gas (GHG) emissions in their use phase. However, it is well known that upstream processes—extraction of raw materials, production of materials and components, transportation, and manufacturing—consume significant amounts of energy and contribute to GHG emissions and other environmental impacts. For a comprehensive assessment of environmental performance, the full life cycle of production, use, and end-of-life has to be taken into account. The method of life-cycle assessment (LCA) [1,2] is widely used for investigation of the life-cycle impacts of conventional and renewable electricity generation technologies.

Today, a great amount of interest exists in the so-called emerging or third-generation photovoltaic technologies (PV). These comprise dye-sensitized solar cells (DSSC), organic photovoltaics (OPV), perovskite solar cells (PSC), quantum-dot photovoltaics (QDPV), and inorganic cells such as the copper–zinc–tin–sulfur–selenide solar cells (CZTSSe) [3]. Their common unique feature is the extremely thin-film technology which enables easy and fast manufacturing, for example, in the form of printing methods [4–7]. From the environmental point of view, emerging PVs are of interest since their thin-film technology is associated with savings of weight and materials. Therefore, the life-cycle impacts of emerging PVs are expected to be lower than those of commercial PVs of the first and second generations.

PVs were investigated in a multitude of LCA studies which led to general insight into their life-cycle impacts [8–15], i.e., about 80% of total life-cycle GHG emissions can be attributed to the production stage [15]. However, different LCA studies on PV revealed large differences in results [11,12], an observation that was also made for LCAs of other electricity generation technologies. This finding obviously compromises the use of LCA for decision support in technology development, as well as in the field of energy policy, since the results are associated with high uncertainty. The reasons for these differences were shown to be legitimate, due to the deviating methodologies, as well as differences and inconsistencies in the technological parameters and assumptions of the respective studies [16]. To tackle this problem, meta-analyses are a suitable means to derive more substantiated results from LCA studies through the combination of a systematic review and the development of technology-specific harmonization approaches. In the field of electricity generation technologies, meta-analyses were conducted and harmonization approaches were developed for first- and second-generation PVs [11,12], concentrating solar power [17], wind power [18], nuclear power [19], and coal-fired power plants [20].

In the case of PV, notably, the two meta-analyses of [11,12] provided a systematic review and harmonization approach, shedding light on the contribution of specific parameters to deviations of studies and reducing deviations of life-cycle impacts [11,12]. However, both meta-analyses exclusively comprised crystalline silicon PVs of the first generation and thin-film technologies of the second generation. In addition, these studies were restricted to GHG emissions in terms of environmental impacts. Consequently, the influences of materials on further impact categories, such as resource depletion and toxicity indicators, were not considered. In view of the fact that material systems for various types of current PVs, notably emerging PVs, largely differ, the identification of possible tradeoffs between impacts is important information from LCA, which requires the inclusion of further impact categories.

With respect to emerging PVs, several LCA studies were conducted [21–43]; however, until now, no comprehensive meta-analysis was performed. Given the high expectations of emerging PVs, thorough and reliable LCA results are crucial. In this study, a meta-analysis of LCAs on emerging PVs is presented, aiming at both the assessment of the current stage of development and possible future prospects. The meta-analysis comprises a systematic review and harmonization of LCA studies and datasets on emerging PVs. The results of this meta-analysis are used to characterize the status quo of environmental performance of emerging PVs with respect to GHG emissions and possible tradeoffs, and to investigate the influencing factors of possible future performance in comparison with first- and second-generation PVs.

2. Methodology

2.1. Overview

As a first step, based on the general methodology of LCA, the technological life cycle of PV is described. From this description, the relevant parameters and characteristics of PV can be derived, which are then evaluated by means of this meta-analysis. Secondly, a systematic review of the literature is performed, from which, according to defined criteria, studies and datasets are selected for inclusion. Finally, the harmonization approach is presented, covering a consistent reference unit for the comparison of LCA results, key indicators, and key modeling assumptions.

2.2. Conceptual Life Cycle of Emerging PVs

2.2.1. Description of the Technological Life Cycle of Emerging PVs

The life cycle of emerging PVs can be divided into upstream, operation, and downstream stages, as shown in Figure 1. The upstream stage refers to the raw material acquisition, consisting of the extraction and processing of raw materials. The raw materials are processed to layer materials. The conceptual solar cell configuration of emerging PVs is composed of five layers: the substrate with front electrode, electron blocking layer, active layer, hole transport material, and back electrode. The layer materials and deposition methods differ considerably; an overview of the most frequently applied materials is given in Table 1. After the PV cell production, the PV cells are interconnected and encapsulated to form a PV module. The PV system of emerging PVs, consisting of the PV module and the balance-of-system (BOS), covers a wider product variety than the first- and second-generation PVs, ranging from a typical rooftop module to building-integrated products or personal gadgets such as mobile chargers or OPV lamps. Consequently, the BOS components vary as well, and they may comprise not only wires and inverters but also Universal Serial Bus (USB) ports or plastic cases.

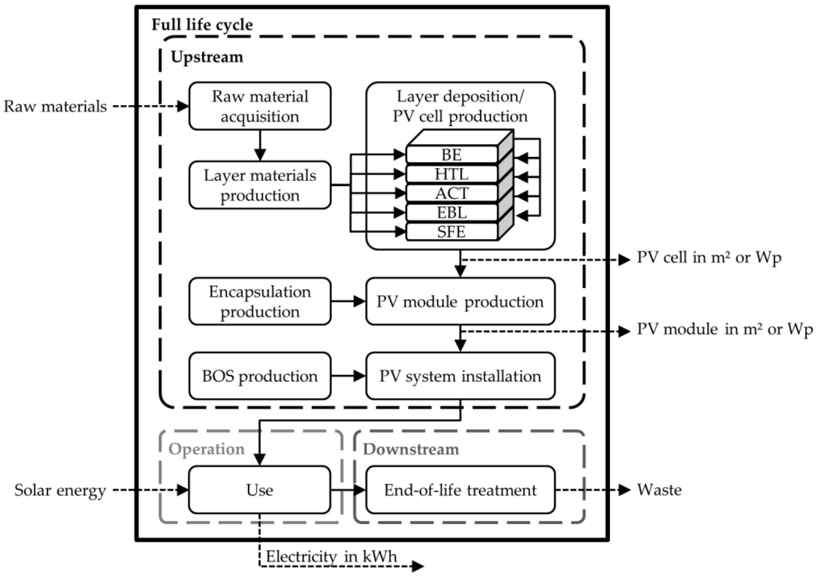

Figure 1. Conceptual life cycle of emerging photovoltaic technologies (PVs) with the technological components and methodological elements such as life-cycle stages, processes, functional units, and input/output flows.

After the installation or distribution of the PV system, its operation or use stage starts. In this stage, impacts only occur during the maintenance, repair, and replacement of PV modules or components. For first- and second-generation PVs, these impacts are very low and negligible [15]. For emerging PVs, there are no data on these impacts, which are expected to be higher due to the shorter lifetime at present. The maximum measured lifetime of emerging PVs ranges from less than one year for QDPV and PSC [44,45] to around seven years for OPV [46]. For DSSC, no data were found. In contrast, first- and second-gen PVs show a lifetime of up to 30 yrs. However, the lifetime of emerging PVs was obtained from laboratory or pilot applications, and it is expected to increase in future.

The downstream stage refers to the end-of-life treatment. For emerging PVs, the end-of-life treatment is not known yet, since there are hardly any PV products available which incorporated emerging PV materials. According to the Waste of Electrical and Electronic Equipment Directive specifying the general requirements for electronic waste in the European Union (EU) [47], end-of-life treatments should comprise recovering or recycling. However, at present, large amounts of electronic products and waste are still landfilled globally; thus, disposal in a landfill has to be considered as well.

Table 1. Overview of the layer materials and deposition methods of emerging photovoltaic technologies (PVs; summarized from life-cycle assessment (LCA) literature); in bold, the most assessed materials and deposition methods of each layer (with frequency) are shown.

Layer	DSSC	OPV	PSC	QDPV	DSSC	OPV	PSC	QDPV
	Materials				Deposition Methods			
BE	**FTO + Ag** (3)	**Ag (40)**, Al, Al+Ca, Al+Cr, C	**Au (12)**, Al or MoOx/Al, Pt, Ag, or C	**ITO (1)**	[21]	**Screen printing,** Gravure printing, N/A, Slot die coating, Evaporation, Sputtering	**Evaporation,** Dip coating, Sputtering	[41]
HTL	**Electrolyt (porphyrin-Co- dye)** (3)	**PEDOT:PSS (37)**, -, MoO_3,TiOx	**Spiro-OMeTAD (14)**, PCBM, Electrolyt (LiI), CuSCN or -	**Al_2O_3 (1)**	[21]	**N/A,** Slot die coating, Screen printing, Gravure printing, Evaporation	**Spray coating,** Screen printing, Sputtering, N/A	[41]
ACT	**Ru-dye (3)**	**P3HT:PCBM (45)**, combination of P3HT or PCBM and other acceptor or donator	**$CH_3NH_3PbI_3$,-ICl_2, -I_2Cl (16)**, $CH_3NH_3SnI_{3-x}Br_x$, $CsPbBr_3$, $FAPbI_3$	**CdSe (1)**	[21]	**Slot die coating,** Gravure printing, Evaporation, N/A, Spin coating, Inkjet printing	**Spin coating,** Dip coating, Evaporation, Slot die coating, Spray coating	[41]
EBL	**TiO_2 (3)**	**ZnO (21)**, PEDOT:PSS, PEDOT:PSS + ZnO, MoO_3, MeOH+ZnO, Ag	**TiO_2 (Comp., Meso.) (16)**, SnO_2, PEDOT:PSS, ZnO	-	[21]	**Slot die coating,** Gravure printing, Screen printing, N/A, Inkjet printing, Spin coating	**Spin coating**, Spray coating/pyrolysi, Screen printing, -N/A, Sputtering	[41]
FE	**Pt + Ag (3)**	**ITO (19)**, Ag, Ag + PEDOT:PSS, PEDOT:PSS, FTO, -, C, Al, Cu	**FTO (19)**, ITO	-	[21]	**Inkjet printing,** Sputtering, Screen printing, Slot die coating, Patterning, N/A	**N/A,** Evaporation, Patterning, Anti-reflex-coating, Sputtering	[41]
S	**Glass (2)**, PET	**PET, PET + UV-Filter, Barrier (63)**, Filter, -, Glass	**Glass (21)**, PET	**Al (1)**	[21]	**N/A**	**N/A**	[41]

S: substrate; FE: front electrode; EBL: electron blocking layer; ACT: active layer; HTL: hole transport layer; BE: back electrode; DSSC: dye-sensitized solar cells; OPV: organic photovoltaics; PSC: perovskite solar cells; QDPV: quantum-dot photovoltaics (QDPV).

2.2.2. Methodological Elements of LCA of Emerging PVs

The assessment of life-cycle impacts follows the LCA method of the ISO standards 14040/14044 [1,2]. According to these standards, the life-cycle impacts are assessed based on the modeled life cycle, the so-called product system, and they are quantified per impact category indicator in relation to the so-called functional unit of the product system. Whereas the functional unit is the quantifier of the function of the product system, used as a reference unit in LCA, the impact category indicator is the quantifier of the impact category. The considered impact categories are selected depending on the potential environmental impacts and the goal of the LCA study. In this meta-analysis, the life-cycle impacts are used to describe the environmental performance of emerging PVs.

In LCAs of PVs in general, the product system is the modeled PV system, encompassing the components of PV cells, PV modules, and BOS, as well as the considered life-cycle stages in terms of the defined system boundaries (upstream, operation, and downstream stage) and the corresponding processes (Figure 1). In contrast to first- and second-generation PVs, the LCAs of emerging PVs do not always assess the full life cycle, but only part of it. Depending on the product system, three functional units are possible for emerging PVs and for PVs in general [48]. Firstly, the functional unit of area, usually 1 m^2, can be used for the comparison of PV cells or PV modules with the same efficiency. Secondly, in the case of emerging PVs with various efficiencies, the functional unit of 1 watt-peak (W_p) should be used for meaningful results. This functional unit is known as the nominal power and takes into account the maximum efficiency of the PV cell or PV module under standard test conditions, which are a light intensity of 1000 W/m^2, cell temperature of 25 °C, and air mass of 1.5, according to the standard IEC 61215 of the International Electrochemical Commission [49]. Third, the functional unit of 1 kWh of electricity fed into the grid is typically used for a mature electricity generation technology installed on an industrial scale. The latter is the only functional unit that enables the inclusion of the operation stage (Figure 1). During the life cycle of emerging PVs, on one hand, the potential environmental impact results from the upstream energy inputs of the layer deposition and the production of the PV cell, PV module, and PV system in relation to the energy output during the use phase, and the inputs or outputs during the end-of-life treatment. This results in the use of energy and corresponding GHG emissions. On the other hand, there are impacts resulting from the layer materials, occurring mostly in the upstream and downstream stages due to the material acquisition or end-of-life treatment. During the use stage, these materials are connected and encapsulated to form the final products and, thus, do not come into direct contact with the environment in LCA studies. In LCA studies, the impacts of these materials may contribute to tradeoffs with respect to resource depletion or toxicity impacts.

2.3. Systematic Review Approach of LCA Literature and Datasets

2.3.1. Literature and Dataset Search

The systematic review covered literature references, i.e., publications and datasets of LCAs on emerging PVs, from literature databases and the openLCA Nexus repository. The literature search was carried out using four literature databases: Web of Science, Wiley online library, ScienceDirect, and SciFinder. Here, combinations of the following keywords were used: life-cycle assessment, dye-sensitized solar cell, organic photovoltaic, perovskite solar cell, quantum-dot photovoltaic, and copper–zinc–tin–sulfur–selenide solar cell. Further considered synonyms are listed in Table S1 (Supplementary Materials). The search strategy focused exclusively on full journal articles. The identified literature references were published between 2001 and 2018.

The openLCA Nexus repository provides more than 130,000 LCA datasets of 20 LCA databases, including well-known LCA databases such as ecoinvent, GaBi LCA Database, and European reference Life Cycle Database (ELCD; last access: 29 January 2019). However, this repository did not include any LCA dataset for the previously used keywords.

2.3.2. Literature and Dataset Selection

The identified literature references were primarily screened, and suitable LCA studies and datasets were selected for inclusion in this meta-analysis. The following inclusion criteria were applied:

- Relevance of the technologies: Only emerging PVs from the fields of DSSC, OPV, PSC, QDPV, and CTZSSe were considered in this meta-analysis.
- Quality and relevance of the LCA study: The underlying LCA study of a literature reference had to be in compliance with the ISO 14040/14044 standards [1,2].
- Completeness and transparency of the LCA study: In this meta-analysis, as a minimum requirement, the product system needed to consider at least the upstream impacts of PV cells (Figure 1). Transparency had to be ensured with respect to basic LCA elements, such as the defined goal with the corresponding information on the functional unit and assessed impact categories.

The primary screening resulted in 28 LCA studies (three DSSC, 16 OPV, eight PSC, one QDPV, and zero CTZSSe) on the considered emerging PVs. In most LCA studies, different layer materials, deposition methods, and end-of-life-treatments were analyzed, resulting in more than one LCA dataset per LCA study. Therefore, the 28 LCA studies were further subdivided into 134 LCA datasets. The following secondary inclusion criteria were applied to select suitable LCA datasets:

(1) The LCA dataset was not published previously in another LCA study.
(2) The LCA dataset included, as a minimum life cycle, impacts of the energy demand or the contributed GHG emissions of the production of PV cells.
(3) The LCA dataset included information necessary for the conversion of the functional unit to m^2, W_p, or kWh.

Finally, a total number of 22 LCA studies (three DSSC, 67 OPV, 23 PSC, and one QDPV) and 94 LCA datasets were included in this meta-analysis. The excluded LCA datasets are summarized in Table S2 (Supplementary Materials). For CTZSSe, no relevant LCA dataset was found. Therefore, this emerging PV was excluded from this meta-analysis.

2.4. Harmonization Approach for LCA Datasets

2.4.1. General Framework

The methodology for harmonization was based on the approach of [11,12], which was conceptually designed for first- and second-generation PVs. Their general framework for harmonizing LCA results for PV is described by Equation (1).

$$\mathrm{GHG} = W/(I \cdot \eta \cdot PR \cdot \tau \cdot A), \quad (1)$$

where GHG stands for the GHG emissions in g CO_2-equivalent (eq) per functional unit of 1 kWh, W refers to the total GHG emitted over the life cycle in g CO_2-eq, I is the irradiation in kWh/(m^2·year), η is the efficiency as a percentage, PR is the performance ratio of PV systems as a percentage, τ is the lifetime in years, and A is the total module area in m^2.

Based on this equation, two levels of harmonization were discerned in [11,12]. The first level involves an in-depth investigation of the underlying LCA studies in terms of the alignment of the total GHG impacts with a consistent life cycle, i.e., including or excluding components and life-cycle stages in or from the numerator W. The second level is less resource-intensive and includes only the harmonization of the GHG impacts according to Equation (1). Whereas both levels were applied in [12], the harmonization approach of [11] was exclusively restricted to the second level, i.e., no alignment of W, whereby standard values of I, η, PR, and τ were defined and the GHG impacts were harmonized to these standard values using a developed spreadsheet-based meta-model.

In this meta-analysis, the harmonization approach encompassed the second level of the definition of the standard values of PR, I, η, and τ as a consistent set, which is generally necessary for the characterization of any PV technology. However, from the systematic review, three requirements were identified to widen the approach of [11] regarding emerging PVs. Firstly, different functional units were found in the LCA datasets on emerging PVs, resulting in additional harmonization to a consistent functional unit. Secondly, the scope of the environmental impacts was widened to include further key indicators in order to account for impacts related to the specific layer materials. Thirdly, to substantiate the comparison of results from the LCA datasets, the consideration of additional methodological specifications was necessary, such as the diverging state of technology development and life-cycle information related to the first level of the harmonization [12]. This information was analyzed in terms of qualitative factors. These requirements resulted in the framework conditions described below for harmonizing LCA results on emerging PVs.

2.4.2. Harmonization to Consistent Functional Units

The LCA datasets on emerging PVs were related to the three definitions of the functional unit: energy, rated power, and area. The rationale behind these definitions of the functional unit was as follows: The comparison of first- and second-generation PVs with each other or with further energy technologies was based on the typical functional unit of 1 kWh of electricity fed into the grid. Accordingly, the functional unit reported for LCA of first- and second-generation PVs in [11,12] was exclusively defined as 1 kWh of electricity fed into the grid. For the comparison of emerging PVs with first- and second-generation PVs, this functional unit was used as well. However, the choice of the functional unit of energy necessarily requires data on module efficiencies, transmission losses in terms of the performance ratio, location-specific irradiation, and lifetime of the PV systems [48]. As a result, notable assumptions on prospective applications and expected lifetime of emerging PVs are mandatory for the calculation. However, at this development stage, there is hardly any knowledge about these applications and the expected lifetime. Therefore, many LCA studies on emerging PVs did not include such highly speculative assumptions and restricted their research question to investigation of the current production of PV cells or PV modules in laboratories or in pilot plants, as well as using the functional units of area or rated power (Figure 1). Accordingly, the definition of the functional unit depends on the research question or goal of the LCA study.

In this meta-analysis, two research questions (hereafter termed as cases) were investigated and resulted in different functional units per case, which were investigated by means of the harmonized results. Firstly, for the case "characterizing the status quo of environmental performance of emerging PVs", the functional unit of 1 W_p provided PV cell, module or system was used. Secondly, for the case of a substantiated discussion on the "possible future environmental performance" in view of a comparison with first- and second-generation PVs, the functional unit was 1 kWh of generated electricity.

2.4.3. Key Indicators (KEYIs)

The key indicators, hereinafter referred to as KEYIs, are the impact category indicators that were selected for a comprehensive description of the potential environmental impacts of the considered emerging PVs and in general for the comparison of PVs. Considering the aforementioned potential environmental impacts, the following five KEYIs were selected for the assessment of the life-cycle impacts, divided into energy-related and material-related KEYIs for the tradeoff consideration:

1. Energy-related KEYIs:
    - Cumulative energy demand (CED): The CED in MJ PE quantifies the primary energy (PE) inputs of the included life cycle stages.
    - Global warming potential (GWP): GWP quantifies the GHG emissions in g of carbon dioxide equivalents (g CO_2-eq) resulting mostly from the energy demand.
2. Material-related KEYIs:

- Resource depletion, mineral, fossil, and renewable resources (RDPf): The RDPf in g of antimony equivalents (g Sb-eq) considers the resource use and impacts on the resource availability.
- Toxicity indicators: These indicators are relevant in assessing the toxicity potential of the included layer materials to the ecosystem and human health, assessed by the following two indicators in this meta-analysis:
  - Ecotoxicity potential for freshwater (ETPf) in comparative toxic units for ecosystems (CTUe);
  - Human toxicity, cancer effects (HTPc) in comparative toxic units for human health impact equivalent to the incidence of cancer (CTUh).

In [50], the consideration of more tradeoffs was highlighted, such as land use or eutrophication. However, for the comparison of emerging PVs, the data coverage is not sufficient (see File S1, Supplementary Materials). Furthermore, the five KEYIs cover the most important tradeoffs for the comparison of PV technologies. Further tradeoff considerations may be important in the case of a comparison with further energy generation technologies. For this case, the harmonization approach is extendable to further impact indicators beyond these five introduced KEYIs.

2.4.4. Key Modeling Assumptions (KEYAs)

The key modeling assumptions, hereinafter referred to as KEYAs, summarize methodological specifications that may influence the total life-cycle impacts of emerging PVs:

1. LCA type, temporal coverage, and technology scale: These KEYAs were interrelated in LCA studies on emerging PVs. The term LCA type stands here for the modeling approach of the LCA study. It was differentiated into the following:

   - Conventional LCA, representing the common approach of LCA studies, particularly commercial technologies which are established on the market and show sufficient primary data quantities for the assessment of the status quo;
   - Prospective LCA/ex ante LCA, representing an approach particularly for the assessment of emerging technologies to assess their prospective developments in comparison with commercial technologies [51,52].

   Accordingly, the temporal coverage of a conventional LCA is based on present conditions of technologies, whereas prospective LCAs consider future scenarios and developments of technologies. Moreover, the technology scale of the assessed technology depends on the LCA type as well. The technology scale characterizes here the stage of development of the assessed emerging PV, and it is an important specification for the characterization and differentiation of emerging PVs in LCA studies. In conventional LCAs, technologies are assessed based on the current technology scale and stage of development. On the contrary, in prospective LCAs, the technology scale is upscaled by the consideration of likely future scenarios and, consequently, emerging technologies are assessed based on higher technology scales. In particular, for a fair comparison between emerging PVs and commercial technologies or technologies at higher or lower development stage, the technology scale of the assessed technology needs to be indicated. A common method for characterizing the technology scale is the concept of technology readiness levels (TRLs), consisting of nine TRLs established by National Aeronautics and Space Administration (NASA) [53]. However, none of the included LCA studies reported TRLs. Therefore, the following classification scheme based on the TRL concept was introduced and applied for the characterization of the technology scale of the LCA datasets on emerging PVs:

- TRL 1 ("basic principles observed and reported") was omitted since it may be relevant for LCA studies of new technology concepts but not for the included emerging PVs [53];
- Laboratory scale, referring to TRLs 2–4 ("research to prove feasibility");
- Pilot scale, referring to TRLs 5–7 ("technology demonstration");
- Industrial scale, referring to TRLs 8–9 ("system test, launch, and operations").

2. Product system: The considered product system of emerging PVs can be distinguished into the three options: (1) PV cell, (2) PV module, and (3) PV system. As shown in Figure 1, the PV system includes more components than the PV cell. Each component has its own impact and, consequently, the consideration of its contributions and tradeoffs is necessary.
3. Layer components: The different layer options as components of the PV cell are relevant to the life-cycle impacts resulting from the energy requirements of the deposition and from possible hazardous elements or materials. Therefore, the further subdivision of the PV cell into the layer components is necessary to track and compare the life-cycle impacts and the contribution of the layer materials and deposition methods.
4. System boundary: As mentioned above, the minimum requirement for the selection of a dataset was the inclusion of the upstream stage, i.e., the production of the PV cell. In addition, studies could also include also the operation stage or cover the full life cycle, including the downstream stage. While the inclusion of the operation stage yields electricity generation and, thus, is covered by the respective functional units of energy, the inclusion of the downstream stage is often omitted and hinders the comparison of results. However, since the LCA studies gave very limited information on end-of-life treatment, the contribution of the downstream stage could not be added to the overall result; thus, an important source of tradeoff was not fully considered. Therefore, the influence of the system boundary was taken into account as KEYAs.

2.4.5. Key Performance Parameters (KEYPs)

The key performance parameters, hereinafter referred to as KEYPs, characterize the performance of the PV system, and they were significant for the determination of the maximum electricity yield during the operation stage. The KEYPs were as follows:

1. Efficiency of the PV cell or PV module (η);
2. Performance ratio of the PV system (PR);
3. Irradiation on the installed PV system (I);
4. Lifetime of the PV system (τ) and its components.

3. Results

3.1. Systematic Review of LCA Datasets on Emerging PVs

The 22 reviewed LCA studies with the number of respective LCA datasets are given in Table 2, along with information on the functional units, KEYIs, KEYAs, and KEYPs. For each LCA dataset, the considered KEYIs were specified; CED was the most commonly considered KEYI, with 67 of the 94 LCA datasets considered; GWP was the second most widely considered KEYI, with 59 LCA datasets considered. RDPf and the two toxicity indicators were assessed for almost all LCA datasets on PSC. However, for the other emerging PVs, these KEYIs were only considered in three LCA studies, with 8–11 LCA datasets on OPV and none on DSSC and QDPV considered. For OPV, 67 LCA datasets from 14 LCA studies could be selected and, for PSC, 23 LCA datasets from six LCA studies could be selected. However, for DSSC and QDPV, only one LCA study with three and one LCA datasets, respectively, could be found.

Table 2. Reviewed LCA studies with number of data sets on DSSC, OPV, PSC, and QDPV (22 studies, 94 LCA datasets), considered key indicators (KEYIs) with corresponding functional unit, key modeling assumptions (KEYAs) and assumptions on the four key performance parameters (KEYPs).

LCA Studies with Number of Included LCA Data Sets		KEYIs [a]				KEYAs [b]				KEYPs [c]			
Author (Year)	**DS**	**FU**	**CED**	**GWP**	**RDPf/Tox**	**LCA type/TS**		**PS**	**SB**	η_R	τ_R	I_R	PR_R
			in MJ PE	*in g* CO_2*- eq*	*in g Sb -eq or CTU*				*Down-stream*	*in %*	*in years*	*in kWh/* m^2*·year*	*in %*
DSSC													
Parisi et al. (2014) [21]	3	1 kWh	✓	✓	–/–	P	PI	S	□	8	20	1700	75
OPV													
Anctil et al. (2013) [22]	13	1 W_p	✓	–	–/–	C	L	M	□	3.0–7.7	N/A	N/A	N/A
Darling and You (2013) [54]	1	1 m^2	✓	–	–/–	C	PI	M	□	1	2	1700	75
Espinosa et al. (2011a) [23]	1	1 m^2	✓	✓	–/–	C	IN	M	□	2	15	1700	80
Espinosa et al. (2011b) [24]	1	104 cm^2	✓	–	–/–	C	IN	S	□	2–3	2	N/A	N/A
Espinosa et al. (2012a) [25]	1	1 m^2	✓	✓	–/–	P	PI	M	□	1	15	1700	80
Espinosa et al. (2012b) [26]	10	1 m^2	✓	–	–/–	C	PI	M	□	1	15	1700	N/A
Espinosa et al. (2013) [27]	6	1 m^2	✓	–✓	–✓/–	C	PI	M	□	2	N/A	1700	N/A
Espinosa et al. (2014) [28]	5	1 m^2	✓	–	–/–	C	IN	M/S	□	2.2/1.6	1	1700	80
Espinosa et al. (2016) [29]	8	1 kWh	–	✓	✓/✓	C	PI	M	■	0.7–1	2	-	N/A
García-Valverde et al. (2010) [30]	1	1 m^2	✓	✓	–/–	C	L	M	□	5	15	1700	80
Roes et al. (2009) [31]	2	1 W_p	✓	✓	✓/–	C	L	S	□	5	25	1700	75
Søndergaard et al. (2014) [32]	3	1 m^2	✓	–	–/–	C	PI	M	■	2	N/A	1700	80
Tsang et al. (2015) [33]	3	1 W_p	✓	✓	–/–	P	PI	C	□	5	N/A	1700	75
Tsang et al. (2016) [34]	12	1 W_p/1 kW_p	✓	✓	–/–	P	PI/IN	S	■	5	25/5	1300	75
PSC													
Celik et al. (2016) [35]	3	1 kWh	✓	✓	–/✓	P	IN	C	□	15	5	1700	75
Espinosa et al. (2015) [36]	2	1 kWh	✓	✓	✓/✓	C	L	C	□	11.5/15.4	1	1700	N/A
Gong et al. (2015) [37]	2	1 m^2	✓	✓	–/–	P	PI/IN	M	■	9.1/11	2	1960	80
Serrano-Lujan et al. (2015) [38]	3	1 kWh	✓	✓	✓/✓	C	L	C	□/■	6.4–9.2	1	1700	80
Zhang et al. (2015) [39]	3	1 cm^2	–	✓	✓/✓	C	L	S	□	6.5	N/A	N/A	N/A
Zhang et al. (2017) [40]	10	1 cm^2	✓	✓	✓/✓	C	L	S	■	4.88–20.0	1	1700	75
QDPV													
Şengül et Theis (2011) [41]	1	1 m^2	✓	✓	–/–	P	PI/IN	S	□	14	25	1700	80

[a] KEYIs: key indicators: FU: functional unit; CED: cumulative energy demand; GWP: global warming potential; RDPf: resource depletion, mineral, fossil, and renewable resources; Tox: one of the two toxicity indicators; ✓ considered in LCA datasets and compliant with the introduced KEYIs/ – not considered or not compliant; [b] KEYAs: key modeling assumptions: LCA type: C: conventional; P: prospective; TS: technology scale with options: L: laboratory scale; PI: pilot scale; IN: industrial scale; PS: considered product system with options: C: cell; M: module; S: system; SB: system boundaries with options: ■ downstream stage included/ □ only upstream stage; [c] Reviewed KEYPs: key performance parameters: η_R: efficiency; τ_R: lifetime; PR_R: performance ratio; I_R: irradiation; DS: number of LCA data sets per study; N/A: data not available.

The systematic review of the KEYAs was conducted according to the four qualitative factors. None of the reviewed LCA studies reported the TRLs nor distinguished between conventional and prospective LCAs, since the latter distinction emerged recently in [51,52]. Therefore, the classification of LCA type and the technology scale was conducted based on keywords and data sources of the reviewed LCA datasets (see File S1, Supplementary Materials, for more information on this classification). In particular, for the LCA studies on PSC, based on primary data sources, specified keywords such as "laboratory production" [30], "laboratory-scale experiments" [39], and "pilot line facility" [27] allowed a clear classification of the technology scale and LCA type. In contrast, there were LCA studies based on secondary data sources and prospective assumptions on future development for which a clear classification of the technology scale was difficult, since the prospective assumptions were not specified in a transparent manner. Therefore, the classification of the upscaled technology scale was not clear. For these prospective LCA studies, the technology scale was not differentiated between pilot and industrial scale (PI/IN). The systematic review showed that OPV was mostly assessed by prospective LCAs (16 of 67 LCA datasets) or based on pilot- or industrial-scale manufacturing routes (35 of 67 LCA datasets). For PSC, only two LCA studies considered prospective assumptions, but most LCA datasets (18 of 23) were assessed based on the current laboratory scale, with the number of TRLs lower than four. The DSSC and QDPV datasets both came from prospective LCAs. Consequently, the assessed OPV was more mature than the other three emerging PVs considering the reviewed LCA datasets in this meta-analysis.

Regarding the considered product system, most LCA datasets on OPV considered PV modules and those on PSC considered PV systems. The latter is surprising since the PV system includes the BOS components that are highly dependent on the unknown future application of PSC. Consequently, this is a highly speculative assumption at this stage of development. The layer components of the reviewed LCA datasets are summarized in Table 1 (more detailed layer information per LCA dataset can be found in File S1, Supplementary Materials). Considering the system boundaries, the full life cycle was only assessed in two LCA studies. The downstream stage was only included in 27 of the 94 LCA datasets. In most LCA data sets, the focus lay in the upstream stage (47 of the 94 LCA datasets).

The systematic review on the KEYPs showed high variations, varying from too pessimistic to too optimistic, influenced by the KEYAs. The assumed efficiency of the reviewed LCA datasets ranged from 0.7% to 7.7% for OPV and from 4.88% to 20.0% for PSC. In spite of these high variations, it was observed that the efficiency of PSC was generally higher than OPV as confirmed in the literature [3]. However, the efficiency of OPV was assumed pessimistically considering the current maximum reported efficiency of 15.6%, trackable by the best research cell efficiency chart of the National Renewable Energy Laboratory (NREL) [3] or by the solar cell efficiency tables by [55]. The single values for DSSC and QDPV rather fell into the range of PSC efficiency, even though their current maximum reported efficiencies were in the range of the OPV maximum. Taking into account the KEYAs, the influence of the technology scale was low. Despite the low TRLs of PSC, they showed efficiencies in the range of first- and second-generation PVs. In contrast, the considered product system and the layer components had high influences on the reviewed efficiencies. Due to the larger active area of PV cells, they showed higher efficiencies than PV modules or PV systems. In contrast to the best reported ones, the efficiency of the PV cells was influenced strongly by the layer components and the included materials, e.g., the PSC with lead in the active layer showed generally higher efficiency than the one with tin. The system boundaries had no influence at all. The reviewed lifetimes varied for all four emerging PVs between one and 25 years. These figures should generally be rated as highly speculative assumptions due to the three reasons. Firstly, they cannot be proven by the maximum reported lifetimes. Secondly, low lifetime assumptions (1–2 years) result from the current state of research and are currently more realistic. Thirdly, the lifetime assumptions are not influenced by the choice of product systems, layer components, and system boundaries. The other two KEYPs, I and PR, were assumed as 1700 kWh/(m^2·year) and 80% in almost all reviewed LCA datasets. The irradiation represents the average yearly solar energy achievable per m^2 and depends on the location of the operation stage of the PVs. The value of 1700 kWh/(m^2·year) was the typical value of southern Europe; however, in central Europe, lower values were obtainable, while higher values were obtainable in the southwestern part of the United States. The product of irradiation and efficiency specifies the direct current generated by the PV cell, module, or system. In contrast, the performance ratio indicates the share of the direct current that is finally fed into the grid as alternating current after deduction of the system-related losses. Eighty percent is the typically used value for ground-mounted systems [48]. Currently, even higher values of 90% are possible due to improvements in inverter efficiencies, as well as the design and maintenance of PV systems in recent years [48,56]. Both KEYPs were only relevant for the operation stage.

3.2. Harmonization of LCA Datasets on Emerging PVs

3.2.1. Mathematical Procedure of the Harmonization

The progressive alignment of the KEYIs of each reviewed LCA dataset to the harmonized KEYIs was performed according to Equations (2)–(7), as given in Table 3. Due to the fact that different functional units were encountered in LCA studies, the calculation encompassed two steps. In the first step, the values of the KEYIs were converted to the functional unit of 1 m^2 according to Equation (2), which was independent of the dataset-specific KEYPs (η, PR, I, τ). For this conversion, three conversion factors depending on the functional unit of the reviewed LCA datasets were necessary (Equations (3)–(5)). As described before, the unit of areas was independent of the dataset-specific KEYPs; thus, the conversion factor was 1 (Equation (3)). In contrast to this, the units of power and energy were influenced by these KEYPs and, consequently, the conversion aimed for the mitigation of their influences by removing the dataset-specific information (Equations (4) and (5). In the second step, the values per 1 m^2 were converted to the case-specific functional unit of 1 W_p or 1 kWh by the use of standard values of η, PR, I, and τ (see next section), as shown in Equations (6) and (7), respectively.

Table 3. Mathematical procedure of the extended harmonization approach of Equation (1) and the used standard values of the four KEYPs.

Harmonization Equations		Parameter/Units	Abbreviations	Standard Values
Conversion of the reviewed KEYIs to W				
$W = KEYI_R \cdot CF$	(2)	Total life-cycle impacts of the LCA dataset in LCIA/m^2	W	-
		Reviewed key indicator in LCIA/FU	$KEYI_R$	-
		Conversion factor	CF	see Equations (3)–(5)
Conversion factors depending on the reviewed functional unit (FU)				
CF = 1 (FU = 1 m^2)	(3)			
$CF = E \cdot \eta_R$ (FU = 1 W_p)	(4)	Light intensity in W/m^2 according to IEC 61215 [49]	E	1000
$CF = \eta_R \cdot PR_R \cdot I_R \cdot \tau_R$ (FU = 1 kWh)	(5)	Reviewed KEYPs	η_R, PR_R, I_R, τ_R	-
Harmonization of the case "characterizing the status quo"				
$KEYI_H = \frac{W}{E \cdot \eta_H}$	(6)	Harmonized key indicator in Case "status quo": LCIA/Wp Case "prospects": LCIA/kWh	$KEYI_H$	-
		Standard values of the KEYPs: • efficiency in %	η_H	DSSC: 6 OPV/QDPV: 8 PSC: 12
Harmonization of the case "possible future performance"				
		• performance ratio in %	PR_H	80
$KEYI_H = \frac{W}{\eta_H \cdot PR_H \cdot I_H \cdot \tau_H}$	(7)	• irradiation in kWh/(m^2·year)	I_H	1700
		• lifetime in years	τ_H	-

3.2.2. Standardization of the KEYPs

For the alignment of the harmonized KEYIs, the standard values of the four KEYPs were needed, i.e., η_H as the percentage per module area A in m^2, PR_H as a percentage, I_H in kWh/(m^2·year), and τ_H in years. The values were identified as described below.

In the case of efficiency η_H, the standardization was drawn on the reporting of progress and achievement of efficiency increase for the best PV research cells provided by [3] and [55]. Here, the emerging PVs were ranked from the highest to the lowest measured best cell efficiencies as follows: PSC (23.7%), QDPV (16.6%), OPV (15.6%), and DSSC (11.9%) [3]. To define a standard value of each emerging PV, the ratio of the best cell efficiencies to the harmonized module efficiencies of the first- and second-generation PVs in [11,12] was considered, which resulted in a ratio of 50% for all technologies (see Table S3, Supplementary Materials, for more information). The final standard values used for the harmonization of the four emerging PVs are given in Table 3. The values assume uniform efficiencies per emerging PV even though the emerging PVs might be further subdivided per morphology. To obtain the most promising morphology, i.e., most efficient and stable cells, using the bulk heterojunction approach was one of the biggest challenges of the current research [57–60]. To account for the variations in the efficiency assumptions depending on the morphology, a sensitivity analysis on the efficiency from 1% to 20% was conducted.

The irradiation I_H in kWh/(m^2·year), performance ratio PR_H as a percentage of the PV system, and operating lifetime τ_H in years were only needed for the case of a functional unit of 1 kWh of generated electricity. While I_H and PR_H are set to 1700 kWh/(m^2yr) and 80%, respectively, according to [11,12], where no standard value of τ_H was defined. Due to the high uncertainty, the influence of the lifetime was assessed by means of sensitivity analysis. The sensitivity analysis covered the range of lifetimes from one year, which was the lowest estimate of studies and, thus, the worst-case assumption, to 30 years, which was the typical lifetime of first- and second-generation PV applications. It should be noted that the latter value is purely hypothetical at this stage of development and is only used for comparability reasons.

The two spreadsheet-based meta-models for the harmonization of the KEYIs using these standard values of the KEYPs can be found in File S1 (Supplementary Materials).

3.3. Status Quo of the Environmental Performance of Emerging PVs

The environmental status quo was evaluated based on the median and the interquartile range (IQR) (75th minus 25th). For OPV and PSC, as a result of harmonization, the IQR distributions decreased for all KEYIs. For the medians and the other two emerging PVs, there was no clear finding. Here, the medians decreased for all KEYIs in the case of OPV and only for CED and GWP in the case of PSC, since the standardized η_H values were higher than the assumptions of the reviewed LCA datasets. In contrast, the medians of the other KEYIs increased due to higher efficiency assumptions. For DSSC and QDPV, the single values for the two KEYIs, CED and GWP, increased as well due to the high speculative assumed efficiencies of their reviewed LCA datasets. Overall, there was a correlation between CED and GWP; both medians decreased by about 60% for OPV and by about 10% for PSC, as well as increased by about 30% for DSSC and by 75% for QDPV. The rationale behind the correlation was that the energy demand was still covered to a large extent by fossil fuels, responsible for large extents of GHG emissions and, consequently, for high GWP impacts. For the other three KEYIs, no quantifiable correlation was identified at this point (see Table S4, Supplementary Materials).

In Figure 2, the results of the environmental status quo are presented as boxplots of the five harmonized KEYIs, indicating the median, IQR, and the minimum and maximum values. In order to depict the influence of the standardized efficiencies η_H, the results of the sensitivity analysis of the median are included in Figure 2. For the discussion of the results, three premises were used. Firstly, as the median of each KEYI decreased, so did the life-cycle impacts that occurred, together with an improvement in the environmental performance. Secondly, as the IQR decreased, the harmonized KEYIs became more robust; however, here, the number of studies was taken into account since a small

IQR resulting from a small number of datasets, possibly from one study with common assumptions, may have been subject to uncertainties. Thirdly, a sharper decrease in the median for the sensitivity analysis resulted in a stronger influence of the efficiency on the result.

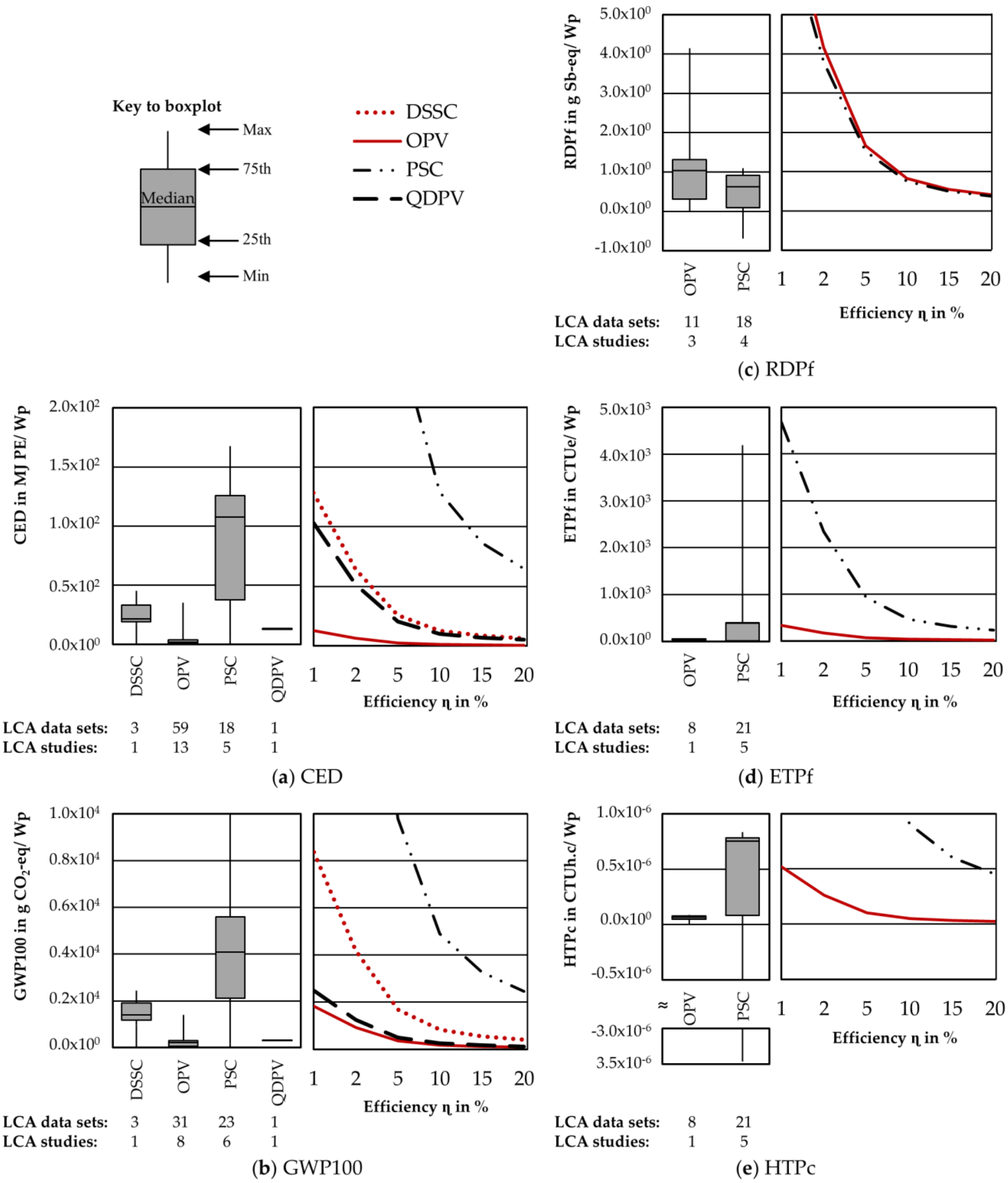

Figure 2. Current environmental status quo. Boxplots of the five key indicators (KEYIs) harmonized to the consistent functional unit of 1 W_p and standard values of the efficiencies (Table 3) (left), as well as influence of the efficiency range (1–20%) on the medians (right).

For CED and GWP, the best environmental performance in terms of the lowest and most robust results was found for OPV: 2 MJ PE/W_p and 228 g CO_2-eq/W_p, respectively. The highest and least robust results were indicated for PSC, with the lowest results in the range of the OPV median and the highest results over 100-fold higher. Both findings were based on a substantial number of LCA studies (between five and 13 studies, providing between 18 and 59 datasets). For DSSC and QDPV, only CED and GWP were assessed. Both KEYIs were higher than OPV but lower than PSC. However, the findings on DSSC and QDPV were limited to a single LCA study, including three or fewer LCA datasets. In contrast to OPV, the medians of both KEYIs decreased sharply with increasing efficiency for PSC, DSSC, and QDPV. However, DSSC and QDPV came close to the OPV values in the case of an efficiency of 20%, but there was still a wide gap with PSC. Accordingly, the results of PSC, DSSC, and QDPV were highly influenced by efficiency increase.

For the other three KEYIs, RDPf, ETPf, and HTPc, results were only available for OPV and PSC. Here, OPV again performed better than PSC for the two toxicity indicators, although it should be noted that this finding resulted from only one LCA study providing eight LCA datasets with similar assumptions; thus, little to no deviations existed. The boxplots and sensitivity analyses showed similar curves for the toxicity indicators compared with CED and GWP. Even though there was no quantifiable correlation between the CED and the two toxicity indicators, there was an apparent dependency. Contrary to this, the results indicated that there was no correlation at all between the CED and the related high fossil fuel share and RDPf. The medians of RDPf, resulting from three and four LCA studies with 11 and 18 LCA datasets, were similar to OPV and PSC, with a slightly higher value for OPV. Although fossil fuels and mineral resources were included in RDPf, this KEYI was more influenced by the mineral resources due to their higher characterization factors. However, the characterization factors of silver and gold as the most used materials of the back electrode of OPV and PSC were over 8 kg Sb-eq/kg; for fossil fuels, they were less than 1.0×10^{-7} kg Sb-eq/kg. The sensitivity analysis also showed that both emerging PVs had similar curves. However, considering, in general, the higher efficiency of PSC, PSC performed better than OPV for RDPf. Accordingly, there was no shift in negative environmental impacts from the energy-related and material-related KEYIs and, consequently, no tradeoffs were expected.

For an in-depth interpretation of the results, the influences of the KEYAs on the KEYIs and the tradeoffs occurring during the life cycle of PVs were evaluated. The evaluation was based on the single included LCA datasets and the single options of the KEYAs, which were laboratory vs. pilot/industrial for the technology scale, PV cell vs. PV module/system for the considered product system, and upstream vs. downstream impacts for the system boundary.

Regarding technology scale, the pilot or industrial scale was obviously predominated by the OPV dataset results, while, in the case of PSC, the majority of LCA datasets were distributed to the laboratory scale. For PSC, this difference in the technology scale resulted in both higher values and a larger distribution of PSC results compared with OPV, in particular for the three following KEYIs: CED, GWP, and HTPc (Figure 3). The reasons for this might have been the influence of the technology scale and tradeoffs resulting from the layer materials and deposition methods used in laboratories and might not have resulted from tradeoffs during the life cycle, indicated by the considered product system or system boundaries. In order to verify this finding, disaggregated information on each layer of the PSC cells was evaluated. The evaluation indicated three kinds of tradeoffs originating from the layer materials and deposition methods, as discussed below.

Firstly, the selection of layer materials influences the environmental performance of each layer and is expected to be different for industrial and laboratory productions. For example, for PVs, gold, as the typically used material for the back electrode on the laboratory scale, has a much higher impact than silver and aluminum used on the pilot or industrial scale [35–37,40]. Secondly, in the laboratory, the thickness of a layer is not of great relevance and often not measured, so more material than necessary for the optimal performance is used. Thirdly, energy-inefficient deposition methods are applied on the laboratory scale compared with the pilot or industrial scale. Several publications support this finding, e.g., the CED of the back electrode was reduced by six-fold from the laboratory deposition of gold by thermal evaporation (36 MJ PE/W_p) [40] to the industrial scale in which gold was substituted by C-paste and deposited by spray coating (4 MJ PE/W_p) [35]. For the active layer, even higher reductions of up to 15-fold were reported. Similar results were observed for OPV development. Starting with a CED of 47 MJ PE/W_p for manufacturing an OPV cell on the laboratory scale, including typical laboratory manufacturing surroundings such as a nitrogen atmosphere and deposition methods such as spin-coating and annealing for depositing the active layer and thermal evaporation for the electrodes [33], the CED was reduced significantly to 6.3 MJ PE/W_p [23] and 0.7 MJ PE/W_p [32] by enhancing the PV cell manufacturing to roll-to-roll production with the deposition method of slot die coating and screen printing without nitrogen atmosphere.

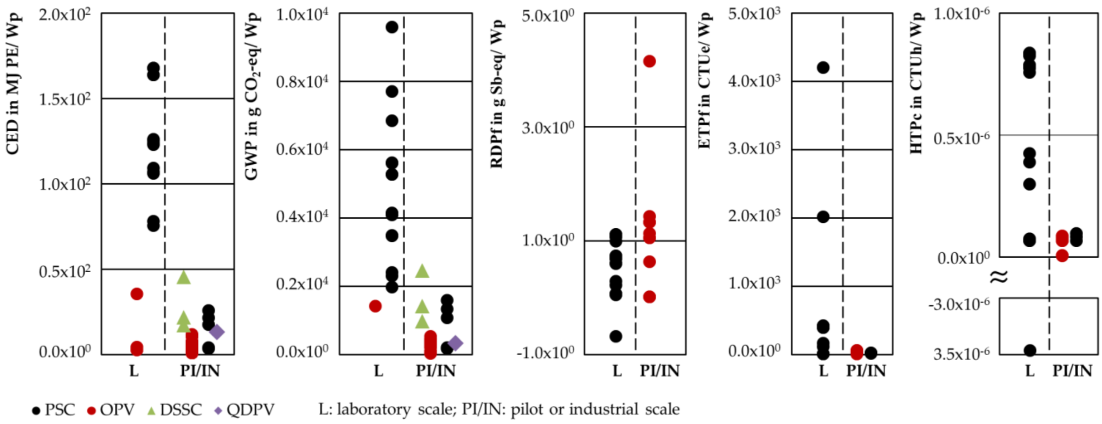

Figure 3. Influence of the technology scale and their single values, laboratory (L) vs. pilot/industrial (PI/IN) scale, on the single harmonized life-cycle assessment (LCA) dataset points of the five KEYIs.

For the considered product system, no influence could be determined due to the limited number of LCA datasets reporting the contributions of the additional components of the PV modules, the encapsulation, and the PV system (the BOS). Nonetheless, for PSC only, three LCA studies enabled the consideration of the additional components. However, in contrast to the literature [50], no tradeoffs of the additional components could be determined since their contributions were less than 5% [37,39,40]. This might be explained by the high impacts resulting from the production of the PSC cells compared with the small contributions of the additional components. For the other three emerging PVs with lower impacts, the additional components, especially the BOS, showed high contributions to all five KEYIs, ranging from 11% to 48% [50].

Regarding system boundaries, in the case of the status quo analysis, the operation phase was excluded by definition, and the only two possible options were the upstream stage and the combination of up- and downstream stage. The inclusion of the downstream stage led to a rather minor increase in results for CED. However, the influence of the downstream stage on CED was negligible compared with the upstream impacts, since the impacts were less than 5% in the case of landfill as end-of-life treatment and even lower in the case of incineration [37,40]; this mattered for the other four KEYIs. In particular, for ETPf, there were two outliers (2000 CTUe/W_p and 4200 CTUe/W_p). Looking only at the downstream stage, the different choices of end-of-life treatment led to higher differences in the KEYIs. Landfill and incineration without lead recycling, had higher impacts with respect to HTPc and ETPf. Particularly, for ETPf, landfill as end-of-life treatment significantly increased the toxicity potential due to the released lead to the environment [38]. Incineration with lead recycling showed less impacts compared with landfill for ETPf and even negative impacts for HTPc and RDPf [38]. Except for ETPf, the influence and tradeoffs of the end-of-life treatment were minor compared with the high upstream impacts of the manufacturing in laboratories.

3.4. Future Prospects of Emerging PVs

For the assessment of future prospects of environmental performance, in the first step, the status quo of emerging PVs was contrasted with commercial first- and second-generation PVs, thus providing a benchmark for the technological development of emerging PVs. In the second step, the possible contribution of environmental performance resulting from changes in the most influencing factors, including efficiency, lifetime, and upscaling of production, by means of sensitivity and scenario analyses, was assessed.

The conversion of the KEYIs to the functional unit of 1 kWh was based on the consistent KEYPs (η_H, PR_H, I_H), given in Table 3. To depict the current state of development as the basis of the sensitivity analysis, the maximum reported lifetimes of seven years for OPV [46] and one year for PSC and QDPV were used [44,61]. For DSSC, no lifetime assumptions were found; thus, one year was used as well. As benchmarks representing the two first-generation PVs, monocrystalline silicon (Mono-Si) and multicrystalline silicon (Multi-Si), the harmonized results of Hsu et al. [11] were applied; also, for the three second-generation PVs, amorphous silicon (a-Si), cadmium–telluride solar cells (CdTe), and copper–indium–gallium–diselenide solar cells (CIGS), the results of Kim et al. [12] were applied. As both studies reported only results for GWP, the comparison with commercial PVs was limited to this KEYI. In Figure 4, the results of this comparison are presented as boxplots of each PV technology; insights into the other KEYIs can be drawn from the results of the status quo. OPV is the only emerging PV that presently meets the benchmark of the commercial technologies, although OPV has only a seven-year lifetime compared with the 30 years of commercial PVs. The median of OPV was in a similar range to CdTe, the commercial PV with the lowest GWP impacts. The other PVs were 5–70-fold higher than the commercial benchmarks.

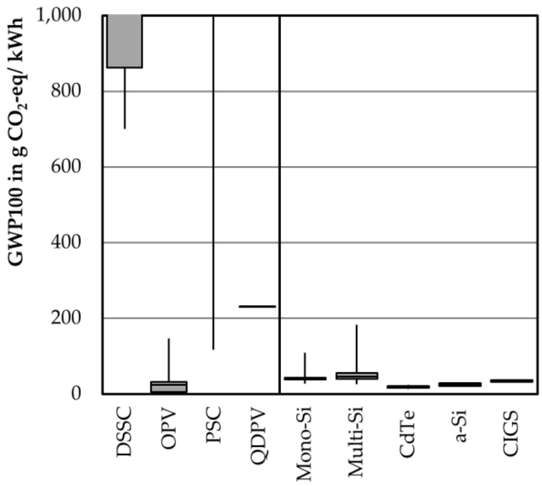

Figure 4. Global warming potential (GWP) status quo of current development of emerging PVs as presented in the LCA datasets and harmonized to the key performance parameters (KEYPs) in Table 3 and current maximum reported lifetimes of one and seven years. The comparison was based on benchmarks of the first- and second-generation PVs based on the standard values of the KEYPs (I_H = 1700 kWh/(m^2·year); PR_H = 80%; τ_H = 30 years; Mono-Si: η_H = 13%; Multi-Si: η_H = 12.3%; CdTe: η_H = 10.9%; a-Si: η_H = 6.3%; CIGS: η_H = 11.5%) taken from References [11,12].

To analyze the influence of development on the efficiency, lifetime, and upscaling, the following assumptions for the sensitivity analyses were made:

1. Efficiency increase from 1% to 25% (the latter value was set as the most optimistic assumption based on the maximum reported efficiency [3]);
2. Lifetime increase from the minimum reported lifetime of one year to the most optimistic assumption of 30 years as the typical lifetime of first- and second-generation PVs;
3. Upscaling of production from the laboratory to industrial scale was depicted as changes in the energy demand from −90% to 90% (as a proxy of the environmental impact in general) and, consequently, of the GWP impacts in the same range as a consequence of this technology scale leap.

The results of the three sensitivity analyses are presented in Figure 5. The efficiency increase had the lowest influence. An efficiency increase would achieve lower results for OPV than for CdTe, but for PSC, an increase to 25% would result in 40-fold higher GWP than Multi-Si, the most common commercial PV with the highest GWP impact of 47 g CO_2-eq/kWh. DSSC and QDPV showed values that were many times more than the commercial PVs as well. The lifetime increase to 30 years showed the highest contributions to GWP reduction. For OPV, the GWP could be decreased to 29% of CdTe and even 12% of Multi-Si; for PSC, the GWP was still higher but could be decreased to twice the Multi-Si impact. DSSC and QDPV were in the range of the benchmarks after lifetime increases to 20 and five years, respectively. The change in technology scale with stagnation of lifetime would result only in competitive GWPs for OPV, by an increase of 90% of the GWP impacts, and for QDPV, by reductions of 90%. Considering that GWP correlated directly to the energy demand, a reduction by 90% of the energy demand resulted in a reduction of 90% of the GWP impact.

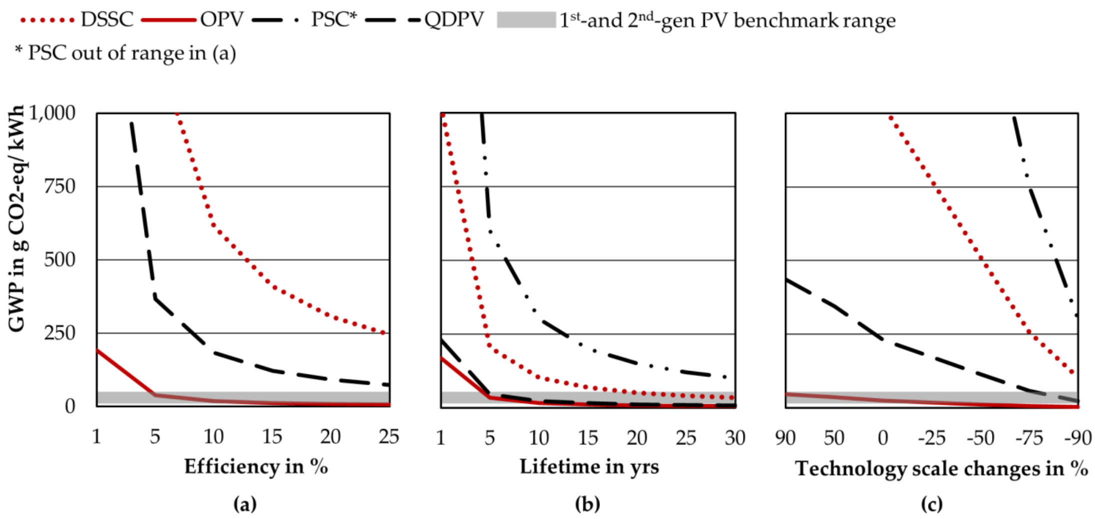

Figure 5. Sensitivity analyses of the prospective development of (**a**) efficiency, (**b**) lifetime, and (**c**) upscaling of the four emerging PVs compared with the range of the benchmarks.

In particular, for PSC and DSSC, combinations of improvement of the influencing factors in order to reach the benchmarks were needed. In Figure 6, the most promising combinations are presented as scenario analyses of lifetime increase combined with efficiency increase and upscaling reduction. Based on this, PSC would need a 90% reduction and a five-year lifetime, only a 50% reduction but a lifetime of 30 years, or a lifetime of 15 years and an efficiency of 20%. The scenario analyses of the other combinations were not as promising; they can be found in Figure S1 (Supplementary Materials). Although the reduction of 90% is on one hand, arbitrary and not substantiated by a specific study, the review of the literature indicated that this is an optimistic but realistic assumption due to the expected improvements from laboratory to industrial scale regarding the material selection, material quantities, and efficiency of deposition methods.

Based on the insights from the status quo analysis, the behavior of the material-related KEYIs was quantitatively envisaged. They are expected to behave similarly to CED and GWP regarding lifetime and efficiency changes, since this behavior is described based on Equation (7). Accordingly, no tradeoffs were expected from these factors. In contrast to this, the KEYIs would behave differently regarding upscaling and change in energy demands. In particular, for RDPf, no significant changes would be expected from a decrease in energy demand during production due to the low contribution of the energy-related fossil fuel resources to this KEYI. For the other two KEYIs (HTPc and ETPf), lower energy demands would be expected to result in reductions, even if not to the same extent as for GWP. Here, tradeoffs between life cycle stages might be expected. The reduction of the upstream impact might result in increasing contributions of the downstream impact.

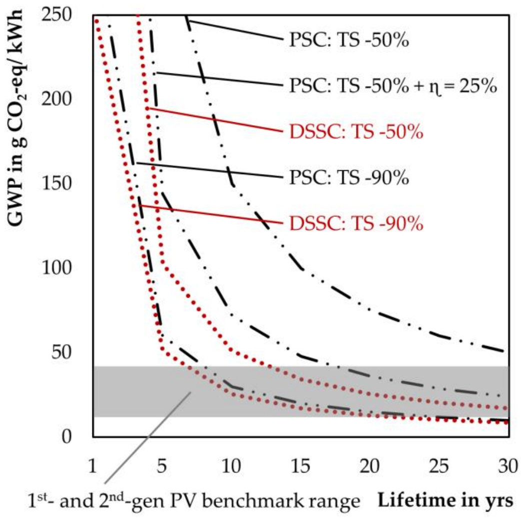

Figure 6. Summary of the scenario analyses of the three influencing factors, efficiency, lifetime, and upscaling, for perovskite solar cells (PSC) and dye-sensitized solar cells (DSSC); the single-scenario analyses of each combination of the influencing factors are given in Figure S2 (Supplementary Materials).

4. Discussion

The environmental performance of emerging PVs was investigated based on a meta-analysis, including a systematic review and harmonization approach of 94 LCA datasets on DSSC, OPV, PSC, and QDPV. The systematic review showed that the definitions of the KEYPs, as well as the KEYAs, especially the technology scale, were not reported and explained sufficiently. For transparency reasons, the report of these values and the classification of the technology scale are highly recommended. The benefits of the harmonization approach are twofold. Firstly, it reduces the deviations of LCA results through the use of standard values of the KEYPs. Secondly, the alignment of LCA results to two alternative functional units enables a substantiated discussion of the environmental performance of emerging PVs for the two cases of status quo and future prospects. The status quo encompasses technology scales from the early laboratory state; here, the functional unit of 1 W_p restricted the comparison of the material-related property related information of PV only to the industrial manufacturing scale. Here, in contrast, the functional unit of 1 kWh included additional information on the application by integrating the lifetime into the comparison. Thus, a comparison of emerging to commercial technologies was feasible in view of identifying benchmarks of environmental performance; based on these benchmarks, the high uncertainty as to a future use phase was tackled by means of sensitivity analysis, leading to a scenario approach for different strategies of further technology development.

The analysis of the status quo based on the harmonized KEYIs showed the differences between the four assessed emerging PVs in terms of the median and IQR. In general, it should be noted that, for DSSC and QDPV, only a very limited number of LCA datasets were available, which generally restricted the validity of conclusions for these two technologies. For OPV, which was based on 67 LCA datasets, by far the lowest values for the median, i.e., best environmental performance, were found for all KEYIs except for resource depletion, RDPf, where the difference to PSC was low. Also, IQR was by far the lowest for OPV. The analysis of the KEYAs confirmed that these findings stood for a rather mature technology from the environmental perspective that is ready to enter the market; the good environmental performance could be mostly attributed to the low impact from production and less to the efficiency. On the contrary, for PSC, a far higher median was found; also, after harmonization, high deviations of results depicted a large IQR. As the functional unit of 1 W_p represented the material-related properties of the PV only, the reasons for these results may have come from two contributions: the kind of layer material and the energy demand of the layer deposition, i.e., the stage of technology development. The KEYAs and an in-depth analysis of the underlying LCA studies confirmed the high share of LCA datasets that were based on the early stage of development, associated with inefficient manufacturing methods of laboratory components and, thus, high energy demand. RDPf was the only KEYI not influenced by high energy demand and, for which, PSC could keep up at the current stage of development with OPV due to its higher efficiency. Based only on the material, the downstream phase could also be investigated as part of the status quo analysis. Based on the assumption of an advanced waste management, the influence of end-of-life treatment in general was low compared with the upstream impact.

For the analysis of future prospects, the use phase was included as additional information, notably the lifetime of the respective emerging PV. Based on the results of the current stage of development and assumptions on lifetime from the literature, the comparison with commercial PVs of the first- and second-generation PVs showed that, currently, OPV is the only emerging PV that can compete with commercial PVs, which was in line with the earlier finding that, out of the four investigated technologies, OPV is the only mature one. The future prospects of the other three technologies could be explored by sensitivity analysis of the three influencing factors of efficiency, lifetime, and upscaling; for the latter, the energy demand was used as a proxy for environmental impact in general. The results of the sensitivity analysis showed that efficiency increase had the lowest influence. Consequently, enhancement of efficiency alone could not make any of the three emerging technologies competitive with respect to the environmental performance of commercial PVs. Lifetime and energy efficiency had a greater influence and might be important, notably for DSSC, QDPV, and PSC. In general, a combination of improvements in each of the three influencing factors would be the most promising way to competitiveness. For this, the sensitivity analysis could be widened to a scenario analysis in order to identify successful combinations of improvements, where each contribution could be substantiated by the current state of evidence from the laboratory. This was explored in detail for PSC and DSSC. Current LCA results confirmed that considerable potential for improvement lies in the combination of a lifetime increase from five to 30 years and upscaling to the industrial scale, with expected reductions of more than 90%.

5. Conclusions

The application of LCA for emerging technologies has contradictory requirements. On one hand, the room for maneuvering in terms of freedom of design is largest in the early stages of technology development, which calls for a very early application in support of the development process. On the other hand, uncertainty of data for the technology alternatives for the future use phase compromises the usefulness of results from LCA for decision support. The developed harmonization approach for emerging PV presents a structured way not only to reduce uncertainty but also to extract significant information from the point of view of different stages of technology development. For the status quo analysis, information was reduced to the material-related properties, thus removing the high uncertainties resulting from assumptions of the future use phase. For the analysis of future prospects, the uncertainty of the use phase was handled by means of sensitivity and scenario analyses, where comparison with commercial PVs had the function of a benchmark that could be used for analysis of the current stage and strategies of technology development.

The important findings for the status quo concerned the characterization of the differences between PV technologies related to their selected materials and their current stage of development. The harmonized KEYIs showed important differences between technologies, and also within the technology of PSC, which could be attributed to the underlying material systems. Conclusions from the analysis of these differences were twofold. Firstly, possible tradeoffs between impact categories, notably those related to energy and those related to toxicity, were not as relevant as might have been expected. An important caveat is that this conclusion was based on a future end-of-life phase that met the requirement of a state-of-the art waste management system, ensuring sound management of toxic compounds of PV materials. Interestingly, a positive contribution from the end-of-life phase to the environmental performance of emerging PVs could possibly be envisaged from advanced recycling technologies for materials that are currently not well developed and, thus, not reflected by LCA studies. Secondly, a significant influence of different material systems can be seen for the energy-related KEYIs, which resulted from the interdependence of selected material system and layer manufacturing techniques. The latter indicated the high contribution of inefficient laboratory manufacturing to the status quo performance of emerging PV. Future LCAs could be supported by a more in-depth investigation of upscaling, yielding information on methods, materials, and cell configurations of industrial manufacturing.

The investigation of future performance of emerging PVs showed that, to meet today's technology benchmarks, a combination of improvements in the factors of lifetime and upscaling would be most promising for PSC. OPV already meets the performance level with respect to KEYIs per kWh of today's best technologies. However, the low efficiency and the related high demand of area in combination with the still low lifetime of far below 20 years hinders its application as a surrogate of today's roof application. In the case of PSC, energy savings from upscaling, as well as the possible lifetime, are crucial factors for application. Current studies gave evidence that, for PSC, an increased environmental performance from upscaling can be expected with a high probability. Regarding possible lifetimes of PSC in real world conditions, until now, no reliable statement can be made. However, if the challenge of a high lifetime can be managed successfully by technology improvement, in view of the already high efficiency, this technology might be a future substitute or supplement for roof application, competing with or even exceeding the performance of today's PVs. Here, one development went for tandem application with enhanced efficiencies [3,62,63]. With respect to the other two emerging PVs, DSSC and QDPV, as of now, the available literature is too small to draw conclusions for future prospects.

As a general conclusion regarding LCA studies on emerging technologies, these insights point to the importance of the intended application of a technology that received little attention in LCA studies for PVs until now. Most current studies implicitly assumed that emerging PVs will substitute existing ones or other electricity generation technologies feeding the grid. However, due to their novel properties, emerging PVs might have many other applications even at shorter lifetimes than today's PVs, such as small devices, e.g., mobile chargers, lamps, clothes, and other gadgets. Due to the change in intended application, other benchmarks for technology development and comparisons of the environmental performance need to be considered for these devices. As a first example, in [64] an LCA of a mobile charger with an integrated OPV cell was performed and the environmental performance in comparison with substituted electricity from the grid as a benchmark was analyzed. Obviously, for such novel applications, behavioral aspects in the use phase, as well as different requirements for the end-of-life management, might substantially influence environmental performance in the life cycle [64]. Thus, for a comprehensive picture of future environmental performance of emerging technologies, not only the technology itself but also emerging applications of technologies should be considered in LCA studies.

Supplementary Materials: The following are available online at http://www.mdpi.com/1996-1073/12/22/4228/s1: Table S1: Keywords and synonyms of the database search; Table S2: Overview of the excluded LCA datasets per collected LCA study after the secondary screening; Table S3: Ratio between best research cell efficiencies and standard values of first- and second-generation PVs; Table S4: Comparison of the descriptive statistics of the KEYIs harmonized to the consistent functional unit of 1 W_p and after full harmonization (including the standard values of the efficiency), subdivided by the five KEYIs; Figure S1: Influence of the KEYAs on the single harmonized LCA dataset points of the five KEYIs (a) technology scale (laboratory (L) vs. pilot/industrial (PI/IN)); (b) product system (cell (C) vs. module/system (M/S)); (c) system boundaries (cradle-to-gate (Gate) vs. cradle-to-grave (Grave); Figure S2: Detailed scenario analyses of the three influencing factors, efficiency, lifetime, and upscaling, for PSC and DSSC; File S1: Supplementary meta-analysis results.

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Nomenclature

PVs	**Photovoltaic technologies**
Mono-Si	Monocrystalline silicon
Multi-Si	Multicrystalline silicon
a-Si	Amorphous silicon
CdTe	Cadmium–telluride solar cells
CIGS	Copper–indium–gallium–diselenide solar cells
CZTSSe	Copper–zinc–tin–sulfur–selenide solar cell
DSSC	Dye-sensitized solar cell
OPV	Organic photovoltaic
PSC	Perovskite solar cell
QDPV	Quantum-dot photovoltaic
KEYIs	**Key indicators**
CED	Cumulative energy demand in MJ PE (primary energy)
ETPf	Ecotoxicity potential for freshwater in CTUe (comparative toxic units for ecosystems)
GHG/GWP	Greenhouse gas/global warming potential in g CO_2-eq (carbon dioxide equivalents)
HTPc	Human toxicity, cancer effects in CTUh (comparative toxic units for human health impacts equivalent to incidence of cancer)
RDPf	Resource depletion, mineral, fossil, and renewable resources in g Sb-eq (antimony equivalents)
KEYAs	**Key modeling assumptions**
C	Conventional
P	Prospective
TS/TRL	Technology scale/technology readiness level
L	Laboratory scale
PI/IN	Pilot/industrial scale
KEYPs	**Key performance parameters**
η	Efficiency
τ	Lifetime
I	Irradiation
PR	Performance ratio
Further	
BOS	Balance-of-system
LCA	Life-cycle assessment
W_p	Watt-peak

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3 Scheme for Generating Upscaling Scenarios of Emerging Functional Materials Based Energy Technologies in Prospective LCA (UpFunMatLCA)

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METHODS ARTICLE

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Scheme for generating upscaling scenarios of emerging functional materials based energy technologies in prospective LCA (UpFunMatLCA)

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Abstract

Upscaling scenarios are indispensable elements of prospective life cycle assessment (LCA). However, current studies reveal confusing terminology and a wide range of approaches in this area. Therefore, we first defined the term upscaling scenario as the description of a possible future target stage of emerging technology, including the development pathway from a current stage within the course of research and development to this future stage. Second, we developed the novel systematic scheme UpFunMatLCA for generating explorative scenarios based on possible development pathways of the specific group of emerging functional material (FunMat)-based energy technologies, including status quo developments. UpFunMatLCA represents a three-step extension of conventional LCAs to upscale the life cycle inventory of emerging FunMats. UpFunMatLCA is based on a clear definition of a current status quo (conceptual, lab, or pilot stage) and a target matured (fab) development stage. A core part of UpFunMatLCA is the so-called upscaling module, providing specific modeling methods and data for the upscaling of FunMats. Using perovskite solar cells, photovoltaic devices based on several FunMats and attached with great expectations regarding the future efficient provision of solar energy, we demonstrate the application of UpFunMatLCA, focusing on the upstream greenhouse gas (GHG) emissions of the prospective manufacturing. In the discussion, we point out the application area of UpFunMatLCA and the possible extension to depict further environmental impacts beyond GHG to contribute to the sustainability assessment of emerging technologies in the early stages of development.

KEYWORDS
emerging technology, industrial ecology, LCA at early development stage, process learning, technology development, upscaling scheme

1 | INTRODUCTION

The energy transition to sustainable, renewable, and low-carbon technologies is also a material transition. Energy technologies such as photovoltaics (PV), batteries, or fuel cells are highly dependent on the development and advancement of the so-called functional materials (FunMat) (Kuznetsov & Edwards, 2010; Schebek et al., 2019). In contrast to structural materials characterized mainly by their mechanical, load-bearing capacity, FunMats are featured by their physical–chemical properties responding to electrical, magnetic, optical, or chemical influences and cover glass, metals, polymers, carbons, ceramics, composites, and semiconductors, which form the basis of sustainable energy technologies (Chung, 2021; Kuznetsov & Edwards, 2010). Furthermore, fostering sustainable development of energy technologies research initiatives such as Horizon 2020 demand the inclusion of environmental assessment methods such as the life cycle assessment (LCA). Accordingly, LCA integrated into fundamental research projects enables sustainable guidance of the research and development of emerging FunMats at the point with the highest design freedoms. However, this stage is also the stage with the highest uncertainties about the future performance of mature technology. Therefore, LCA, as designed for matured technologies, requires a thorough interpretation for application to emerging technologies.

The comparability of LCA on emerging and mature technologies is highly dependent on the technology maturity and stage of development. Gavankar et al. (2015) found a dependence of the technology maturity on environmental performance and recommended the interpretation of LCA results exclusively under the specification of the technology maturity using known classification schemes such as the technology readiness level (TRL) (National Aeronautics & Space Administration (NASA), 2007) and manufacturing readiness level (MRL) (US DoD, 2015). Both concepts describe the technology or manufacturing development from the lowest, the conceptual fundamentals (TRL/MRL 1) to the highest levels, the proven applicable technology (TRL 9) or the full rate manufacturing (MRL 10). For example, looking at perovskite solar cells (PSC), one promising emerging PV technology with an outstanding record power conversion efficiency of 25.7% (UNIST Korea) in the laboratory (lab) (TRL < 4) in 2022 (National Renewable Energy Laboratory (NREL), 2022), a review on the environmental performance of emerging PVs showed two things (Weyand et al., 2019). First, LCAs on PSC mainly focus on upstream emissions of lab manufacturing and are based on lab data. Second, these LCAs indicate much higher cumulative energy demands, greenhouse gas (GHG) emissions, and other environmental impacts than mature technologies of the first and second PV generation and other emerging PVs, although PSC manufacturing is expected to show lower upstream impacts. As the main contributor, the inefficient manufacturing with energy-intensive equipment in lab compared with mature technologies fabricated commercially (fab) was identified (Weyand et al., 2019). Therefore, a final statement as to whether PSCs could become more environmental friendly than their competitors is challenging based on these LCAs.

In the LCA community, this challenge of LCA on emerging technologies has been recently acknowledged under the term prospective or ex ante LCA (Arvidsson et al., 2017; Cucurachi et al., 2018). This term distinguishes traditional so-called conventional or ex post LCAs, which assess mature technologies at a current development stage (status quo) with real-world data, and prospective or ex ante LCAs. Both terms encompass the environmental assessment of emerging technologies as guidance of technology development. The difference is that ex ante LCAs focus on the assessment before market introduction (van der Giesen et al., 2020), whereas "an LCA is prospective when the (emerging) technology studied is in an early phase of development (…), but (…) is modeled at a future, more-developed phase" using the definition of Arvidsson et al. (2017). Consequently, prospective LCA also allows assessing future developments of established technologies integrating forecasting methods, as van der Giesen et al. (2020) stated. In our study, we use the broader term, prospective LCA. The model or "procedure that projects how (…) [an emerging] technology currently available at a lower TRL may look and function at a higher TRL" is defined as upscaling method using the definition of Tsoy et al. (2020) in the following.

Current literature identifies confusing terminology regarding the term upscaling and a wide range of upscaling methods (Bergerson et al., 2020). Systematic reviews on the challenges of prospective LCAs only touch upon the topic of upscaling methods regarding the projection of future process performances and the modeling of life cycle inventory data subdivided into the foreground and background systems and the prediction of future performances due to an increase of the physical process size (Hetherington et al., 2014; Moni et al., 2020; Thonemann et al., 2020; van der Giesen et al., 2020). In some studies, the development of scenarios is recommended to upscale technology maturity and inventory data using data sources such as "scientific articles, patents, expert interviews, [or] unpublished experimental data" (Arvidsson et al., 2017) or estimation methods such as process simulation, manual calculations, molecular structure models, or proxy (Tsoy et al., 2020). Even though Thonemann and Schulte (2019) do not directly use the term scenario, their presented four-step approach includes the assessment of the status quo and two prospective upscaled processes, the "best-case" and "scaled process," which are similar to a baseline, best-case, and realistic scenario. Generally, scenarios in prospective LCAs often focus merely on a hypothetical future technology maturity but not on the development pathways to this technology maturity. However, the term scenario, as initially intended in future research, encompasses both the "conceptual future" and the "paths of development (…) from which a specific conceptual future results" (Kosow & Gassner, 2008). Therefore, we introduce the term upscaling scenario and define it as the description of a possible future stage of emerging technology, including the development pathway from a current stage within the course of research and development to this future stage.

The upscaling framework of van der Hulst et al. (2020) introduces experience mechanisms taking into account the size and learning effects as main drivers of technology development from TRL 1 to TRL 9 and above using MRL and market penetration levels (MPL), as another classification

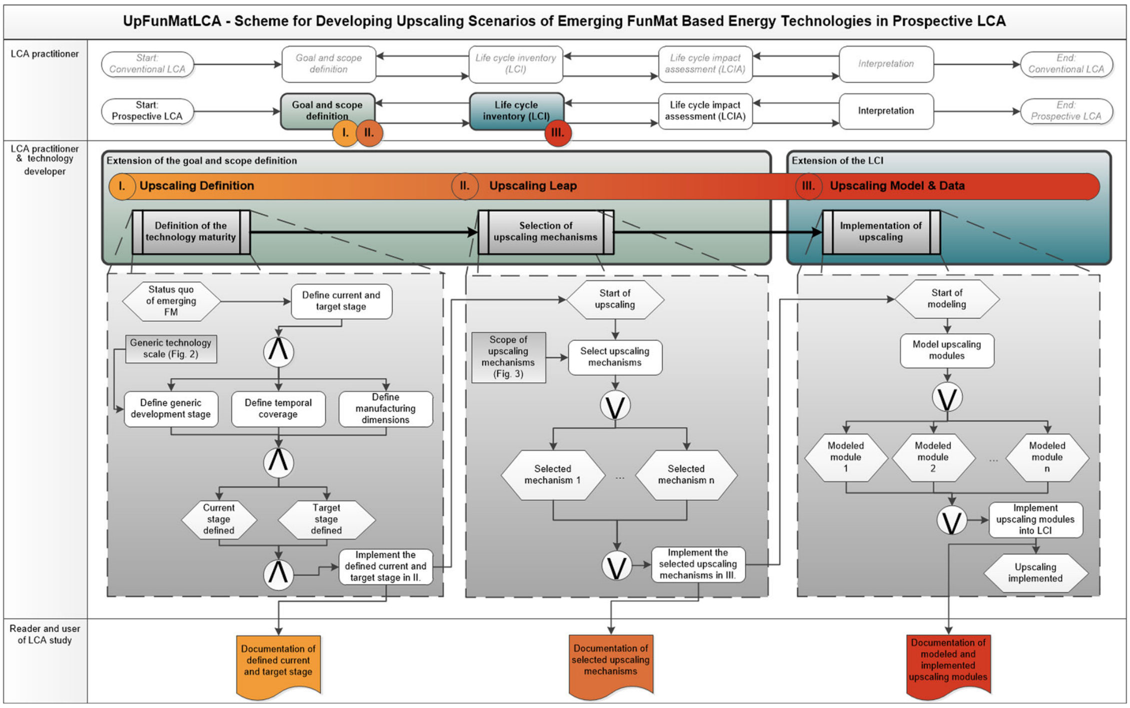


FIGURE 1 Workflow of the UpFunMatLCA with the three upscaling Steps I–III (marked with orange circles) as extensions to the four life cycle assessment (LCA) phases in prospective LCAs and the division of the three user groups—LCA practitioner, cooperation with technology developer, and user of prospective LCA study (symbols are used according to ISO 5807 (ISO 5807 1985)).

scheme. Whereas the size effect stems from the mere increase of the physical dimensions, such as the manufacturing size of products, the learning effect covers all changes resulting from experience gain of daily routines at production sites. Other authors provide a comprehensive summary of available upscaling methods with linkage to TRL developments (Buyle et al., 2019) or focus on single experience mechanisms based on size effects (Caduff et al., 2011; Kawajiri et al., 2020) or learning effects (Bergesen & Suh, 2016; Thomassen et al., 2020). Accordingly, previous studies and frameworks support structuring a prospective LCA case study and developing upscaling scenarios in terms of identifying key drivers or descriptors. However, the term scenario is not used in these studies.

Considering the gap between the theoretical and practical implementation of upscaling scenarios in prospective LCA case studies on emerging FunMats, we present a scheme for generating upscaling scenarios of emerging FunMat-based energy technology called UpFunMatLCA. UpFunMatLCA aims to generate fast and easily qualitative and quantitative scenarios for the transfer into the life cycle inventory (LCI) of prospective LCA. It enables the selection of suitable upscaling methods based on selected upscaling leaps to generate one or more scenarios from predefined development pathways in a consistent, transparent, and comparable manner for modeling foreground and background systems and upscaling LCI data. The selection of these predefined development pathways does not aim to generate best- or worse-case scenarios but somewhat realistic scenarios that intend to represent possible development pathways of FunMats based on current technology developers' knowledge or specific decisions during technology development. Therefore, the generated scenarios are explorative in the sense that they assess possible technology developments focusing on salient characteristics and interactions of main contributors or key drivers. The predefined development pathways are not complete for all available and forthcoming FunMats but can be extended analogously by further expert knowledge or new research insights. Using the case of GHG emissions of PSC from lab to fab, we illustrate the application of UpFunMatLCA and provide all vital information and data for generating upscaling scenarios.

2 | METHODOLOGY OF UPFUNMATLCA—SCHEME FOR GENERATING UPSCALING SCENARIOS OF EMERGING FUNMAT-BASED ENERGY TECHNOLOGIES IN PROSPECTIVE LCA

UpFunMatLCA, shown in Figure 1, stands for the systematic arrangement of three developed upscaling steps as an extension of conventional LCAs for attaining and integrating upscaling scenarios into the first two LCA phases, goal and scope definition and LCI, according to the ISO standards 14040 (2006) and ISO 14044 (2006). The other two LCA phases, encompassing life cycle impact assessment (LCIA) and interpretation, are out of the scope of UpFunMatLCA and are conducted as in conventional LCAs. The upscaling scenarios, as defined in the introduction, are applied for an emerging FunMat "for which there is just an experimental proof of concept, a validation in the lab, or pilot plant" (Cucurachi et al., 2018) and which shows the possible application in future energy technology. The three upscaling steps of UpFunMatLCA were developed from the five phases of the scenario technique of Kosow and Gassner (2008), combined with a systematic review of upscaling in LCA and the involvement of technology expertise. More information on the development of UpFunMatLCA is explained in Table S1 of the Supporting Information S1.

Following the scheme, the technology developer and LCA practitioner are jointly guided through the selection of predefined development pathways representing possible future design choices and their evaluation supporting the process of data acquisition and specification of assumptions that forms the basis of the upscaling scenarios. Thus, a mutual understanding is fostered within the working process, which will serve as the common ground for understanding and interpreting LCA results and support sound decision making.

The three steps of UpFunMatLCA are specified as follows:

Step I. Upscaling Definition:

For a stringent definition of the term upscaling in terms of the technology maturity, the starting point or baseline scenario, referred to as the current stage of the technology development, and the forecasted endpoint after upscaling must be defined, referred to as the target stage.

Step II. Upscaling Leap:

The upscaling leap representing the technology maturity of emerging FunMat from the current to the target stage is defined by the so-called upscaling mechanisms. According to van der Hulst et al.'s (2020) experience mechanisms, the upscaling mechanisms describe the changes or innovations expected during technology development.

Step III. Upscaling Model and Data:

The implementation of a specific upscaling leap and modeling of upscaling mechanisms takes place in Step III. To this end, the so-called upscaling modules are introduced. These modules reflect independent units that include upscaling methods and data specified for the upscaling of FunMats and are ready for the implementation in LCI of prospective LCAs.

Documenting each upscaling step is essential for two reasons: First, the readers of prospective LCAs are a broad audience consisting of LCA practitioners in general but mainly of non-LCA experts, such as technology developers, who are interested in the environmental performance of their technology or forced to conduct similar LCAs themselves, or policymakers, who are interested in incorporating LCA results into decision making. Second, in contrast to conventional LCAs, the scenario assumptions in terms of the high design freedoms result in a high dependency on the decisions made on future conditions, materials, and manufacturing processes and the results in terms of the environmental performance of emerging technologies. To this end, we introduce a documentation template that gives an overview and summary of the salient characteristics of each upscaling scenario (Table S2 of the Supporting Information S1 or applied in Table 1).

In the following, each step of UpFunMatLCA is explained in more detail.

2.1 | Step I—Upscaling Definition: Definition of the technology maturity

Theoretically, the definition of the technology maturity at the current and target stage can be done by the selection of each level using the standard classification schemes of TRL (NASA, 2007) and MRL (US DoD, 2015). However, even though the detailed assignment of TRLs/MRLs is desirable in technology development (NASA, 2007), the interest of LCA on emerging FunMats is not in upscaling between closely spaced or adjacent TRL/MRL levels but between general stages of development—such as "from lab to fab." Additionally, in practice, this level of detail is not feasible since changes in technologies with TRLs lower than 7 (MRLs lower than 8) occur iteratively, and available LCI data often cannot be attributed to a detailed TRL/MRL or stem from different levels in LCA. Therefore, we combine both classification schemes into one generic technology scale with five generic development stages to define the current and target stages. Furthermore, this technology scale incorporates the MPL similar to van der Hulst et al. (2020) to classify the dissemination of the technology after market launch. Using the characteristics summarized in Figure 2, the current stage, which represents an emerging material or technology at the status quo, is defined as either the conceptual, lab, or pilot stage; whereas the target stage, which represents the projected matured technology, is defined as either the fab-early or fab-mature stage. In addition, the definition of technology maturity encompasses the definition of the temporal coverage in terms of the base year and the target year of modeling and the definition of the manufacturing dimensions or product sizes of the current and target stages.

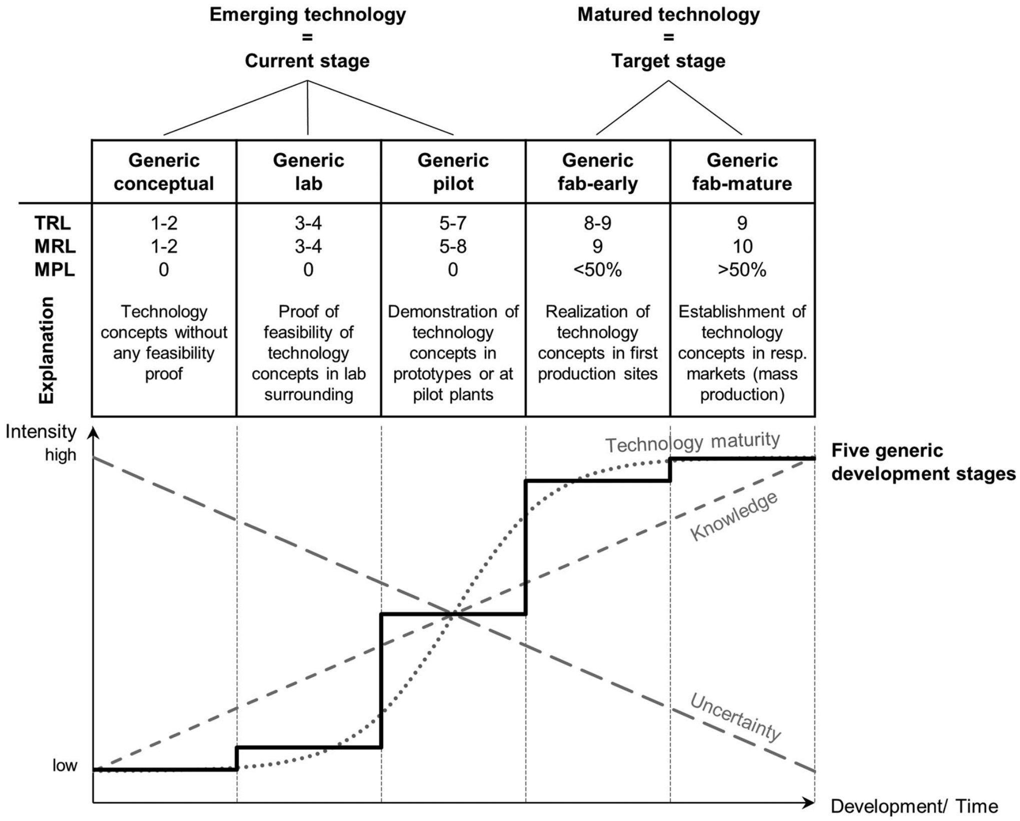


FIGURE 2 Generic technology scale for the definition of the modeled development stages illustrating the schematic dependency of the intensity of technology maturity, knowledge, and uncertainty on the five generic development stages (as summary and extension of Arvidsson et al., 2017; Bergerson et al., 2020; Grübler, Nakićenović, and Victor 1999; van der Hulst et al., 2020; National Aeronautics & Space Administration (NASA), 2007; US DoD, 2015), more details are available in Table S3 of the Supporting Information S1).

2.2 | Step II—Upscaling Leap: Selection of upscaling mechanisms for describing the leap from current to target stage

Upscaling mechanisms are the key drivers of the scenarios or the descriptors of the upscaling leap from the current to the target stage. These mechanisms are specified for FunMats based on thorough literature research and exchange with technology developers, aiming to select predefined development pathways consistently, transparently, and without additional extensive research. Therefore, we focus on the following upscaling mechanisms.

2.2.1 | Generic upscaling mechanisms for FunMat

Focusing on the upstream life cycle processes, including raw material processing and manufacturing of emerging FunMats, we discern three general upscaling mechanisms: changes in the (A) manufacturing processes, (B) materials, and (C) external developments. Whereas (A) and (B) belong to changes in the foreground system, (C) depends on background system's changes. The characteristics of each upscaling mechanism are summarized in Figure 3 and as follows:

A. **Process learning** subsumes innovations regarding the manufacturing processes.
   - **A-1 Technological learning** reflects changes in the type of manufacturing processes from the current to the target stage. Accordingly, the manufacturing equipment changes in the type and requires mapping from current to target stage equipment. Furthermore, the change in manufacturing processes can occur between any development stage, from lab to fab-early (Figure 3).

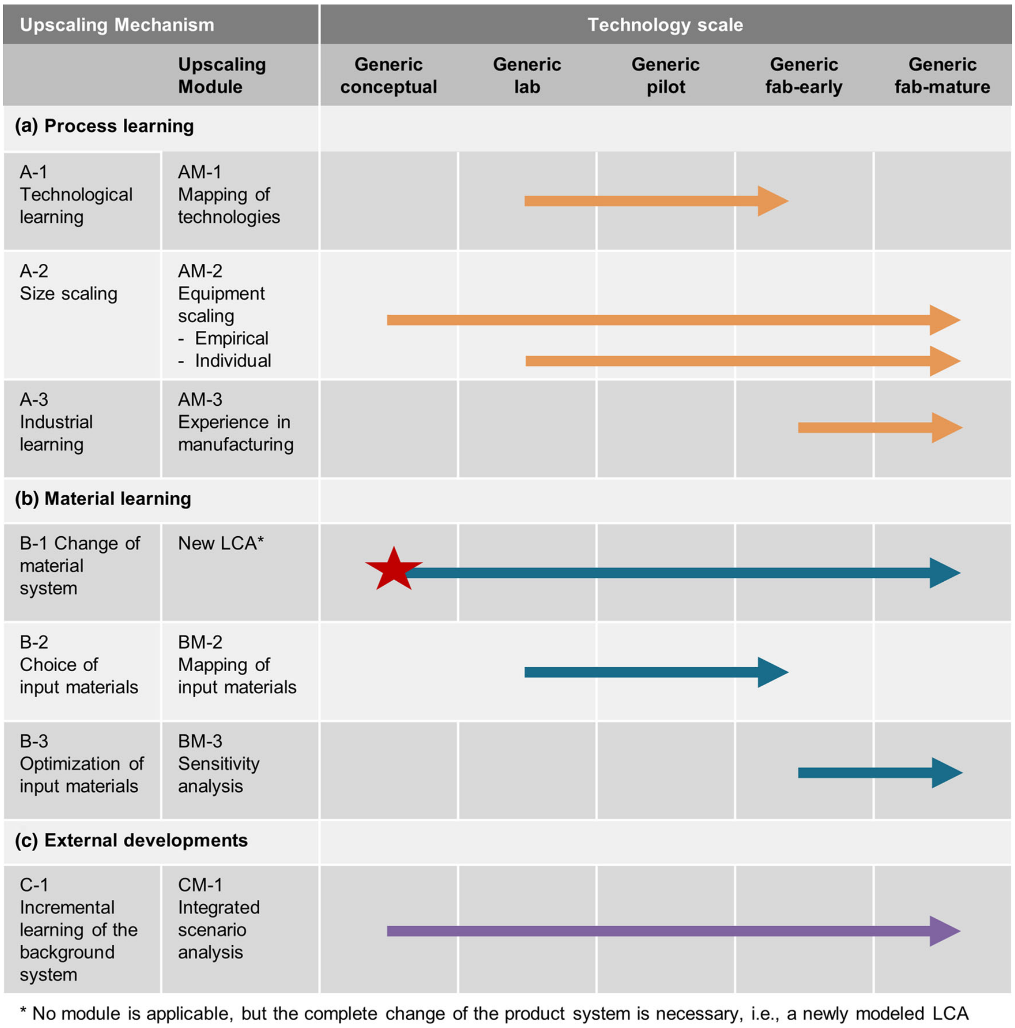


FIGURE 3 Schematic illustration of the scope of the upscaling mechanisms concerning a specific "leap" from one to another generic development stage for the upscaling of emerging FunMat-based technologies. Legend: orange arrows, possible leap of the process learning modules; blue arrows, possible leap of the material learning modules; purple arrows, possible leap of the external developments module; red star, change of material system is always related to a conceptual change, resulting in a new life cycle assessment.

- **A-2 Size scaling** displays the size effect resulting from the improvements due to the increase of the manufacturing size from current lab samples in square centimeters to target mass-produced modules in the square meter range. This mechanism can be applied at each development stage for upscaling from general conceptual to fab-mature or in between (Figure 3) if the respective manufacturing equipment changes only in size but not type.
- **A-3 Industrial learning** incorporates efficiency increase due to the experience gained from daily routines at production sites of industrial manufacturing, the so-called experience effect (Abell & Hammond, 1979). Accordingly, industrial learning occurs only between fab-early and fab-mature (Figure 3).

B. **Material learning** subsumes innovations regarding the material system, including the related raw materials, and is intimately linked to the natural science-based development process of novel materials.

- **B-1 Change of material system** results in a conceptual change of the entire considered product system independently of the current stage. One example would be the change from a dye sensitized to a PSC, which corresponds to a new technology system and thus requires an entirely new LCA.
- **B-2 Choice of input materials** encompasses the optimization of material systems in terms of change of single input materials (e.g., the substitution of lead by tin in PSC or the change of substrate material from glass to plastic).

B-3 Optimization of input materials involves minimizing material inputs by either directly reducing production losses or recycling production waste.

C. **External developments** subsume innovations resulting from the external progress of the background system over time.

C-1 Incremental learning of the background system includes, for example, efficiency gains during the extraction of raw materials or transition of the energy system to renewable technologies.

2.2.2 | Selection of the upscaling mechanisms

At the start of the upscaling, the upscaling leap from the current to the target stage preselects the relevant upscaling mechanisms using Figure 3. Then, the final upscaling mechanisms are selected considering the following three options: (1) all preselected upscaling mechanisms, (2) focus on a single upscaling mechanism, for example, the main contributor at the current stage, (3) interactions between the upscaling mechanisms, for example, the manufacturing process depends on the choice of materials, and, thus, a combination of the process and material learning mechanisms is necessary.

2.3 | Step III—Upscaling Model and Data: Implementation of upscaling—modeling of upscaling modules for process learning

In Step III—Upscaling Model and Data (Figure 1), the implementation of upscaling takes place. To this end, we focus on the three upscaling modules (AM-1–3) of the process learning mechanism, introduce their general upscaling methods and explain the associated additional data collection processes compared to conventional LCI.

2.3.1 | AM-1 Technological learning module "mapping of technologies"

According to van der Hulst et al. (2020), the modeling method of this module includes learning "from existing industrial processes through an analysis of functions, dimensions, and similarities." Therefore, a qualitative mapping from the current manufacturing process to the target counterpart is recommended for implementing technological learning based on comprehensive research of technical literature and patents. Furthermore, the quantitative implementation of this module can be done according to the size scaling module (see below).

2.3.2 | AM-2 Size scaling module "equipment scaling"

For the mathematical implementation of the size effect, we translate the two published models of Kawajiri et al. (2020) into the assumption that the energy demand of a manufacturing process and the power demand of the respective equipment will decrease per manufactured square meter by increasing manufacturing size of the FunMat from current to target stage. Accordingly, for implementing the size effect, the empirical data sets of the two technical parameters, nominal power and maximum manufacturing area of respective equipment, need to be collected from technical data sheets and product specifications of respective manufacturing equipment. The modeling is based on the two scaling parameters, scaling factor b and scaling coefficient c. Both scaling parameters are derived from the log-form relationship between the two technical parameters using the ordinary least square regression method. For FunMat, we adjust the two models as follows and use Equations (1)–(3) to project the energy demand per manufactured area at the target stage.

Model 1 is referred to as empirical scaling since only empirical data of the manufacturing processes and respective equipment is used. Here, the power demand P_{it} per manufacturing process i at the target stage t is calculated based on Equation (1), where b_j, c_j stand for the scaling factor and coefficient of the respective equipment j and S_{it} for the equipment capacity of the manufacturing process i in terms of the manufacturing area at the target stage t:

Model 1: Empirical scaling:

$$P_{it} = c_j \cdot {S_{it}}^{b_j} \tag{1}$$

In contrast, Model 2 is referred to as individual scaling since individual data measured at the current stage is integrated into the calculation of P according to Equation (2). Here, P_{it}, S_{it}, b_j, and c_j are used as in Equation (1), and P_{i0} stands for the measured power demand of each manufacturing process i and S_{i0} for the manufacturing area at current stage 0:

Model 2: Individual scaling:

$$P_{it} = P_{i0} \cdot \left(\frac{S_{it}}{S_{i0}} \right)^{b_j} \tag{2}$$

Finally, the power demands P_i at the target stage t are used to calculate the resulting energy demand using Equation (3):

$$E_{t\_total} = \sum_{i=1}^{n} P_{it} \cdot tp_{it} \tag{3}$$

where E_{t_total} is the total upscaled energy demand at target stage t, P_{it} the power demand and tp_{it} the processing time at target stage t per manufacturing process i.

This upscaling module uses empirical data based on historical findings. In many cases, this data is helpful since similar equipment is provided in most labs. However, historical findings might be missing in the case of new manufacturing processes; thus, this upscaling module cannot be applied.

2.3.3 | AM-3 Industrial learning module "experience in industrial manufacturing"

Based on production-site-specific data, the standard methods of the experience concept can be applied, as shown in Bergesen and Suh (2016) and Louwen et al. (2016). For emerging technologies, there is usually no data from mass production. For the sake of completeness, this module is vital to mention here. The implementation of this module can be done qualitatively, or the effect of industrial learning can be studied based on general information on industrial learning of related technologies and applied to emerging technologies.

3 | CASE STUDY: UPSTREAM GHG EMISSIONS OF PSC FROM LAB TO FAB

The goal of the case study is to present the application of UpFunMatLCA by upscaling the GHG emissions of PSC samples manufactured at the lab (current stage) but projected and evaluated as fab PV material (target stage). In particular, the extra data collection processes to fill the three upscaling modules AM-1–3 with data are demonstrated.

3.1 | Case study description

The PSC samples selected were manufactured as part of the material development of the Surface Science Group of the Technical University of Darmstadt, aiming for the optimization of PSC's performances to the physical optimum (Dachauer et al., 2019; Mortan et al., 2019, 2020; Wittich et al., 2018). They represent a typical PSC device, including several FunMats and manufacturing processes (Figure 4) commonly used in many research labs (Chen et al., 2017). The modeled life cycle of PSC samples as the product system, divided into upstream, operation, and downstream processes, is illustrated in Figure 4. As the system boundary, we focus on upstream processes. Therefore, key performance parameters, such as the efficiency necessary to model the use phase, are not considered. Accordingly, as recommended by Weyand et al. (2019), the functional unit is defined as "1 m^2 manufactured PSC area." The inventory data of the foreground system is generated from primary data collection for the current stage. For the target stage, the inventory is modeled based on the developed upscaling modules (see later). Data from literature and GaBi Professional (version: SP36, 2018) substitutes missing foreground data. The LCA database ecoinvent (version 3.7.1 cut-off) is used as background data. The GHG emissions are reported in kg CO_2-eq using the characterization model and factors of the Global Warming Potential for 100 year time horizon (GWP100) from the Intergovernmental Panel on Climate Change (IPCC) (2013).

Furthermore, we distinguish the resulting GHG emissions into the material-embedded and processing energies related emissions to investigate the hypothesis that the processing energy is the main contributor to the GHG emissions of lab-scaled PSC samples.

3.2 | Developed upscaling scenarios

Using UpFunMatLCA, three upscaling scenarios are generated, including the current and two target stages. Each step of the scenario generation (Steps I–III) is summarized in Table 1 using the documentation template of UpFunMatLCA. The extra data collection processes of the three applied upscaling modules (AM-1, AM-2, and AM-3) to the conventional LCI are explained in the following.

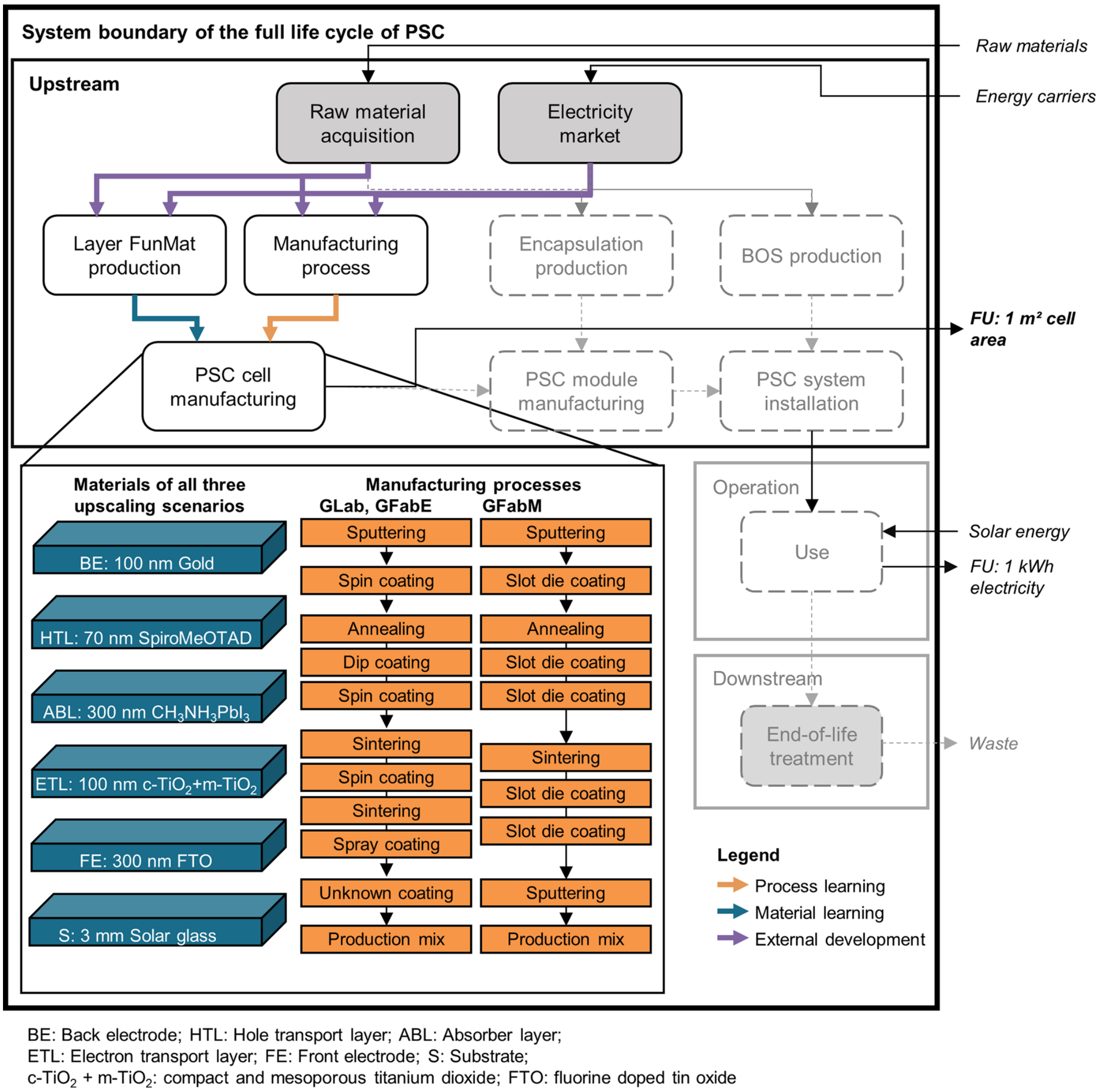


FIGURE 4 Product system of the selected perovskite solar cell samples at the status quo (extended from Weyand et al., 2019), differentiated into (1) foreground (white filled boxes) and background processes (grey filled boxes), (2) considered (black border) and unconsidered (grey dashed border) upstream, operation and downstream processes. The colored arrows mark the involvement of the upscaling mechanisms. Elementary flows are marked by italic font.

3.2.1 | AM-1 Mapping of technologies

For this upscaling module, we conducted patent and literature research. However, only the literature review provided relevant data for the technological mapping. In addition, the patent review included only scattered data on future manufacturing processes. Table 2 summarizes the mapping results from the current to target stage manufacturing processes. There are several target manufacturing processes with related equipment from which one must be selected. The patent and literature review are available in Supporting Information S2, Tabs "AM1[…]."

3.2.2 | AM-2 Equipment scaling—empirical and individual

For developing this upscaling module, two types of data were used:

TABLE 1 Key characteristics of the three generated upscaling scenarios using UpFunMatLCA.

	Current stage	Target stages	
Step I—Upscaling Definition			
Name	GLab (baseline)	GFabE	GFabM
General description	Status quo: PSC samples manufactured with a size of 20×20 mm^2 in lab surroundings; primary data was collected during lab manufacturing of 20 PSC samples in total over the period from 2016 to 2020. The cell architecture with corresponding layer FunMats and manufacturing processes is illustrated in Figure 4.	Prospective 1: Aims for the demonstration of the size scaling module, thus, increasing manufacturing size from 20×20 mm^2 to 5 m^2; same layer FunMats, same manufacturing processes used as at status quo. 2030 is assumed as market introduction year of PSC materials with low MPL (<50%).	Prospective 2: Aims for the demonstration of all three process learning upscaling modules, thus, increase of manufacturing size from 20×20 mm^2 to 5 m^2; same layer FunMats, new prospective manufacturing processes, mass production. 2050 is assumed as the year with MPL > 50%.
Generic development stage	Lab	Fab (early)	Fab (mature)
Temporal coverage	2020	2030	2050
Manufacturing dimensions	20×20 mm^2	5 m^2	5 m^2
Step II—Upscaling Leap			
Selected upscaling mechanisms (details to preselection are shown in Figure S4, Supporting Information S1)	None	A-1 Technological learning A-2 Size scaling	A-1 Technological learning A-2 Size scaling A-3 Industrial learning
Step III—Upscaling Data and Model			
Modeled modules (description see below)	None	AM-1 Mapping of technologies (Figure 4, Table 2) AM-2 Equipment scaling—individual (Supporting Information S2, Tabs “AM2[…]”)	AM-1 Mapping of technologies (Figure 4, Table 2) AM-2 Equipment scaling—empirical (Figure 5) AM-3 Experience in manufacturing

I. Over 250 empirical data sets to derive regression models of the six manufacturing processes (Table 1) for applying both the empirical (Model 1, Equation 1) and individual scaling (Model 2, Equation 2);
II. LCI data of the status quo for the individual scaling (Model 2, Equation 2).

Figure 5 provides the upscaling module, “AM-2 Equipment scaling—empirical,” including the regression models (Figure 5a) and corresponding data with model accuracy evaluation of the six manufacturing processes (Figure 5b). For five manufacturing processes, the model accuracy results in a good to moderate application of this upscaling module. Only the model of spray coating is not in compliance with the set data quality. Here, R^2 is below 0.3, which means that the manufacturing area does not describe the course of the power demand from lab to fab and, thus, that no statement can be made about the development of the power demand via the manufacturing area (see Supporting Information S2, Tabs “AM2[…]” for more details on the data quality and model accuracy evaluation). There are three possibilities for modeling the spray coating process in GFabE: (1) using the upscaling model despite the low accuracy of the upscaling data, (2) linearly scaling using the collected lab data, or (3) excluding this process due to a lack of representative data. All three cases increase the uncertainty. In (1), the consistency and scenario uncertainty is reduced due to the modeled fab scale, but the parameter uncertainty increases due to the non-representative upscaling data. In (2) and (3), the scenario and parameter uncertainty increase due to the linear scaling of the lab data and the lack of representative upscaling data, respectively. Therefore, the impacts of the spray coating on the results should be investigated. In our case, we assessed the impacts using a sensitivity analysis and found that the effects of the spray coating are negligible for the three modeling ways, with less than 1%. The detailed results of the sensitivity analysis are summarized in Table S5 of the Supporting Information S1.

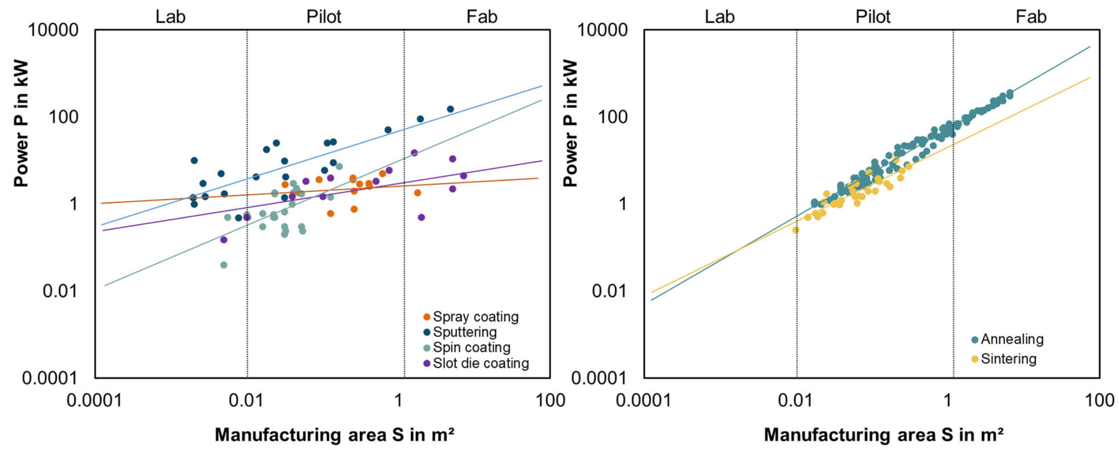
The upscaling module “AM-2 Equipment scaling—individual” is provided in the Supporting Information S2. In addition, all empirical data sets, derived regression models, scaling parameters, model accuracy evaluation, and collected individualized data are available in the Supporting Information S2.

TABLE 2 Upscaling data of the upscaling module "AM-1-Mapping of technologies": Qualitative mapping of the current process to selectable target stage process for PSC-FunMats.

FunMat	Current stage processes	Current equipment	Target stage processes	Target equipment
spiroMeOTAD (HTL), m-TiO_2 (ETL), PbI_2 (ABL precursor)	Spin coating	Spin coater	Spin coating Slot die coating Physical vapor deposition Chemical vapor deposition Printing techniques (gravure, inkjet, screen)	Spin coater Slot die coater Customized equipment Customized equipment Printer
c-TiO_2 (ETL)	Spray coating	Spray coater	Spray coating Slot die coating Physical vapor deposition Chemical vapor deposition Printing techniques (gravure, inkjet, screen)	Spray coater Slot die coater Customized equipment Customized equipment Printer
FTO (FE), Au (BE)	Sputtering (sputter coating and vacuuming)	Sputter coater with vacuum pump	Sputtering Physical vapor deposition Printing techniques (gravure, inkjet, screen)	Sputter coater Vacuum chamber with effusion cell equipment Printer
CH_3NH_3I (ABL precursor)	Dip coating	Manually	Dip coating Slot die coating Printing techniques (gravure, inkjet, screen)	Slot die coater Printer
$CH_3NH_3PbI_3$ (ABL)	Annealing	Hot oven	Annealing	Hot oven Various customized systems (infrared, hot air, contact dryer, fluid bed dryer)
c-TiO_2 + m-TiO_2 (ETL) PbI_2 (ABL precursor) CH_3NH_3I (ABL precursor) $CH_3NH_3PbI_3$ (ABL)	Heating, drying	Hot plate	Heating, Drying	Hot plate Various customized systems (infrared, contact dryer, fluid bed dryer)
c-TiO_2 + m-TiO_2 (ETL)	Sintering	Hot plate	Sintering	Hot oven Various customized systems (infrared, sintering machines, infrared)

(a) Regression models of six manufacturing processes divided into

- **Deposition processes**
- **Material property conversion processes**



(b) Upscaling data with accuracy evaluation

Manufacturing		Scaling parameter with CI		Parameter accuracy factors			Model accuracy
Process	**Equipment**	**b (95 % CI)**	**log c (95 % CI)**	**R²**	**Manufacturing area S (min-max)**	**n**	
Spray coating	Spray coater	0.08 (0.07 – 0.09)	0.41 (0.20 – 0.61)	0.02	0.032 – 1.77 m²	14	Bad
Sputtering	Sputter coater	0.55 (0.52 – 0.59)	1.70 (1.42 – 1.99)	0.67	0.002 – 5.0 m²	22	Good
Spin coating	Spin coater	0.74 (0.73 – 0.75)	0.99 (0.79 – 1.19)	0.33	0.005 – 0.17 m²	25	Moderate
Slot die coating	Slot die coater	0.27 (0.26 – 0-28)	0.46 (0.13 – 0.79)	0.44	0.005 – 210 m²	15	Moderate
Annealing	Hot oven	1.01 (1.00 – 1.01)	1.70 (1.68 – 1.73)	0.98	0.02 – 7 m²	159	Good
Sintering	Hot plate	0.86 (0.85 – 0.86)	1.28 (1.20 – 1.36)	0.84	0.01 – 0.31 m²	33	Good

CI: confidence interval; R²: Coefficient of determination; n: Number of data sets

FIGURE 5 Upscaling module "AM-2 Equipment scaling—empirical": (a) Regression models divided into deposition and material conversion property processes; (b) upscaling data including scaling parameters and accuracy evaluation per manufacturing process/equipment. The detailed regression models and their model accuracy evaluation are available in the Supporting Information S2, Tab AM2-Upscaling module.

3.2.3 | AM-3 Experience in manufacturing

For PSC, no mass production data is available. Therefore, we use experience rates from commercial PVs (Louwen et al., 2016). Here, for matured first-generation PV , mono- and multicrystalline silicon solar cells, experience rates of the manufacturing demands derived from over 40 years of development indicate reductions of the GWP by 17%–24% (Louwen et al., 2016). This data can be assumed to be a gross estimate for the mass production of emerging PVs in 2050. To this end, the averaged experience rates of GWP of 20% are implemented into this upscaling module.

3.3 | Prospective upstream GHG emissions from lab to fab

The prospective upstream GHG emissions using UpFunMatLCA are shown in Figure 6. Figure 6a shows the results of the three upscaling scenarios, GLab, GFabE, and GFabM, and compares them with literature data as validation. GLab with 490 kg CO_2-eq/m^2 is in the middle of other LCA results, which assessed PSC at the lab scale. GFabE with only applied size scaling module results in a reduction of 59% for the increased manufacturing area of 5 m^2 and lies between the pilot and fab scale LCA results. GFabM, including all three process learning modules, lies in the range of the three LCA studies with projected fab scale PSCs. In contrast to our case study, these three studies allow only the evaluation of a single fixed target stage, which (1) partly included prospective materials and processes for commercial fabrication, but was then filled with data from the lab (Celik et al., 2016), (2) dismissed and reduced materials to "those strictly necessary to assemble the module" (Alberola-Borràs et al., 2018), or (3) used lab materials and manufacturing processes taken from PSC literature but calculated the energy demand of manufacturing processes "with (…) typical commercially

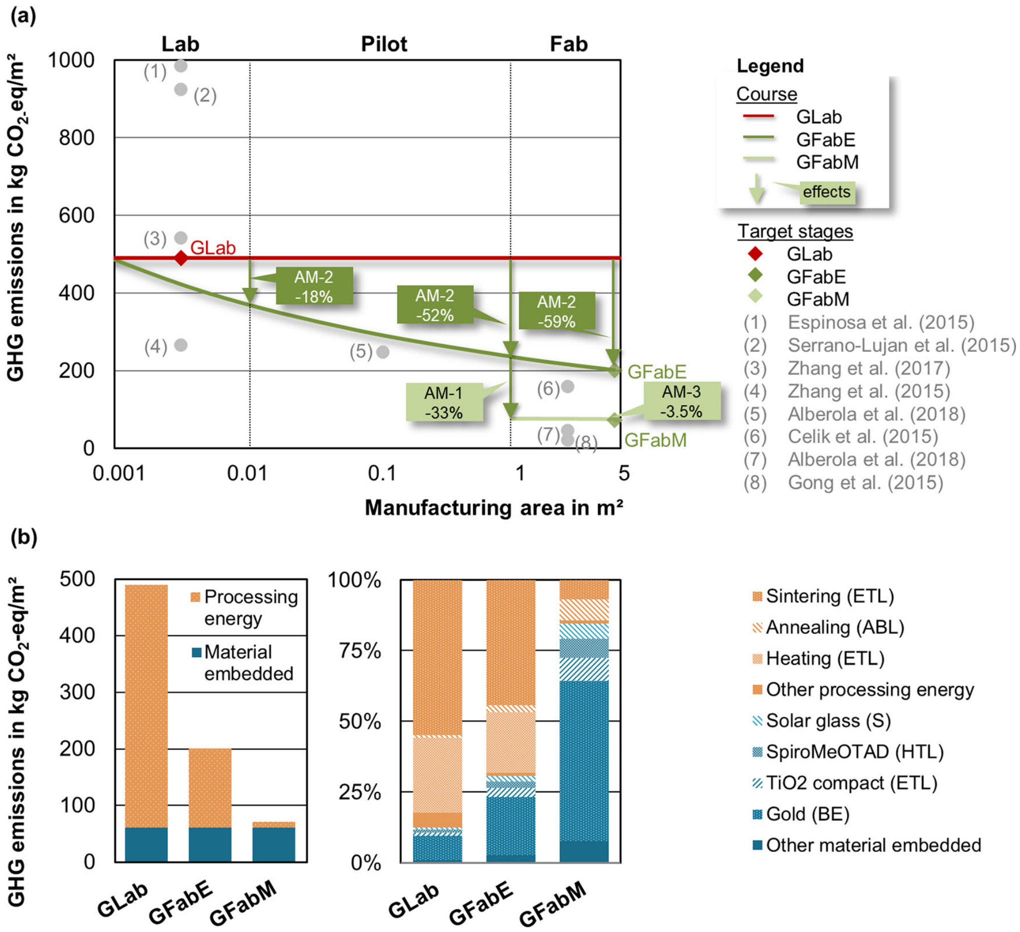


FIGURE 6 Projection of the upstream greenhouse gas emissions of the selected perovskite solar cell samples from lab to fab (a) course of the greenhouse gas (GHG) emissions per manufactured m^2 of the status quo and the two upscaled scenarios, compared with harmonized literature results averaged per study and classified technology scale, (b) resulting GHG emissions of GLab, GFabE, and GFabM and main contributions of the layer FunMats and manufacturing processes. Underlying data for Figure 6 are available in the Supporting Information S3.

available equipment" (Gong et al., 2015). Even though these studies include upscaling methods similar to UpFunMatLCA, they do not allow the evaluation of the way from a current to a target stage and the flexible integration of possible junctions during technology development.

In contrast to the literature results, the application of UpFunMatLCA enables the evaluation of the various development pathways and the flexible and transparent inclusion of possible junctions, such as the change of manufacturing processes. Figure 6a also illustrates the course of the GHG emissions representing the development pathway from lab ($S < 0.1$ m^2) to fab ($S > 1$ m^2) and the single effects of the three applied process learning modules. Applying the size scaling and industrial learning modules result in continuous reductions. For size scaling, the reduction increases with increasing manufacturing area. Comparing the current and target stages shows reductions per manufactured m^2 of 18% for a target manufacturing area of 0.1 m^2, 52% for 1 m^2, and even 59% for the defined manufacturing area of 5 m^2. Technological learning results in a discontinuous reduction as soon as a manufacturing process change occurs. In our case, GFabM includes the change to slot die coating as a deposition method, which occurs at the transition to commercial fabrication and results in a reduction of GHG emissions by 85% compared to GLab and 63% compared to GFabE.

Figure 6b confirms the hypothesis that the processing energy with 87% is the main contributor to GHG emissions at the current stage and shows the correlation between the processing energy and the GHG emissions. The GHG emission reductions result exclusively from the reductions of the processing energies due to the application of the process learning modules. The high share of fossil fuels in the energy supply of the background system can explain this correlation between processing energy and GHG emission. This correlation is expected to change in future due to the decarbonization of the energy system. However, this change is out of the scope of our case study and might be modeled with the inclusion of upscaling mechanism (C) as discussed below. The material-embedded GHG emissions play a minor role at the current scale. However, these emissions become more relevant with a more realistic estimation of the processing energy, as shown for GFabE and GFabM. Here, the share of the material-embedded impacts increases to 30% and 85%, respectively. Accordingly, the impacts of the materials become pivotal, and the extension of the material learning upscaling module is necessary. Similar correlations are expected for other impact categories such as International Life Cycle Data System (ILCD) midpoint 2011, human toxicity or freshwater ecotoxicity (European Commission, Joint Research Centre, Institute for Environment & Sustainability, 2012), as discussed in Weyand et al. (2019).

In contrast, tradeoff categories, such as ILCD midpoint 2011, resource depletion—mineral and fossil (European Commission, Joint Research Centre, Institute for Environment & Sustainability, 2012), might be unaffected by high processing energies. Here, characterization factors of the mineral resources such as silver or gold are much higher than those of fossil resources. However, the tradeoff evaluation is part of further work and, thus, out of the scope of our case study.

4 | DISCUSSION

The benefit of UpFunMatLCA is threefold. First, it is clearly focused on evaluating the technology maturity of a specific group of emerging technology, the FunMat-based energy technologies. Thus, UpFunMatLCA contributes to precise terminology in LCA of emerging technologies and the guidance of technology development using upscaling scenarios. Moreover, it can be combined with other effects that require other methodological approaches in prospective LCA, notably with market maturity (Bergerson et al., 2020). Second, UpFunMatLCA is comprehensive in the sense that it predefines development pathways in terms of upscaling mechanisms relevant to the specific technology group of emerging FunMat-based energy technologies. It offers a structured and transparent way to develop upscaling scenarios for prospective LCA and get first insights of the projected technology, specifically of emerging FunMats, even for LCA practitioners without precise knowledge of the FunMat to be modeled or technology developers with basic LCA knowledge. Despite this, we always recommend the cooperation of both experts to conduct LCAs on emerging technologies. Third, the transparent allocation of upscaling modules to upscaling mechanisms enables transparency and flexible use and advancement of UpFunMatLCA during technology development. For example, for emerging FunMat, we showed the key mechanism of process learning and introduced upscaling modules to evaluate the GHG emissions more representatively. In addition, the upscaling mechanisms can be extended by other life cycle phases, such as the use and end-of-life phase.

4.1 | Generalization and limitations of UpFunMatLCA

UpFunMatLCA is generally applicable for LCAs on FunMats, not only on PSC, but also on other emerging technologies since these LCAs face the four similar challenges as those presented for PSC: (1) lab-stage processes representing fab-stage, (2) testing of various materials to find physical optimum, (3) missing data as shown for FunMats in Smith et al. (2019), and (4) processing energies or manufacturing processes representing the main contributor to environmental impacts as shown for the case studies on piezoelectric ceramics (Ibn-Mohammed et al., 2016), capacitors (Smith et al., 2018), or fuel cells (Kawajiri & Inoue, 2016) as examples. These challenges are also present for other emerging materials such as nanomaterials (Hetherington et al., 2014) or biochemicals (Ögmundarson et al., 2020a), or emerging technologies in general (Thonemann et al., 2020; Tsoy et al., 2020). Even though nanomaterials come from a novel scientific field with emerging manufacturing processes, completely novel materials, and unknown environmental implications (Simon et al., 2016), parts of UpFunMatLCA are still generally applicable to generate upscaling scenarios considering the following limitations.

The upscaling definition (Step I, Figure 1) and upscaling leap (Step II, Figure 1) could generally be used to define the current and target development stage and to identify the key factors in terms of upscaling mechanisms. However, some materials or technologies require extensions of Figure 3 in terms of additional upscaling mechanisms or modules. The same applies to the implementation of the upscaling model and data (Step III, Figure 1). For example, the equipment scaling might be replaced by another module for upscaling the manufacturing of emerging biochemicals (Ögmundarson et al., 2020b), for which quantitative process simulations using software, such as ASPEN PLUS®, are commonly used for size scaling of bioreactors rather than empirical data of manufacturing equipment. Another example relates to the abovementioned embedded manufacturing processes of our upscaling modules. Standard processes such as annealing or sintering can be easily upscaled using our data, regardless of the FunMat or emerging technology. However, some FunMats, such as piezoelectric ceramics or capacitors, require additional manufacturing processes, such as ball milling (Ibn-Mohammed et al., 2016) or calcining (Smith et al., 2018), which are not included in our upscaling modules. Accordingly, these processes must be supplemented in the same way as presented above for the two upscaling modules, technological learning and size scaling. After that, both modules can be easily applied to further FunMats or emerging technologies.

Besides the modeled process learning modules, the material learning and impacts resulting from the materials are relevant to prevent unintentional tradeoffs to other impact categories such as toxicity or resource depletion. For this purpose, future research should include the upscaling modules of material learning as proposed in our study.

In addition, the upscaling module of the external development of the background system should be included. This module is not exclusively related to FunMats; thus, existing models and data can be used. For example, the PREMISE approach of Sacchi et al. (2022) enables the modeling of prospective background databases by combining integrated assessment models, including the shared socioeconomic pathway scenarios, with common LCA background databases.

4.2 | Position relative to previous literature

UpFunMatLCA can be classified into the context of the technology maturity in contrast to the market maturity and represents an important contribution to the development of structured guidelines for the cooperation of LCA practitioners and technology developers, particularly for material scientists, as called for in Bergerson et al. (2020). Above this, UpFunMatLCA contributes to the specifications of general frameworks on LCA of emerging technologies such as van der Hulst et al. (2020), Thonemann et al. (2020) and Tsoy et al. (2020) and represents a merge and harmonization of several upscaling methods, particularly of Kawajiri et al. (2020) and Piccinno et al. (2016).

The general framework of van der Hulst et al. (2020) is specified regarding selecting upscaling mechanisms and modeling these mechanisms using the introduced upscaling modules, particularly for emerging FunMats. In this context, we decided to distinguish between material and process learning mechanisms instead of using a chronological distinction of technology maturity from low to high. This distinction enables the focus on key mechanisms such as process learning, which focuses on the main environmental impacts resulting from the processing energies of lab-manufactured FunMats. We also concretized the suggested modeling methods per mechanisms by modeling the introduced upscaling modules, which are applicable directly in the LCI of prospective LCAs. Similar to van der Hulst et al. (2020), we merged different methods from previous literature for modeling the upscaling modules; worth mentioning here are size scaling, as shown in Kawajiri et al. (2020) and Caduff et al. (2014); technological learning as shown for chemical processes in Piccinno et al. (2016) and industrial learning as shown in Louwen et al. (2016) and Arvesen et al. (2018).

Like Tsoy et al. (2020), we discern three upscaling steps in UpFunMatLCA. Tsoy et al. (2020) derived these steps from the review of ex ante case studies and focused on the target or referred to there as the “projected” stage. Their upscaling steps give a good overview of available and applicable data estimation methods. A decision tree guides the LCA practitioner to the most suitable method depending on the research question of the emerging technology to be assessed. In contrast, our three steps were derived from and specified for the case of emerging FunMats aiming to model both the current and target stage and the direct implementation into standard LCA practice. To this end, we predefine the modeler’s decision regarding the data estimation method and provide finalized upscaling modules filled with data directly applicable in LCAs on FunMats but also on other emerging technologies, as discussed above. Furthermore, these upscaling modules represent a specification of the four-step approach of Thonemann et al. (2020) regarding the definition of the assumptions made for upscaling from the current stage (" lab-scale") to the two target stages proposed there, " best-case" and " scaled" for PVs based on PSC.

4.3 | Implication of UpFunMatLCA and future studies

The integration of UpFunMatLCA into the methodology of LCAs is a vital way to assess the future chances and risks of an explicit group of emerging technology, that is, emerging FunMat-based energy technologies from an early development stage on, despite contradictory requirements of high uncertainties and room for maneuvering in terms of freedom of design. The UpFunMatLCA presents a structured way to integrate likely future development pathways into prospective LCA and gain meaningful information on these developments’ environmental impacts. These potential impacts provide essential insights for future research by indicating possible levers of environmentally friendly technology progress. Therefore, the comparison with benchmarks is not seen as a final exclusion criterion for emerging technology but rather as an indicator that if the emerging technology develops in this way, it is highly likely to present the following chances or risks compared to a mature counterpart. The development of similar uniform schemes is also essential for other technology groups to increase comparability and support the comprehensiveness of the LCA results on emerging technologies compared to mature technologies. UpFunMatLCA provides an important example to concretize the development of upscaling scenarios for other technology groups.

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CONFLICT OF INTEREST STATEMENT

The authors declare no conflict of interest.

DATA AVAILABILITY STATEMENT

The data that supports the findings of this study are available in the supporting information of this article.

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SUPPORTING INFORMATION

Additional supporting information can be found online in the Supporting Information section at the end of this article.

How to cite this article: Weyand, S., Kawajiri, K., Mortan, C., & Schebek, L. (2023). Scheme for generating upscaling scenarios of emerging functional materials based energy technologies in prospective LCA (UpFunMatLCA). *Journal of Industrial Ecology*, 1–17. https://doi.org/10.1111/jiec.13394

4 Are perovskite solar cells an environmentally sustainable emerging energy technology? Upscaling from lab to fab in life cycle assessment,

This chapter contains Publication 3, Weyand et al. (2023b):

> Weyand S, Kawajiri, K., Mortan, C., Zeller, V., Schebek L. Are perovskite solar cells an environmentally sustainable emerging energy technology? Upscaling from lab to fab in life cycle assessment. ACS Sustainable Chemistry & Engineering, DOI: 10.1021/acssuschemeng.3c03019.

The full article is available at: 10.1021/acssuschemeng.3c03019 or use QR code.

5 Discussion

This chapter synthesizes the three publications regarding key findings, contributions and recommendations of the novel upscaling methodology for future research. Figure 5.1 illustrates the application area of the developed methodology and frames it relative to recent research trends. Finally, implications for decision-makers and limitations are discussed.

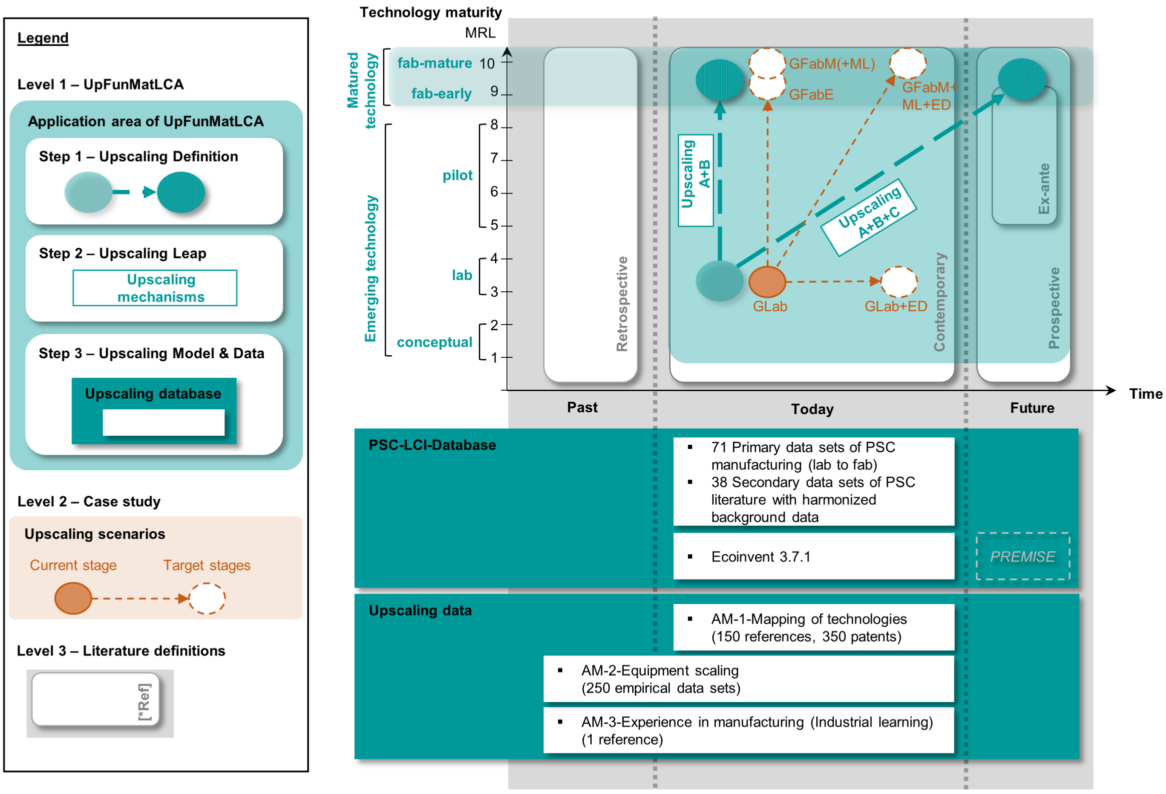

Figure 5.1: Upscaling levels for framing the novel methodology of this thesis relative to recent research trends (Level 3): Level 1: Illustration of the UpFunMatLCA application area (Publication 2, Weyand et al. (2023a)) with summary and temporal coverage of the collected LCI and upscaling data (Publication 2 and 3, Weyand et al. (2023a), Weyand et al. (2023b)), Level 2: Upscaling scenarios of the PSC case study assessed in (Publication 2 and 3, Weyand et al. (2023a), Weyand et al. (2023b)), Level 3: LCA terminology according to Arvidsson (2023) (*Ref),

5.1 Summary of the key findings

In this thesis, **a novel structured methodology for a clear, transparent, and comprehensive integration of upscaling into prospective LCA was developed**. First, it focuses clearly on evaluating the environmental performance of a specific group of emerging technology, the

FunMat-based energy technologies considering the status quo and future prospects. Furthermore, the term **upscaling is clearly defined**, and key parameters (KEYPs), key indicators (KEYIs), and generic technology scales are introduced to foster transparent cooperation with technology developers. Second, the novel methodology is **comprehensive** in the sense that it predefines development pathways in terms of upscaling mechanisms relevant to the specific technology group of emerging FunMat-based energy technologies. Third, it provides a structured and **transparent** allocation of upscaling modules to upscaling mechanisms to apply and adapt upscaling in a flexible way as technology development progresses.
The following novel methods are part of the novel upscaling methodology and evolved from the three publications (sorted in chronological order):

1) **Meta-analysis approach for the systematic review and harmonization of the environmental performance of emerging FunMat-based energy technologies (Chapter 2, Publication 1, Weyand et al. 2019):** A clear set of KEYIs, KEYPs, and key modeling assumptions (KEYAs) was introduced for the systematic review and the harmonization of the LCA results in terms of the KEYIs. Two key methodological findings were drawn from this publication: First, the functional unit is a KEYA that can be harmonized to evaluate the environmental performance of emerging PVs and compare them with commercial benchmarks. For this comparison, we recommended using the functional unit of an average 1 kWh generated electricity during the lifetime of PV technologies and introduced a mathematical procedure for harmonizing the environmental performance accordingly (Chapter 2, Table 3). Second, the technology scale is a KEYA that cannot be harmonized retrospectively in meta-analysis but prospectively in LCA studies by integrating upscaling steps into the modeling, as shown in Chapter 3.

2) **UpFunMatLCA for harmonizing the technology scale and upscaling the environmental performance of emerging FunMat-based energy technologies (Chapter 3, Publication 2, Weyand et al. (2023a)):** UpFunMatLCA is a novel systematic scheme for generating explorative upscaling scenarios based on predefined development pathways, including status quo developments. It follows a three-step approach to upscale emerging FunMat-based energy technologies in prospective LCA (Figure 5.1). A core part of UpFunMatLCA is the so-called upscaling module, providing specific modeling methods and data for the upscaling of FunMats.

3) **PSC-LCI-Database for evaluating the environmental performance of emerging and upscaled FunMat-based energy technologies (Chapter 4, Publication 3, Weyand et al. (2023b)):** The PSC-LCI-Database provides a comparable foundation of the predefined development pathways for generating upscaling scenarios. It includes over 200 data sets, primary data of the PSC's manufacturing processes, layer materials, and deposition methods measured during lab manufacturing and based on leaching experiments, secondary data for modeling the technological learning and the size scal-

ing depending on the manufacturing area, and secondary data of PSC literature with harmonized background data.

4) **Environmental break-even time (e-BET) for interpreting the environmental performance of possible future FunMat-based energy technologies (Chapter 4, Publication 3, Weyand et al. (2023b)):** e-BET was introduced to indicate how likely the environmental sustainable PSC's deployment will be in future as an example of an emerging FunMat-based energy technology. Remarkably, this indicator is practical for PSC, as lifetime is currently the most significant uncertainty in its assessment. Using e-BET, it was possible to calculate what lifetime PSCs would have to achieve to keep up with commercial benchmarks.

5.2 Contributions

This thesis provides the following two significant contributions:

- UpFunMatLCA is a pioneer for upscaling a specific technology group
- Transparency of the technology maturity and upscaling for proper interpretation of prospective LCAs

5.2.1 UpFunMatLCA is a pioneer for upscaling a specific technology group

So far, implementing upscaling in prospective LCAs has been done case-specific (Celik et al. 2016, Kawajiri & Inoue 2016, Piccinno et al. 2016) or at a general level (Tsoy et al. 2020, van der Hulst et al. 2020). One has led to using single upscaling methods, which makes upscaling challenging to follow, and the comparability of results is not given, as shown in Publication 1, Weyand et al. (2019). The general approaches to modeling technology development are beneficial for structuring prospective LCAs, but the results are not comparable because each study uses its own data, methods, etc. This is where UpFunMatLCA comes in, as it breaks down general techniques for a specific technology group, the FunMats, and stores them with data so that upscaling is structured and based on a comparable data basis and methods. Therefore, UpFunMatLCA represents a pioneer for upscaling a specific technology group in prospective LCA. The adaptation of UpFunMatLCA to other technology groups is essential to increase comparability and support the comprehensiveness of the LCA results on emerging technologies compared to benchmarks. UpFunMatLCA is structured so that it can be easily transferred to other technology groups. To this end, the upscaling mechanisms and upscaling modules need to be adjusted to the requirements of different technologies. UpFunMatLCA provides a vital example to concretize the development of upscaling scenarios for other technology groups.

5.2.2 Transparency of the technology maturity and upscaling for proper interpretation of prospective LCAs

This thesis contributes significantly to the transparency of 1) previous LCA studies of emerging PVs regarding the assessed technology scale, 2) the interpretation of future LCAs applying UpFunMatLCA.

In Publication 1, Weyand et al. (2019), the meta-analysis attributed the significant discrepancy between the LCA results of different emerging PVs and within one PV technology, particularly PSC, to the technology maturity underlying the assessment. However, most case studies were not transparent regarding the assessed technology‘s maturity. Therefore, each case study was reviewed, and the classification of the technology maturity was implemented based on the study's content in Publication 1, Weyand et al. (2019). This classification of the technology maturity or reporting of the development stage is reasonable since the technology maturity impacts the results, as shown in Gavankar et al. (2015).

In Publication 2, Weyand et al. (2023a), UpFunMatLCA was developed that allows the specification of the development stage and the harmonization of the technology maturity transparently using upscaling scenarios. Three essential elements of UpFunMatLCA contribute to the transparent modeling in future studies:

1) Definition of the status quo and upscaled development stage, referred to as current and target stage.

2) Selection of relevant upscaling mechanisms for FunMats that summarizes the key drivers of the technology development of FunMats.

3) Modelled upscaling modules, including the upscaling methods and data for use in LCI. This transparent modeling, combined with the developed documentation template (6), allows the reader to understand and comprehend the upscaling assumptions quickly. In addition, this transparency on the upscaling assumptions enhances the understanding of the LCA results for various audiences by combining the language of LCA practitioners and material scientists.

5.3 Position relative to recent research trends

The recently published typology of Arvidsson (2023) is beneficial for framing the developed upscaling methodology of this thesis relative to the recent research trends (Figure 5.1).

This typology of Arvidsson (2023) includes the three dimensions: Positionality, maturity, and causality. In particular, the first two are similarly used in Publication 2, Weyand et al. (2023a), Figure 2. Instead of positionality, we referred to "development/ time" to differentiate between the emerging technology's current status quo and the target stage as the future, more-developed phase. Arvidsson (2023) supplements this with the time perspective past. The retrospective is useful for illustrating the temporal coverage of the upscaling data in this thesis, partly based on historical for industrial learning or empirical data for size scaling (Figure 5.1).

As maturity from TRL low to high, we use “technology maturity”, meaning the same but classify it differently. As shown in Figure 5.1 and Publication 2, Weyand et al. (2023a), Figure 2, the technology maturity was aggregated into five development stages. The three stages – conceptual, lab, pilot – describe the emerging technology’s status quo, and the two stages – fab-early and fab-mature - refer to the point around the market breakthrough and dissemination. To this end, to classify the dissemination phase, the TRLs had to be combined with the two classification schemes: manufacturing readiness (MRL) and market penetration levels (MPL).

The last dimension, causality, considers the LCA mode or LCA modeling way between attributional and consequential LCA modeling (Arvidsson 2023). Besides the different modeling ways, this dimension differentiates between time-integrated, all data and environmental impacts have the same time stamp, and time-resolved, different time stamps are included in the assessment. As described in the introduction, both modeling ways can be combined with the developed upscaling methodology (see 5.1). The distinction between time-integrated and time-resolved data is further discussed in the limitation of this thesis.

Furthermore, with the updated prospective LCA definition (Arvidsson 2023), “ex-ante” and “prospective” can be more clearly distinguished. Ex-ante assesses a current emerging technology at a future point when it is mature (van der Giesen et al. 2020), and thus, is part of a prospective LCA. Broadening the prospective LCA term is also beneficial for framing the developed UpFunMatLCA-scheme (Figure 5.1) as its scope is not limited to ex-ante, but generally covers future developments. Therefore, the broad definition of prospective is still more appropriate than ex-ante for applying UpFunMatLCA. Even though ex-ante now seems more suited to characterize the assessment of emerging technologies at a higher maturity.

In distinctions to these terms, we also generated and assessed the three upscaling scenarios – GFabE, GFabM, and GFabM+ML (Figure 5.1) - focussing solely on changing technology maturity based on contemporary data thus, did not consider prospective or ex-ante in the classical sense. Arvidsson’s typology helps illustrate the different dimensions of assessing emerging technologies and transferring them for upscaling. However, the question remains about how to describe the upscaling of technological maturity, as ex-post is not the correct term. As suggested Figure 5.1, extending ex-ante would be a way of not throwing more terms into the “LCA soup”, following Guinée et al. (2018). Ex-ante would stand here to describe a future situation based on data from the present.

5.4 Recommendations for future research

Table 5.1 summarizes the findings from this work as recommendations for future LCA studies of FunMats. Both status quo and future assessments are included there. Based on the research question, there are different requirements for the goal and scope definition. Table 5.1 also provides recommendations on when and what upscaling mechanisms and data are required.

Table 5.1: Recommendations on the goal and scope definition of future LCA studies of FunMats

Goal of the LCA			Scope of the LCA									Thesis
ID	Research questions (adjusted to FunMats [1]	FunMat Examples	FU	Benchmark	Time	Technology maturity	LCA mode	KEYPs	KEYIs	Upscaling Mechanisms	Data	Pub.
(1a)	How have FunMats been manufactured? Which manufacturing route/ process/ layer materials has the lowest environmental impacts?	Characterizing the environmental performance of PSC samples with the same efficiency but based on different layer materials/ manufacturing processes	1 m^2 provided PV cell, module		Today	Generic Lab to Generic Fab Mature	ALCA, status quo	-	Single KEYIs, e.g., GWP, CED	-	LCA-DB	P1, P2
(1b)	How could FunMats be produced in the future? Which production route/process/layer materials would have the least environmental impact?	Characterizing the environmental performance of PSC samples with the same efficiency but based on different layer materials/ manufacturing processes	1 m^2 provided PV cell, module		Today	Generic Lab to Generic Fab Mature	ALCA, prospective	-	Single KEYIs, e.g., GWP, CED	Process or material learning	LCA-DB +UpD	P3
(2a)	What are the environmental impacts of an emerging FunMat as its currently intended function?	Characterizing environmental performance of FunMats applied in emerging PVs	1Wp provided PV cell, module, or system		Today	Generic Conceptual to Generic Pilot	ALCA, status quo	T: Efficiency η in % (measured at status quo)	GWP, CED, (*RDP(m+f), ETPf, HTPc*)	-	LCA-DB	P1
(2b)	What are the environmental impacts of an emerging FunMat as its prospective function?	Characterizing environmental performance of FunMats applied in PV modules	1Wp provided PV cell, module, or system		Today	Generic Conceptual to Generic Pilot	ALCA, status quo	T: Efficiency η in % (prospective estimate)	GWP, CED, (*RDP(m+f), ETPf, HTPc*)	-	LCA-DB	P1
(3a)	What are the expected environmental impacts of an upscaled FunMat as its prospective function based on today's conditions?	Prospective environmental performance of PSC upscaled and integrated into a PV module compared with commercial benchmarks	1 kWh of averaged converted electricity	first- and second-generation PVs, other renewables, etc.	Today	Generic Fab Early or Mature	ALCA, prospective	T: Efficiency η in % T: Lifetime τ in yrs S: Performance ratio in % S: Irradiation in kWh/m^2yr T: Temperature coefficient in K	GWP, CED, RDP(m+f), ETPf, HTPc, further KEYIs	Process and material learning	LCA-DB +UpD	P3
(3b)	What are the expected environmental impacts of an upscaled FunMat as its prospective function based on future conditions?	Prospective environmental performance of PSC upscaled and integrated into a PV module compared with commercial benchmarks	1 kWh of averaged converted electricity	first- and second-generation PVs, other renewables	Future	Generic Fab Early or Mature	ALCA, prospective	T: Efficiency η in % T: Lifetime τ in yrs S: Performance ratio in % S: Irradiation in kWh/m^2yr T: Temperature coeff. in K	GWP, CED, RDP(m+f), ETPf, HTPc, further KEYIs	Process and material learning, external development	LCA-DB +UpD + PREMISE	-

Table 5.2: Recommendations on the goal and scope definition of future LCA studies of FunMats (continued)

(4a)	What is the consequence of the market introduction of an prospective FunMat based on today's conditions?	Environmental performance of an OPV solar charger as a substitute for the country-specific electricity mix to charge a mobile phone	10 Wh of electricity is drawn and stored in the mobile phone battery	Substituted technology	Today	Generic Fab Early or Mature	CLCA, prospective	T: Efficiency η in % T: Lifetime τ in yrs S: Performance ratio in % S: Irradiation in kWh/m²yr T: Temperature coeff. in K U: Use-intensity	GWP, CED, RDP(m+f), ETPf, HTPc, further KEYIs	Process and material learning	LCA-DB +UpD	P4
(4b)	What is the consequence of the market introduction of an prospective FunMat based on future conditions?	Environmental performance of an OPV solar charger as a substitute for the country-specific electricity mix to charge a mobile phone	10 Wh of electricity is drawn and stored in the mobile phone battery	Substituted technology	Future	Generic Fab Early or Mature	CLCA, prospective	T: Efficiency η in % T: Lifetime τ in yrs S: Performance ratio in % S: Irradiation in kWh/m²yr T: Temperature coeff. in K U: Use-intensity	GWP, CED, RDP(m+f), ETPf, HTPc, further KEYIs	Process and material learning, external development	LCA-DB +UpD + PREMISE	-

Research questions: [1] questions originally from Guinée et al, 2018 adjusted to FunMats and framed to the novel upscaling methodology **FU: Functional unit; LCA mode:** ALCA: Attributional; CLCA: Consequential; **KEYPs:** C: Country-specific; S: Standard value T: Technology-specific; U: User-dependent; **KEYIs:** GWP: Global warming potential; CED: Cumulative energy demand; RDP(m+f): Resource depletion potential, mineral and metals/ fossil energy carriers; ETPf: Ecotoxicity potential for freshwater; HTPc: Human toxicity, cancer effects; **Data:** LCA-DB: Standard LCA Databases; UpD: Upscaling data as shown in Figure 5.1; PREMISE as prospective background database; **Thesis:** Link to publication; **Pub:** Publication; P1: Publication 1, Weyand et al. (2019); P2: Publication 2, Weyand et al. (2023b); P1: Publication 3, Weyand et al. (2023a); P1: Publication 4, Glogic, Weyand et al. (2019).

5.5 Importance for decision-making

The developed upscaling methodology aims to accompany and advance emerging FunMat-based energy technologies from an environmental perspective and supports the following decisions during technology development:

1) The main target group is the material scientists, scientists researching PSCs or FunMats, or technology developers in general. The newly developed upscaling methods enable the assessment of the current and target prospective environmental performance of emerging FunMat-based energy technologies with integrated realistic scenarios generated from potential development pathways. Thus, it incorporates a system-wide understanding of potential environmental impacts into the technology development and supports the identification of environmental hotspots, risks, or unintended consequences. The earlier these are known, the earlier actions can be taken. Therefore, decisions of this target group are supported regarding how to design environmentally-friendly future technologies starting from the conceptual stage. Accordingly, this thesis endorses the integration of prospective LCA into basic research and the understanding of the resulting environmental impacts. The performance of LCA by technology developers is simplified by generating upscaling scenarios using UpFunMatLCA. Furthermore, this thesis disseminates the LCA methodology among non-LCA experts.

2) The second target group is the LCA practitioners supported in systematically modeling and upscaling emerging technologies. Notably, for PSC or other FunMats, UpFunMatLCA might be applied by LCA practitioners without direct cooperation with technology developers since the knowledge of several development pathways is included in UpFunMatLCA. For assessing different development pathways or advanced technology development, collaboration is useful to update the formed development pathways, for example.

3) Policymakers in funding agencies or policymakers, in general, are supported in understanding the challenges of prospective LCAs and LCAs based on different development stages. They are kept in prioritizing research activities and decisions concerning the directions of new funding programs and research initiatives regarding the design of sustainable products and technologies. At this point, it should be stressed that evaluating emerging technologies is associated with high uncertainties. Decisions based on these studies should be made with deliberation and considerable care, especially regarding findings during fundamental research. However, coming back to Collingridge, he said: "Decision-making under ignorance [is] a more extreme condition than uncertainty" (Collingridge 1980). In this respect, the newly developed upscaling methods significantly contribute to making decisions not out of ignorance but based on sufficient reflection.

5.6 Limitations

In this thesis, over 200 LCI data sets were provided for emerging PVs, particularly for PSC, over 150 references and over 350 patents were found for the AM1 Mapping of technologies upscaling module, and over 250 empirical data sets were collected for the AM2 Equipment Scaling upscaling module. Nevertheless, the data basis is limited to the following parts:

The LCI data sets cover only one single lab-manufacturing option, the wet chemical deposition with spin coating, spray coating, and dip coating. There are also vapor-based deposition techniques, including co-evaporation. Transferring the modeled upscaling modules to these techniques could be part of further research and cooperation.

The patent analysis was not practical for mapping technologies since it included only scattered data on future manufacturing processes. However, so far, only PSC patents have been reviewed. Expanding the search to the considered manufacturing processes might result in more relevant data sets from patent analyses.

This thesis uses no prospective background database like PREMISE (Sacchi et al. 2022). These databases discern external temporal changes, which are recommended in the UpFunMatLCA. However, including external developments increase uncertainty. Therefore, the question of the case study was what environmental impacts of future PSC modules could be expected under current conditions. Considering this, the used ecoinvent 3.7.1 database (Wernet et al. 2016), representing today's data, was sufficient in this thesis.

Another limitation is the validation of the KEYPs, KEYIs, and e-BET for other FunMat-based energy technologies. So far, they were only validated for emerging PVs in Weyand et al. (2019) and PSC in Weyand et al. (2023b) . For extending the KEYIs, the material learning upscaling modules and their effects on the KEYIs might be interesting for further assessment, similar to the comparison of climate-friendliness and material efficiency in Weyand et al. (2023b). The extension of the considered life cycle stages is relevant to assess the toxicity KEYIs of PSCs, as discussed in Weyand et al. (2023b) . Considering this, future studies should extend the data basis recycling technologies and end-of-life-treatment. The methodology developed can be used for this purpose. Furthermore, the combination with risk assessment should be assessed to identify risks from substances or materials currently not covered in the LCIA, like nanomaterials, as recommended by Guinée et al. (2017), Tsang et al. (2017).

6 Conclusion

This thesis presents a novel structured upscaling methodology consisting of four newly developed methods for evaluating and harmonizing the environmental performance of emerging FunMat-based energy technologies compared to commercial benchmarks. The methodology's core is the UpFunMatLCA, a scheme for generating upscaling scenarios of emerging FunMat-based energy technology to harmonize the technology scale in prospective LCA.

The newly developed scheme UpFunMatLCA was used for the first time to integrate systematically structured upscaling into the technology development of an emerging FunMat-based energy technology and to support the decision on whether PSC is a promising future energy technology considering only lab knowledge. Integrating UpFunMatLCA into the technology development indicates for the case study of PSCs that they are promising regarding climate-friendliness and resource efficiency compared to current country-specific electricity mixes.

The integration of UpFunMatLCA into the methodology of LCAs is a vital way to assess the future chances and risks of an explicit group of emerging technology, i.e., emerging FunMat-based energy technologies from an early development stage on, despite contradictory requirements of high uncertainties and room for manoeuvering in terms of design freedom.

Accordingly, this thesis supports several decisions during technology development: First, for LCA practitioners, UpFunMatLCA presents a structured way to integrate likely future development pathways into prospective LCA and gain meaningful information on these developments' environmental impacts. Second, for the technology developer or material scientist, these potential environmental impacts provide essential insights for future research by indicating possible levers of environmentally-friendly technology progress. Last, for policymakers, the comparison with commercial benchmarks is not seen as a final exclusion criterion for emerging technology but rather as an indicator that if the emerging technology develops in this way, it is highly likely to keep up with commercial counterparts.

All in all, this thesis provides significant improvements concerning the following:

- integrating prospective LCA into basic research,
- understanding LCA results for technology developers,
- disseminating LCA methodology also among non-LCA experts,
- performing LCA of PSC without technology developers,
- performing LCA by technology developers.

UpFunMatLCA is a pioneer in combining theoretical and practical methods for upscaling a specific technology group in prospective LCA. It represents, thus, an important template for other technology groups to develop similar uniform schemes for increasing and supporting the comprehensiveness of the LCA results on emerging technologies compared to commercial benchmarks. The transferability to other technologies would result in the modeling of further upscaling modules and the expansion of the database of UpFunMatLCA to include additional manufacturing processes. Furthermore, including the material learning modules would enable a combination or extension with risk assessment. For example, indicating risks from substances or materials at an early stagewhich are currently not covered in LCIA, like nanomaterials.

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Glossary

Key indicators (KEYIs): The KEYIs are the impact category indicators that were selected for a comprehensive description of the potential environmental impacts of the assessed technology (Weyand et al. 2019).

Key modeling assumptions (KEYAs): The KEYAs, summarize methodological specifications that influence the total life-cycle impacts of the assessed technology Weyand et al. (2019).

Key performance parameters (KEYPs): The KEYPs characterize the performance of the PV system, and they were significant for the determination of the maximum electricity yield during the operation stage. Weyand et al. (2019).

Environmental break-even time (e-BET): The e-BET is defined as the period or point when the upscaled PSC's environmental impacts offset a commercial benchmark. It examines whether and when introducing new technology brings environmental benefits over the current technology landscape (Weyand et al. (2023b)).

Upscaling: The term upscaling is defined in this thesis as transferring the functionality and characterization of an emerging technology to a possible target stage, considering development pathways from a current stage within the course of research and development to this future stage. The upscaling focuses on the manufacturing phase as the main contributor to the environmental performance of FunMat-based energy technologies in this thesis.

Upscaling method: The model or "procedure that projects how (. . .) [an emerging] technology currently available at a lower TRL may look and function at a higher TRL" is defined as upscaling method using the definition of Tsoy et al. 2020 (Weyand et al. (2023a)).

Upscaling scenario: Upscaling scenario is defined as the description of a possible future stage of emerging technology, including the development pathway from a current stage within the course of research and development to this future stage (Weyand et al. (2023a)).

UpFunMatLCA: UpFunMatLCA represents a three-step extension of conventional LCAs to upscale the life cycle inventory of emerging FunMats. UpFunMatLCA is based on a clear definition of a current status quo (conceptual, lab, or pilot stage) and a target matured (fab) development stage. A core part of UpFunMatLCA is the so-called upscaling module, providing specific modeling methods and data for the upscaling of FunMats (Weyand et al. (2023a)).

emerging technology: Emerging technologies are ""technologies for which there is just an experimental proof of concept, a validation in the lab, or pilot plant"" (Cucurachi et al. 2018) and show a TRL lower than 8 (Weyand et al. (2023a)).

Functional material: The performance of renewable energy technologies depends highly on functional materials (FunMat) (Kuznetsov & Edwards 2010, Schebek et al. 2019). FunMats are used as metals, such as rare earths, in wind turbine permanent magnets or as semiconductors in photovoltaic technologies (Kuznetsov & Edwards 2010, Schebek et al. 2019) and possess a distinct electronic structure and physical-chemical properties responding to electrical, magnetic, optical, or chemical influences (Chung 2021).

Attributional LCA: System modelling approach in which inputs and outputs are attributed to the functional unit of a product system by linking and/or partitioning the unit processes of the system according to a normative rule Sonnemann & Vigon (2011).

Consequential LCA: System modelling approach in which activities in a product system are linked so that activities are included in the product system to the extent that they are expected to change as a consequence of a change in demand for the functional unit Sonnemann & Vigon (2011).

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Appendix

Appendix I: Supplementary materials of Publication 1, (Weyand et al. 2019)
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Appendix IV: Additional supplementary materials

Appendix I

Appendix I contains the essential parts of the supplementary materials of Publication 1, Weyand et al. 2019:

> Weyand S, Wittich C, Schebek L. (2019): Environmental Performance of Emerging Photovoltaic Technologies: Assessment of the Status Quo and Future Prospects Based on a Meta-Analysis of Life-Cycle Assessment Studies. Energies; 12(22): 4228, DOI: 10.3390/en12224228.

Supplementary Materials

The following are available online at https://www.mdpi.com/1996-1073/12/22/4228/s1: Table S1: Keywords and synonyms of the database search; Table S2: Overview of the excluded LCA datasets per collected LCA study after the secondary screening; Table S3: Ratio between best research cell efficiencies and standard values of first- and second-generation PVs; Table S4: Comparison of the descriptive statistics of the KEYIs harmonized to the consistent functional unit of 1 Wp and after full harmonization (including the standard values of the efficiency), subdivided by the five KEYIs; Figure S1: Influence of the KEYAs on the single harmonized LCA dataset points of the five KEYIs (a) technology scale (laboratory (L) vs. pilot/industrial (PI/IN)); (b) product system (cell (C) vs. module/system (M/S)); (c) system boundaries (cradle-to-gate (Gate) vs. cradle-to-grave (Grave); Figure S2: Detailed scenario analyses of the three influencing factors, efficiency, lifetime, and upscaling, for PSC and DSSC; File S1: Supplementary meta-analysis results.

The full supporting information is available at: https://www.mdpi.com/1996-1073/12/22/4228 or use QR code.

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Supplementary information

Environmental Performance of Emerging Photovoltaic Technologies: Assessment of the Status Quo and Future Prospects Based on a Meta-Analysis of Life-Cycle Assessment Studies

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Table S1. Keywords and synonyms of the database search.

LCA	CZTSSe	DSSC	PSC	OPV	QDPV
Life cycle assessment	CZTSSe	Dye-sensitized solar cell, Dye-sensitized cell, Graetzel cell	Perovskite solar cell, Perovskite photovoltaic	Organic photovoltaic, Organic solar cell, Polymer photovoltaic, Polymer solar cell Plastic photovoltaic, plastic solar cell	Quantum dot solar cell Quantum dot photovoltaic

Table S2. Overview of the excluded LCA data sets per collected LCA study after the secondary screening.

Author (Year)	ND	Included	Why excluded? Not compliant with		
DSSC			**(1)**	**(2)**	**(3)**
Greijer et al. (2001) [1]	2	×			✓
Kato et al. (2007) [2]	1	×			✓
OPV					
Chatzideris et al. (2017) [3]	*x*	×	✓		
Serrano-Luján et al. (2017) [4]	2*	×		✓	✓
PSC					
Itten and Stucki (2017) [5]	1	×			✓
Alberola-Borràs et al. (2018) [6]	3	×			✓

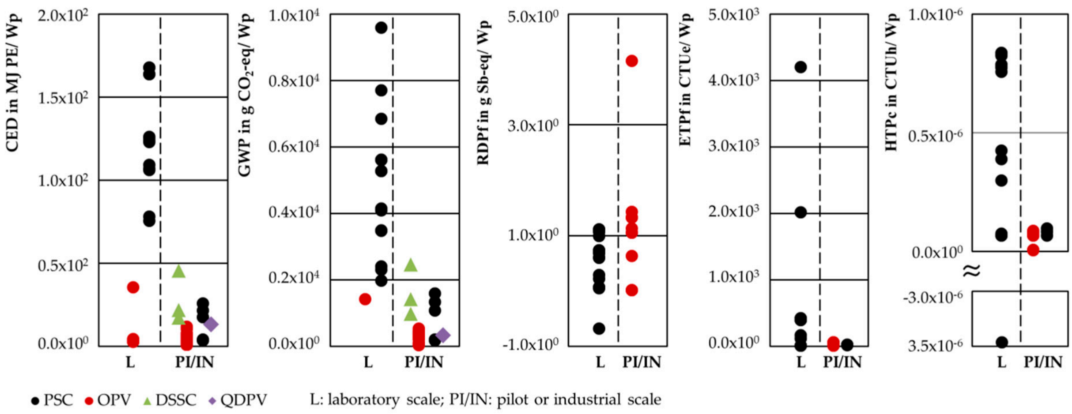
*More country-specific datasets included

Table S3. Ratio between best research cell efficiencies and standard values of first- and second-generation PVs.

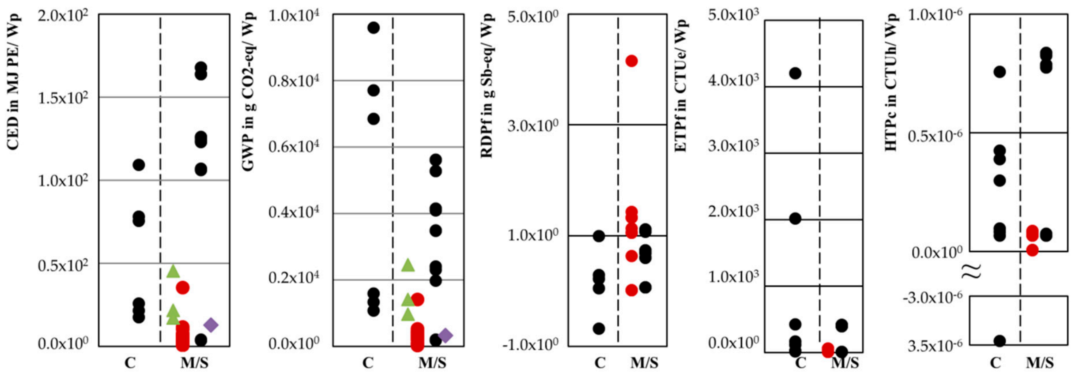
PVs	Best Research Cell Efficiency	Best Research Module Efficiency	Commercial Module Efficiency	Standard Values of the Efficiency in [6,7]	Ratio between Best Research Cell and Standardised
Mono-Si	26.7	24.4	17	13	0.49
Multi-Si	22.3	19.9	17	12.3	0.55
CdTe	21	18.6	16	10.9	0.52
a-Si	14	11	-	6.3	0.45
CIGS	21.7	19.2	-	11.5	0.53

Table S4. Comparison of the descriptive statistics of the five KEYIs harmonized to the consistent functional unit of 1 W_P and after full harmonization (including the standard values of the efficiency).

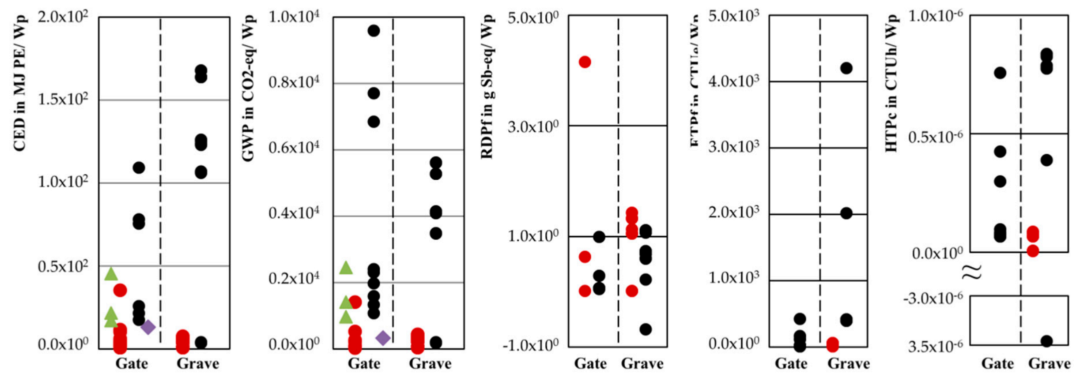
	DSSC		OPV		PSC		QDPV	
	Harmonized to FU of 1 W_P	**Harmonized (All Steps)**	**Harmonized to FU of 1 W_P**	**Harmonized (All Steps)**	**Harmonized to FU of 1 W_P**	**Harmonized (All Steps)**	**Harmonized to FU of 1 W_P**	**Harmonized (All Steps)**
CED in MJ PE/ W_P								
Min	13	17	1	0.5	4	3		
25th	14	19	3	1	35	38		
Median	16	21	5	2	113	108	7	13
75th	25	33	7	4	146	126		
Max	34	45	56	35	262	168		
IQR	11	14	4	3	111	88		
Change in Median		33%		−64%		−5%		75%
Change in IQR		33%		−26%		−21%		75%
GWP100 in g CO_2-eq/W_P								
Min	714	952	35	22	174	159		
25th	880	1173	167	50	3358	2121		
Median	1046	1394	608	228	4400	4083	179	313
75th	1441	1921	1321	305	8514	5596		
Max	1836	2448	2241	1400	32640	25024		
IQR	561	748	1154	254	5157	3475		
Change in Median		33%		−62%		−7%		75%
Change in IQR		33%		−78%		−33%		75%
HTPc in CTUh/W_P								
Min			2.8×10^{-8}	2.4×10^{-9}	-4.5×10^{-6}	-3.5×10^{-6}		
25th			3.8×10^{-7}	4.8×10^{-8}	1.2×10^{-7}	8.0×10^{-8}		
Median			5.2×10^{-7}	6.5×10^{-8}	5.0×10^{-7}	7.5×10^{-7}		
75th			6.3×10^{-7}	7.9×10^{-8}	9.2×10^{-7}	7.8×10^{-7}		
Max			6.7×10^{-7}	8.4×10^{-8}	1.9×10^{-6}	8.3×10^{-7}		
IQR			2.5×10^{-7}	3.1×10^{-8}	8.0×10^{-7}	7.0×10^{-7}		
Change in Median				−88%		51%		
Change in IQR				−87%		−12%		
ETPf in CTUe/W_P								
Min			11	1	2	1		
25th			242	30	11	14		
Median			332	41	306	390		
75th			395	49	815	402		
Max			424	53	5468	4192		
IQR			153	19	804	388		
Change in Median				−88%		27%		
Change in IQR				−87%		−52%		
RDPf in kg Sb-eq/W_P								
Min			1.0×10^{-6}	2.5×10^{-7}	-9.1×10^{-4}	-7.0×10^{-4}		
25th			5.0×10^{-4}	3.1×10^{-4}	1.3×10^{-4}	9.5×10^{-5}		
Median			8.3×10^{-3}	1.0×10^{-3}	4.8×10^{-4}	6.3×10^{-4}		
75th			9.7×10^{-3}	1.3×10^{-3}	1.4×10^{-3}	9.2×10^{-4}		
Max			1.1×10^{-2}	4.1×10^{-3}	2.3×10^{-3}	1.1×10^{-3}		
IQR			9.2×10^{-3}	1.0×10^{-3}	1.3×10^{-3}	8.2×10^{-4}		
Change in Median				−88%		33%		
Change in IQR				−89%		−35%		



(a) Technology scale



(b) Product system



(c) System boundary.

Figure S1. Influence of the KEYAs on the single harmonized LCA data set points of the five KEYIs. (**a**) technology scale (laboratory (L) vs pilot/industrial (PI/IN)); (**b**) product system (cell (C) vs module/system (M/S)); (**c**) system boundaries (cradle-to-gate (Gate) vs cradle-to-grave (Grave).

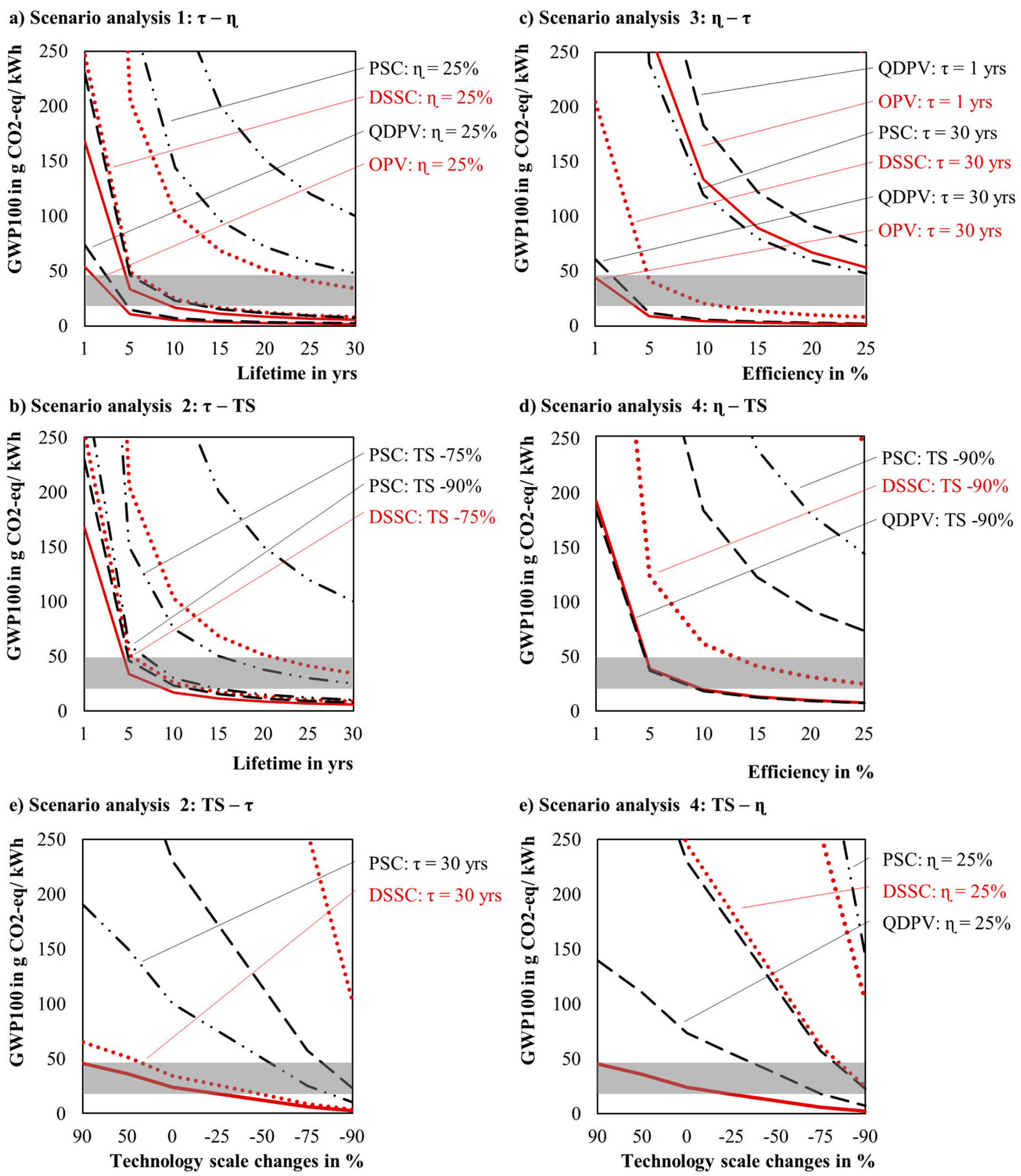


Figure S2. Detailed scenario analyses of the three influencing factors, efficiency, lifetime and upscaling, for PSC and DSSC.

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Appendix II

Appendix II contains the essential parts of the supplementary materials of Publication 2, Weyand et al. (2023a):

> Weyand S, Kawajiri, K., Mortan, C., Schebek L. (2023): Scheme for Generating Upscaling Scenarios of Emerging Functional Materials Based Energy Technologies in Prospective LCA (UpFunMatLCA). Journal of Industrial Ecology, DOI: 10.1111/jiec.13394

Supporting information S1: This supporting information provides more details on the development of the scheme and the data used for the practical implementation of the case study.

Supporting information S2: This supporting information includes modelled upscaling modules and data sets of the UpFunMatLCA scheme. In particular, this includes all collected data sets of the two modelled process learning modules, AM-1 Mapping of technologies and AM-2 Equipment scaling, and is also available at https://doi.org/10.48328/tudatalib-1063.4.

Supporting information S3: This supporting information provides the underlying data for Figure 6.

The full supporting information is available at: https://onlinelibrary.wiley.com/doi/full/10.1111/jiec.13394. The QR codes lead to the single supporting information.

SUPPORTING INFORMATION FOR:

Weyand, S., Kawajiri, K., Mortan, C. & Schebek, L. (2023.) Scheme for Generating Upscaling Scenarios of Emerging Functional Material Based Energy Technologies in Prospective LCA (UpFunMatLCA): General Methodology and Practical Implementation for the Case of Perovskite Solar Cells. *Journal of Industrial Ecology.*

Summary

This supporting information S1 provides more details on the development of the scheme and the data used for the practical implementation of the case study.

1 Introduction – Background on LCA and technology development

1.1 LCA description for technology developer only

LCA is a method standardized in the ISO 14040/14044 (ISO 14040 2006; ISO 14044 2006) for the evaluation of a full range of environmental impacts throughout the life cycle of products and services: It is also applied widely to technologies based on FunMat (Smith et al. 2019). The integration of LCA in the early stages of the maturation process has several advantages: LCA integrates environmental and sustainability indicators into technology development, enables the identification of unintended consequences, and gives environmental-friendly guidance before costly investments and resources are made. Technology developers can thus take actions to eliminate these consequences while supporting the prioritization of research activities (Smith et al. 2019). To this end, the following four LCA phases are applied according to the standards (ISO 14040 2006; ISO 14044 2006):

1) The **goal and scope definition (G&S)** encompasses the framework conditions such as the G&S of the LCA, the so-called functional unit as a reference unit, system boundaries, and the so-called product system. The product system represents the modeled life cycle. It is differentiated into upstream, encompassing processes from the raw material extraction to the manufacturing stage, operation, corresponding to the use phase, and downstream processes, referring to the recycling and end-of-life treatment of materials at the end of the product life cycle.

2) **Life cycle inventory (LCI)**: In this phase, extensive data collection occurs. To this end, the product system is divided into a foreground and background system. Generic or secondary data from LCA databases such as ecoinvent (ecoinvent 2020), IDEA (National Institute of Advanced Industrial Science and Technology 2018), or GaBi Databases (Sphera Solutions Inc. 2020) is usually used for the background system; the foreground system

corresponds to case study-specific data preferably from primary sources. For example, for emerging FunMat, the primary data on material inventories and processing energies are collected either from or together with technology developers during their investigations.
3) In **life cycle impact assessment (LCIA)**, the environmental impacts are quantified per impact category indicator. The considered indicators are selected depending on the G&S of the LCA study and the potential environmental impacts resulting from the assessed technology. For example, regarding climate-friendliness, LCIA focuses on energy-related impacts or other impacts involving GHG emissions rather than on impacts corresponding to materials like resource depletion or release of toxic substances during the extraction of raw materials.
4) In the **interpretation** phase as the last phase, the LCA results are processed as a basis for recommendations and decision-making, addressing uncertainty issues.

1.2 Systematic review on upscaling in prospective LCA

A systematic review was conducted to identify the relevant scientific works published on technology development and upscaling emerging technologies in prospective LCA. The review covered the two literature databases Web of Science and ScienceDirect using the keywords “life cycle assessment”, “LCA” combined with “upscaling”, “up-scaling”, “scale-up”, “learning” and “emerging technology” (with different spelling). As a result, we came up with 36 publications. In a first evaluation round, we checked the abstracts for the scope of the publications and excluded four publications. A second evaluation excluded publications with limited focus on a case study. Here, 19 publications were excluded. Finally, one publication was extended and in total 13 publications were assessed focusing on the topics:

- **Classification schemes of technology maturation considered**
- **Inclusiong of technology maturation**
- **Upscaling data, techniques and models**

Author	Database	Excluded, missing scope	Excluded, only case study
Bergerson et al. (2020)	WoS or Science direct	no	no
Buyle et al. (2019)	WoS or Science direct	no	no
Cucurachi, van der Giesen, and Guinée (2018)	WoS or Science direct	no	no
Gavankar, Suh, and Keller (2015)	WoS or Science direct	no	no
Hetherington et al. (2014)	WoS or Science direct	no	no
Kawajiri et al. (2020)	WoS or Science direct	no	no
Moni et al. (2020)	WoS or Science direct	no	no
Thonemann and Schulte (2019)	WoS or Science direct	no	no
Thonemann, Schulte, and Maga (2020)	WoS or Science direct	no	no
Tsoy et al. (2020)	WoS or Science direct	no	no
van der Giesen et al. (2020)	WoS or Science direct	no	no
van der Hulst et al. (2020)	WoS or Science direct	no	no
Arvidsson et al. (2017)	Additional	no	no

1.2.1 *Upscaling effects: Size, learning and experience effect*

The concept of economy of scale, originating from economic analysis, is the empirical finding that manufacturing at a bigger size with a higher TRL or MRL decreases costs. In 1936, Theodore Wright described this concept mathematically by the so-called size effect as a function of the initial cost C_0 of the first production capacity X_0 to the future cost at any time C_t of the future production capacity X_t and the scaling factor b (Eq. 1) (Wright 1936). Eq. 1 is also known as Wright's law.

$$C_t = C_0 \left(\frac{X_t}{X_0}\right)^b \quad (\text{Eq. } 1)$$

The size effect in a narrower sense means the reduction of unit costs simultaneously by increasing physical dimensions such as the manufacturing size. Consequently, this effect displays any economic, technical, or other effect related merely to the size, volume, or throughput of a process or technology. Thus, factor b is derived from empirical technology data at different dimensions by using regression analysis. The rationales behind this are decreasing marginal costs by dividing overhead costs by a larger number of products and better equipment utilization.

Beyond that, Wright discovered a cost reduction due to gained experience of the employees and an associated productivity increase, the so-called learning effect. Later the Boston Consulting Group (BCG) also established the term experience effect as a collection of various learning effects (Boston Consulting Group 1968). Learning and experience effects cannot be dedicated to single changes and are usually not considered separately. Therefore, we use the term learning effect synonymously for both effects in the following. The learning effect means that technologies can be manufactured more efficiently with each increase of their cumulative production rate due to increased experience of the daily routines at the production site of mass production. This effect is modeled using the so-called experience curve concept, based on data from real manufacturing sites or market data.

2 Methodology of UpFunMatLCA - Scheme for Generating Upscaling Scenarios of Emerging Functional Material Based Energy Technologies in Prospective LCA

In the following, the development of the three-step scheme UpFunMatLCA are explained in more detail. The general scheme is developed using the five phases of the scenario technique of Kosow and Gassner (2008) (Table S1).

Table S1 The connection of the generated upscaling scenarios using the three steps of UpFunMatLCA and the five phases of scenario technique of Kosow and Gassner (2008)

Three steps of UpFunMatLCA	Five phases of Kosow and Gassner (2008)	Explanation
Aim of UpFunMatLCA	**Phase 1: Scenario field identification**	The scenarios' purpose is to upscale an emerging FunMat from the current to a target development stage in prospective LCA. The problem of upscaling is the projection of the future process performances of emerging FunMats and modeling of life cycle inventory data based on the current stage of development. Therefore, the aim is to generate realistic scenarios that intend to represent possible development pathways of FunMats based on current technology developers' knowledge or specific decisions during technology development. These scenarios are used to model the foreground and background system and upscale the life cycle inventory data. The focus of the foreground system is not the full life cycle of FunMats but the limitation to the upstream processes, including processes from raw material extraction to manufactured FunMat.
Step I: Upscaling Definition and Step II: Upscaling Leap	**Phase 2: Identification of key factors**	The key factors or descriptors of the upscaling scenarios are the upscaling mechanisms. These are already explained in more detail in our study. To identify the key factors, we developed Step I and Step II of UpFunMatLCA. Here, first, the current and target stage is defined and results second, in a clear delimitiation of the development path and upscaling leap. Based on the upscaling leap, the relevant upscaling mechanisms are selected.
Step III: Upscaling Model and Data	**Phase 3: Analysis of the key factors**	The analysis of the key factors and the data collection process of the scenarios is implemented as upscaling modules in Step III. The upscaling module includes the upscaling method depending on the selected upscaling mechanism.
Upscaling scenarios	**Phase 4: Scenario generation**	Following the three steps of UpFunMatLCA, upscaling scenarios are generated.
LCIA + interpretation of the upscaling scenarios	**Phase 5: Scenario transfer**	The upscaling scenarios are used to model the foreground and background system and upscale LCI to assess the future possible environmental impacts of emerging FunMats in prospective LCA. Accordingly, the upscaling scenarios are transferred to the LCIA and interpretation.

In Table S2, the template for documenting the salient characteristics of each upscaling scenario is presented.

Table S2 Template for documenting upscaling in a prospective LCA

	Current stage	Target stage
Step I - Upscaling Definition		
Name		
General description		
Generic development stage		
Temporal coverage		
Manufacturing dimensions		
Step II - Upscaling Leap		
Selected upscaling mechanisms		
Step III - Upscaling Data and Model		
Modeled modules		

2.1 Step I – Upscaling Definition: Definition of the technology maturity

The investigation of upscaling in terms of projection of future technology developments has since long been the interest of economics to assess impacts on production costs, unit costs of technical equipment, products, and entire businesses in the future. For this purpose, general classification schemes to describe the maturation process and the status quo of the technology development and concepts for upscaling in economics have been introduced and applied in the LCA of technology development.

In the following, we explain the development of the generic technology scale from common classification schemes of technology development and description of technology maturity.

Table S3 Delimitation of the developed generic technology scale from common classification schemes and literature

Our technology scale		**TRL (NASA, 2007)**		**MRL (US DoD 2015)**	**EARTO (2014)**	**Hulst et al. (2020)**
Emerging	Generic conceptual	1-2	Basic principles and technology concept	1-2	Invention (TRL 1-2)	
	Generic lab	3-4	Proof-of-concept, validation in lab	3-4	Concept validation (TRL 3-4)	
	Generic pilot	5-7	Technology demonstration	5-8	Prototyping and incubation (TRL 5) Pilot production and demonstration (TRL 6-7)	
Mature	Generic fab-early	8-9	System test, launch and operations	9	Initial market introduction (TRL 8)	Industrial early production (MPL 0-5% + 5-50%)
	Generic fab-mature	n.c.		10	Market expansion (TRL 9)	Industrial mature production (MPL 50-100%)

2.2 Step II – Upscaling Leap: Selection of upscaling mechanisms for describing the leap from current to target stage

2.2.1 Generic upscaling mechanism for FunMat

A) Process learning

This mechanism subsumes innovations regarding the manufacturing processes. For a systematic distinction, we restrict process learning to the case of a given, i.e., non-changing material system, where only its specific manufacturing processes will change, i.e., the direct processing and manufacturing of FunMat. Similar to the innovative character of FunMat, these manufacturing processes may also be novel or are often only recently introduced for the respective emerging FunMat. In the terminology of LCA, these processes are attributed to the foreground system. In contrast, the background system comprehends the mining and processing processes of raw materials, the manufacturing of bulk intermediate products, and all infrastructure processes, e.g., power generation. These processes are usually long known technologies, which can generally be expected to undergo mainly incremental efficiency gains. If significant technology changes occur, they are not specific to the manufacturing of FunMat but have broader impacts on the general economy. Thus, the background system is incorporated in the upscaling mechanism C) external developments.

In LCA, the impacts of changing foreground manufacturing processes can be principally assessed via sensitivity analysis, assuming percent improvement of the processes (Glogic et al. 2019). On the one hand, the realistic setting of parameter variation requires in-depth knowledge of the specific processes for the respective FunMat and respective data, which often are not readily available. On the other hand, process changes are the most crucial aspect with impacts notably on the energy demand of emerging technologies. To account for this most crucial step, we discern three sub mechanisms:

A-1 Size scaling: For the mathematical implementation of this size effect into the upscaling module, we use two recently published models for size scaling (Kawajiri et al. 2020) and implement them into the size scaling module according to Eq. 2 and Eq. 3: notably for layer-based FunMat. For these types of technologies, we formulate the assumption specifically in the way that the energy demand of a process will decrease per manufactured square meter by increasing the manufacturing size from the current stage (e.g., lab samples in square centimeter range) to mass-produced goods (in m^2 range).

A-2 Technological learning: This sub mechanism reflects changes in the type of manufacturing processes from the current to target stage. These processes can, in many cases, be applied in the lab as well as large-scale manufacturing, e.g., the sputtering process (Madou 2012). However, in other cases, due to the changing requirements of mass production or automatic production lines, other manufacturing processes have to be anticipated for fab scale.

A-3 Industrial learning: This sub mechanism incorporates experience from daily routines at production sites of industrial manufacturing, displayed in Wright's law as well but based on production-site-specific data. If data from the industrial production site is available, the standard methods of the experience concept can be applied as shown in (Louwen et al. 2016; Bergesen and Suh 2016). However, in case of no data, the effect of industrial learning can be studied based on assumptions from general information on industrial learning of related technologies. In particular, for emerging FunMat, there is hardly any data from mass production.

B) Material learning

This mechanism subsumes innovations regarding the material system, including the related raw materials, and is intimately linked to the natural science-based development process of novel materials.

B-1 Change of material system: This sub mechanism results in a conceptual change of the entirely considered product system independently of the current stage. In LCA, for this case, no general upscaling approach can be conceived; instead, this type of change has to be mirrored by a complete change of the product system, i.e., a newly modeled LCA inventory.

B-2 Choice of input materials: Above the complete change of the material system, material learning may also encompass the optimization of material systems in changing single input materials. One example can be the substitution of lead by tin in PSC or the change of substrate material from glass to PET. In these cases, the original product system is kept, but respective upstream processes are substituted in LCA. However, these changes may directly influence the manufacturing processes since glass withstands higher temperatures than PET. In total, due to the wide variety of possible material changes, material learning can be characterized as a disruptive change for which the implications to another upscaling mechanism also need to be considered.

B-3 Optimization of input materials: Given that information on losses is available, material learning can be mirrored by sensitivity analysis. For example, findings from a study on life cycle losses of commercial PVs showed the material losses during the raw material extraction and manufacturing of two PV technologies (CdTe and CIGS) have been estimated to be between 15-37 % related to the used materials [38]. Consequently, similar projections need to be derived for FunMats used in PSC devices.

C) External developments

C-1 Incremental learning of the background system: This mechanism subsumes innovations resulting from the external progress of the background system over time. Here, integrated LCA models are developed in the literature, notably to integrate energy scenarios in LCA (Arvesen et al. 2018; Hertwich et al. 2015). By using these models, studies showed that considering the life cycle impacts of the energy transition could result in 60 % reductions of the GHG emissions of the electricity mix from 2010 to 2050 (Hertwich et al. 2015). Furthermore, for PV, temporal reductions of the primary energy consumption per energy output of even 70 % are expected from 2010 to 2050 when considering the infrastructural change of the energy system and efficiency gains of various industry sectors over time (Arvesen et al. 2018).

2.3 Step III - Upscaling Model and Data: Implementation of upscaling – modeling of upscaling modules for process learning

AM-1 Technological learning module "mapping of technologies"

No further details are necessary.

AM-2 Size scaling module "equipment scaling"

The empirical scaling is used when no data on the energy or power demands of the current stage is available, but only the kind of manufacturing process (e.g., sintering) and the suitable equipment (e.g., hot plate) is known. Therefore, the empirical scaling can already be applied at the conceptual scale. The empirical data usually includes the nominal power, i.e., the maximum power demand of the equipment is applied in the calculation. Therefore, the empirical scaling represents the worst-case estimation of the target power demand. In contrast, for the individual scaling, individualized consumptions from at least the lab stage are necessary to apply this model. This model is beneficial in case the actual measured power demand is far from the trend of the empirical data.

As a reference model, we define a "linear scaling" to refer to the typical way of scaling in conventional LCAs from "lab to fab" stage without considering size effects – i.e., the "non-scaling". This linear scaling is used to compare the effect of both models on the LCA results.

The graphical illustration of the two scaling models (Eq. 2-3) compared to the linear scaling is presented in Figure S1.

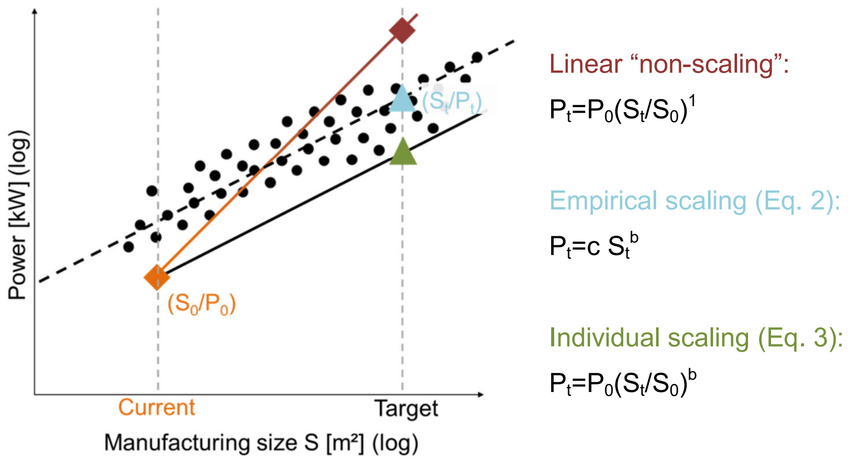


Figure S1 Graphical illustration of the model behind the size scaling module according to (Kawajiri et al. 2020)

AM-3 Industrial learning module "experience of industrial manufacturing"

No further details are necessary.

3 Case study: Upstream GHG Emissions of PSC from Lab to Fab

3.1 Case study description

3.1.1 Selected PSC samples

The PSC samples selected and assessed in this study were manufactured in lab as part of the material development of the Surface Science Group of the Technical University of Darmstadt. The interest of this material development lies in the fundamental understanding of the interplay of each layer or semiconductor band alignment (Hellmann et al. 2019; Wussler et al. 2020) to achieve high efficiencies and to find optimal layer combinations and manufacturing processes (Mortan et al. 2020; Mortan et al. 2019; Wittich et al. 2018; Dachauer et al. 2019). The selected samples are intended to represent a typical PSC material with layer materials and manufacturing methods commonly used in many research laboratories (Chen et al. 2017).

One selected sample have solar cell dimension of 32,5 mm^2 and a mini-module substrate dimension of 4 cm^2 shown in Figure S2. In addition, the detailed layer materials, thicknesses and manufacturing processes are shown in Figure S2. The detailed experimental procedure and flow chart of the manufacturing of the selected PSCs are explained in the following subsections.

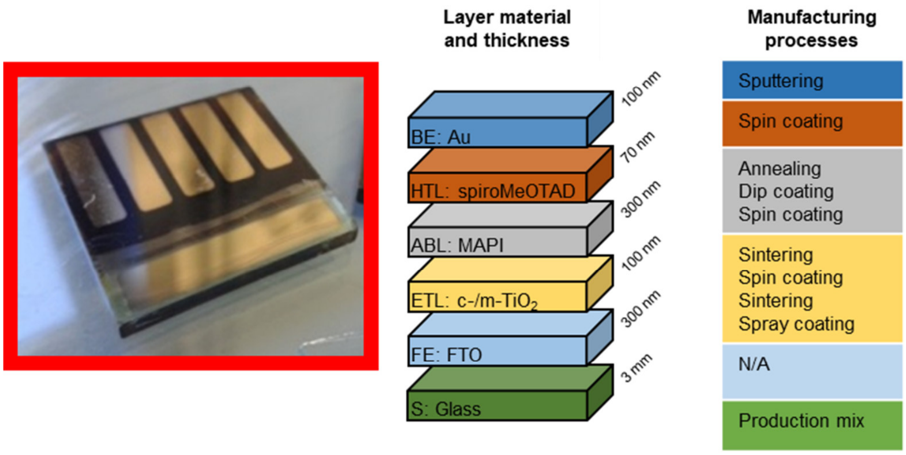


Figure S2 Picture of one selected PSC sample and specifications on the cell architecture and manufacturing of the status quo

The selected samples characterized electrically at the solar simulator setup, respectively through UV/Vis absorption spectroscopy, photoluminescence (PL), scanning electron microscopy (SEM), X-ray diffraction (XRD) and X-ray photoelectron spectroscopy (XPS) show a maximum power conversion efficiency of 15.6 %.

3.1.2 Experimental procedure

Front electrode with substrate (S) and front electrode (FE) (Glass coated with fluorine doped tin oxide (FTO): Pilkington NSG TEC15 FTO glass substrates have been used, cut as 2 cm x 2 cm squares, with a sheet resistance of 12-14 Ω/sq. and a glass thickness of 2.2 mm. The substrates are cleaned with isopropanol, soap, tap water, distilled water and blown dry with a nitrogen gun.

Electron transport layer (ETL) (compact and mesoporous titanium dioxide (c- and m-TiO_2): The c-TiO_2 layer is produced by spray pyrolysis on the glass/FTO substrates. 500 µL of titanium diisopropoxide bis(acetylacetonate), 75 wt. % in isopropanol (TIAA) from Merck is mixed with 18 mL reaction grade Ethanol. This solution is sprayed using oxygen carrier gas onto the glass/FTO substrates, that have been treated for 5 min. in an oxygen plasma oven and heated to 450°C for 25 min. prior to deposition. After the spraying process, the glass/FTO/c-TiO_2 substrates are annealed for 30 min. at 450°C in atmospheric conditions.

The m-TiO_2 layer is deposited by spin coating 100 µL of a 1:7 weight ratio solution of 18NR-T Titania (TiO_2) paste from Greatcell Solar and reaction grade ethanol onto each glass/FTO/c-TiO_2 substrates in atmospheric conditions. The solution is dropped on a substrate, before spinning at 83 rps (revolutions per second) for 45 s. After drying for 10 min. at 70°C, an additional sintering step takes place for 45 min. at 450°C on a hot plate, in atmospheric conditions.

Absorber layer (ABL) (PbI_2- and CH_3NH_3I-precursor): Prior to the deposition of the lead(II)iodide layer, the glass/FTO/c-TiO_2/m-TiO_2 substrates are treated in a UV/ozone oven for 15 min. The deposition takes place in a nitrogen (N_2) filled glovebox. After each substrate has been heated for 2 min. at 80°C on a hotplate, 100 µL of a 555 mg PbI_2 (Alfa Aesar 99.9985%, metal base) in 1 mL DMF (N,N-Dimethylformamide, Merck, 99.8%, anhydrous) solution, that has been stirred for at least half an hour at 80°C is dropped onto the hot substrates, then spun at 108 rps for 90 s. Each substrate is subsequently dried for 10 min. at 80°C.

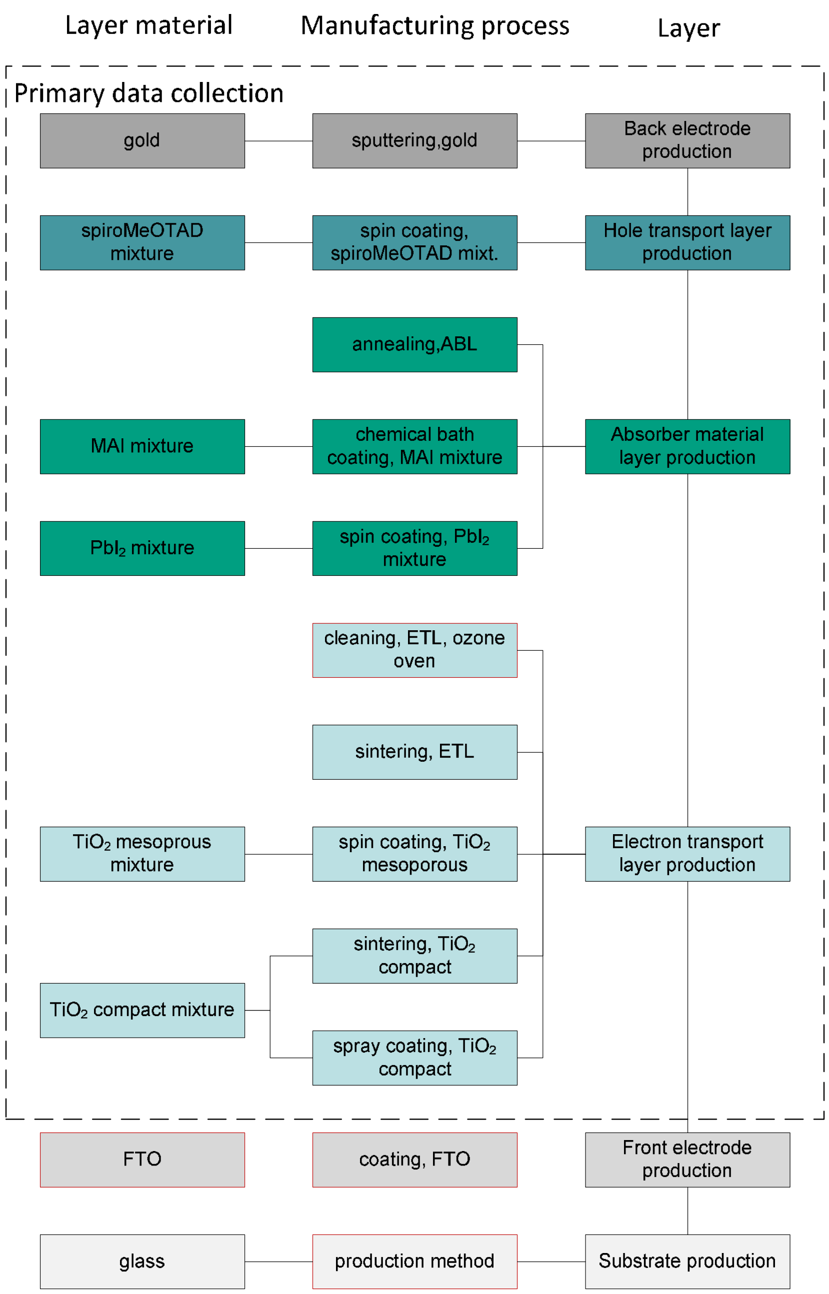
In a nitrogen glovebox, a solution of 400 mg methylammonium iodide (MAI, Greatcell Solar) and 40 mL anhydrous 2-propanol (99.5%, Merck) is stirred at 70°C until dissolved. After reaching room temperature, the solution is added to a Petri dish containing the glass/FTO/c-TiO_2/m-TiO_2/PbI_2 substrates. After 2 min., each substrate is rinsed in a clean 2-propanol bath of excess MAI and immediately blown dry with a pen blower. After additional drying on a hot plate for 15 min. at 50°C in the glovebox, the substrates are annealed in a tube furnace, in atmospheric air for 20 min. at 120°C.

Hole transport layer (HTL) (Spiro-MeOTAD): The deposition of the spiro-MeOTAD layer takes place on the glass/FTO/c-TiO_2/m-TiO_2/MAPI substrates, in a nitrogen glovebox. 80 mg spiro-MeOTAD (Borun New Material, 99.9%) is mixed in 1 mL chlorobenzene (Merck, anhydrous, 99.8%) with 28.5 µL 4-tert-butylpyridine (Merck, 98%) and with 17.5 µL of a solution made from 260 mg Li-TFSI (bis(trifluoromethane)sulfonimide lithium salt, Merck, >99%) and 0.5 mL acetonitrile (Merck, anhydrous 99.8%). 100 µL of the resulted spiro-MeOTAD solution is dropped on a glass/FTO/c-TiO_2/m-TiO_2/MAPI substrate. After a pause of 20 s, it is spun at 23 rps for 30 s and left to dry at room temperature in the glovebox.

Back contact with back electrode (BE) (Gold layer): The gold (Au) layer is deposited by argon sputtering on top to the spiro-MeOTAD layer, in a Quorum Technologies Q300TD machine with 30 mA current for 120 s, using a steel mask for defining the contacts.

3.1.3 Detailed flow chart of the status quo

The detailed manufacturing flow chart collected during lab visits between 2016-2018 are shown in Figure S3



FTO: fluorine doped tin oxide, TiO_2: titanium dioxide, PbI_2: lead (II) iodide, MAI: methylammonium iodide, ETL: Electron transport layer, ABL: Absorber material or active layer

Figure S3 Detailed process flow chart of the foreground system of the manufacturing stage

3.2 Developed upscaling scenarios

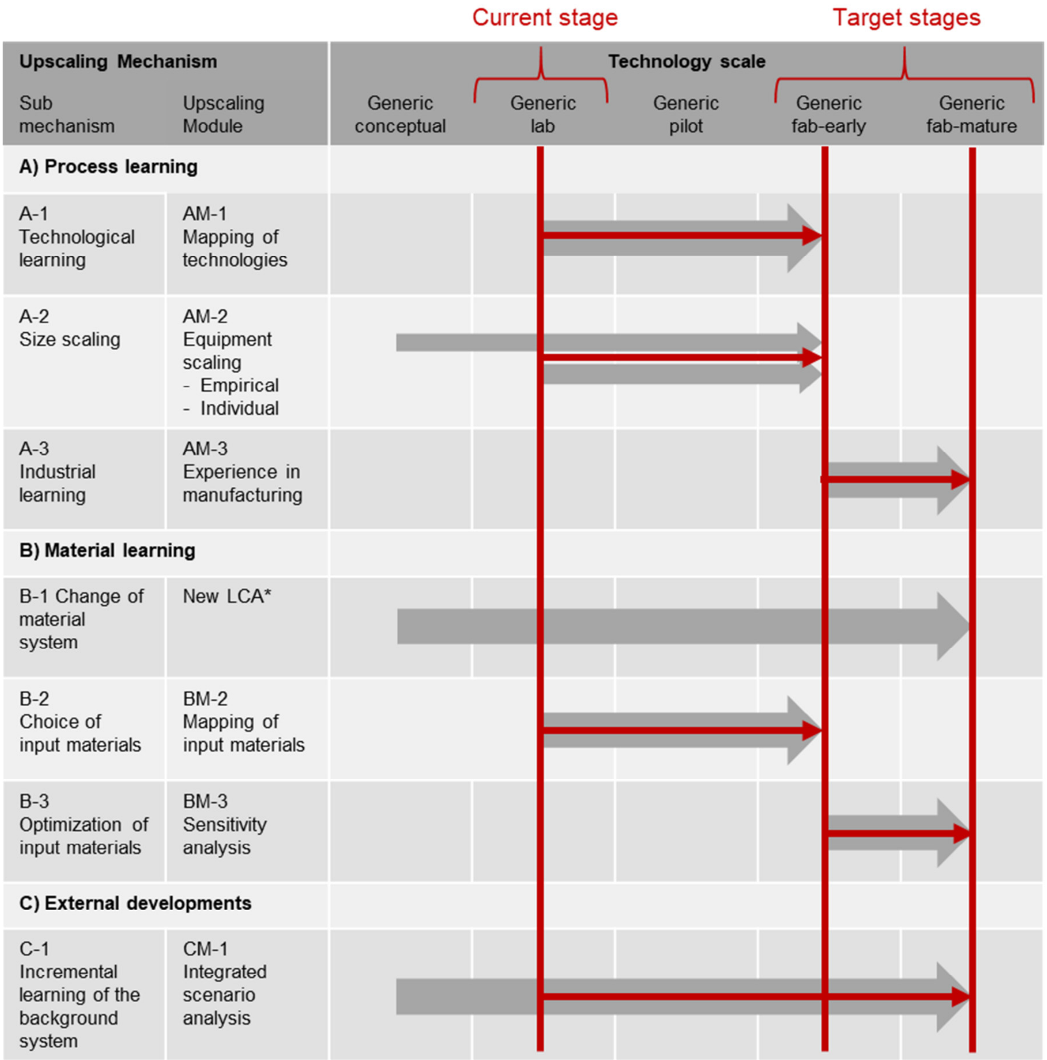
3.2.1 Step 1: Definition of the modelled current and target stages

Table S4 Generic technology scale extended by the standard cell, module, and manufacturing sizes for the definition of the technology maturity of PV case studies (adjusted and combined from (Baliozian et al. 2016; Gavankar, Suh, and Keller 2015; Fischer et al. 2020))

This study	**Generic conceptual**	**Generic lab**	**Generic pilot**	**Generic fab**	
				(early)	**(mature)**
Cell size	-	Not classified	Not classified	166x166 mm²	
Module size	-	>0.01 m²	0.01-1.65 m²	60 cells → 1.65 m² 72 cells →1.98 m²	
Manufactured size	-	>0.01 m²	0.01-1.65 m²	1-6 modules → 1.65 – 10 m²	
Comparison to other literature					
TRL according to (Baliozian et al. 2016)	0	1-4	5-7	8	9
Cell size according to (Baliozian et al. 2016) and updated (Fischer et al. 2020)	-	Not classified	Not classified	125x125 or 156x156 mm² 166x166 or 182x182 or 210x210 mm² (2020)	
Module size (Fischer et al. 2020)		Not classified	Not classified	60 or 72 cells until 2030	

3.2.2 Step 2: Selection of upscaling elements

Upscaling from generic lab to generic fab-early or generic fab-mature results in the preselection of six mechanisms (Figure S4). The change of material system is excluded since the PSC material does not fundamentally change. We focus only on the main contributor, thus only the process learning modules are finally selected.



* No module is applicable, but the complete change of the product system is necessary, i.e., a newly modeled LCA

Figure S4 Selection of upscaling elements

3.2.3 Step 3: Extension of the LCI - Data collections of the modeled process learning upscaling modules

AM-1 Mapping of technologies

The detailed description of this upscaling module AM-1 is available in the Supporting Information S2, Tabs “AM1[…]”.

AM-2 Equipment scaling – empirical and individual

Here, only the results of the sensitivity analysis are shown in Table S5. The detailed upscaling data of this upscaling module is provided in in the Supporting Information S2, Tabs “AM2[…]”..

Table S5 Results of the sensitivity analysis of GFabE in purple (underlying data from Table S5 are available in the Supporting Information S3, purple Tabs “Sensitivity analysis”).

GWP 100 in kg CO2-eq / m2							
sensitive indicators		**GFabE**		**GFabE (linear scaling)**		**GFabE (exclusion of spray coater)**	
perovskite solar cell production, all layers, wet chemical	**kg CO2 eq**	**100.00%**	**200.99226**	**100.76%**	**202.5113**	**100.00%**	**200.99107**
Control calculation		*100.00%*	*200.992281*	*100.76%*	*202.511321*	*100.00%*	*200.991091*
titanium dioxide (TiO2) mixture production, for titanium dioxide (TiC	*kg CO2 eq*	***2.98%***	*5.99376*	***2.98%***	*5.99376*	***2.98%***	*5.99376*
titanium dioxide (TiO2) mixture production, titanium dioxide (TiO2) r	*kg CO2 eq*	*0.12%*	*0.24227*	*0.12%*	*0.24227*	*0.12%*	*0.24227*
market for gold | gold | Cutoff, U - GLO	*kg CO2 eq*	*20.63%*	*41.46658*	*20.63%*	*41.46658*	*20.63%*	*41.46658*
spiroMeOTAD mixture production, hole transport layer - DE	*kg CO2 eq*	*2.47%*	*4.95939*	*2.47%*	*4.95939*	*2.47%*	*4.95939*
methylammonium iodide (MAI) mixture production, active layer - DE	*kg CO2 eq*	*1.70%*	*3.41449*	*1.70%*	*3.41449*	*1.70%*	*3.41449*
lead(II) iodide mixture production, active layer - DE	*kg CO2 eq*	*1.00%*	*2.00635*	*1.00%*	*2.00635*	*1.00%*	*2.00635*
solar glass production, ecoinvent version 3.7.1 cutoff	*kg CO2 eq*	*1.91%*	*3.83278*	*1.91%*	*3.83278*	*1.91%*	*3.83278*
fluorine doped tin oxide (FTO) production, front electrode, Espinosa	*kg CO2 eq*	*0.00%*	*1.0818E-05*	*0.00%*	*1.0818E-05*	*0.00%*	*1.0818E-05*
hot plate operation, during titanium dioxide compact mixture spray	kg CO2 eq	21.34%	42.9003	21.34%	42.9003	21.34%	42.9003
spray coater operation, during titanium dioxide compact mixture	**kg CO2 eq**	**0.00%**	**0.00119**	**0.67%**	**1.35053**	**0.00%**	**0**
hot plate operation, during titanium dioxide compact mixture sinter	kg CO2 eq	25.61%	51.48036	25.61%	51.48036	25.61%	51.48036
hot plate operation, during electron transport layer sintering, per ta	kg CO2 eq	18.56%	37.30461	18.56%	37.30461	18.56%	37.30461
hot plate operation, during titanium dioxide mesoporous mixture sp	kg CO2 eq	0.07%	0.14922	0.07%	0.14922	0.07%	0.14922
spin coater operation, during titanium dioxide mesoporous mixtu	**kg CO2 eq**	**0.00%**	**0.00436**	**0.03%**	**0.05064**	0.00%	0.00436
vacuum pump operation, during gold sputtering, per sputtered targe	kg CO2 eq	0.24%	0.47596	0.24%	0.47596	0.24%	0.47596
sputter coater operation, during gold sputtering, per target substrat	kg CO2 eq	0.17%	0.33722	0.17%	0.33722	0.17%	0.33722
hot plate operation, during methylammonium iodide mixture chemi	kg CO2 eq	0.04%	0.07461	0.04%	0.07461	0.04%	0.07461
hot oven operation, during annealing of active layer, per target sub:	kg CO2 eq	2.48%	4.99422	2.48%	4.99422	2.48%	4.99422
hot plate operation, during lead (II) iodide mixture spin coating, per	kg CO2 eq	0.67%	1.34297	0.67%	1.34297	0.67%	1.34297
spin coater operation, during lead (II) iodide mixture spin coating	**kg CO2 eq**	**0.00%**	**0.00872**	**0.05%**	**0.10129**	0.00%	0.00872
coating operation, during fluorine doped tin oxide coating, per targe	kg CO2 eq	0.00%	0	0.00%	0	0.00%	0
spin coater operation, during spiroMeOTAD mixture spin coating,	**kg CO2 eq**	**0.00%**	**0.00291**	**0.02%**	**0.03376**	0.00%	0.00291
electron transport layer production, titanium dioxide compact r	kg CO2 eq	68.70%	138.07606	68.85%	139.4254	68.70%	138.07487
back electrode production, gold, wet chemical deposition, per	kg CO2 eq	21.04%	42.27976	20.88%	42.27976	21.04%	42.27976
hole transport layer production, spiroMeOTAD, wet chemical (	kg CO2 eq	2.47%	4.9623	2.45%	4.9623	2.47%	4.9623
active layer production, CH3NH3PbI3, wet chemical depositio	kg CO2 eq	5.89%	11.84135	5.85%	11.84135	5.89%	11.84135
substrate production, glass, perovskite solar cell per target sc	kg CO2 eq	1.91%	3.83278	1.89%	3.83278	1.91%	3.83278
front electrode production, fluorine-doped tin oxide, wet chemi	kg CO2 eq	0.00%	1.082E-05	0.00%	1.082E-05	0.00%	1.082E-05
MaE		*30.80%*	*61.9156308*	*30.80%*	*61.9156308*	*30.80%*	*61.9156308*
PEn		69.20%	139.07665	69.95%	140.59569	69.19%	139.07546
Summe		**100.00%**	**200.992281**	**100.76%**	**202.511321**	**100.00%**	**200.991091**

AM-3-PSC Learning rate of PSC

No detailed upscaling data was collected.

3.3 Prospective upstream GHG emissions from lab to fab

The underlying data for Figure 6 are available in the Supporting Information S3.

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SUPPORTING INFORMATION FOR:

Weyand, S., Kawajiri, K., Mortan, C. & Schebek, L. (2023.) Scheme for Upscaling Scenarios of Emerging Functional Material Based Energy Technologies in Prospective LCA (UpFunMatLCA). *Journal of Industrial Ecology.*

This supporting information includes modelled upscaling modules and data sets of the UpFunMatLCA scheme. In particular, this includes all collected data sets of the modelled process learning modules AM1 (Technological learning module “mapping of technologies”) and AM2 (AM-2 Size scaling module “equipment scaling”) and is also available at https://doi.org/10.48328/tudatalib-1063.4.

Content: UpFunMatLCA - Process learning upscaling modules AM1 and AM2 - model and data

AM1	**Upscaling module: AM-1 Mapping of technologies**	
AM1		
	AM1	Search criteria of the systematic literature search and patent analysis
	AM1	All literature results
	AM1	Evaluation of the manufacturing processes for manufacturing area > 5cm²
	AM1	Evaluation of the manufacturing processes for flexible PSC
	AM1	Patent database

AM2	**Upscaling module: AM-2 Equipment scaling**	
AM2	**Summary of all empirical data sets and detailed regression models**	
	AM2	Spray coating - Spray coater
	AM2	Sputtering - Sputter coater
	AM2	Sputtering - Vacuum pump
	AM2	Spin coating - Spin coater
	AM2	Slot die coating - Slot die coater
	AM2	Annealing - Hot oven (harmonized to substrate area)
	AM2	Sintering/ Heating - Hot plate

Appendix III

Appendix III contains the supplementary materials of Publication 3, Weyand et al. (2023b).

> Weyand S, Kawajiri, K., Mortan, C., Zeller, V., Schebek L. (2023): Are perovskite solar cells an environmentally sustainable emerging energy technology? Upscaling from lab to fab in life cycle assessment. ACS Sustainable Chemistry & Engineering, DOI: 10.1021/acssuschemeng.3c03019.

Supporting information provides more details on the practical implementation of the case study and is available below.

SUPPORTING INFORMATION FOR:

Are perovskite solar cells an environmentally sustainable emerging energy technology? Upscaling from lab to fab in life cycle assessment

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Summary

This Supporting Information S1 provides more details on the practical implementation of the case study and includes:

Number of pages: 14

Number of figures: 1

Number of schemes: -

Number of tables: 4

More supporting material to this article

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Introduction

Environmental sustainable energy technologies are those that are climate-friendly and, at the same time, show a low potential of trade-offs to other environmental impacts in terms of resource use or effects on human health or ecosystem quality. The key indicators, referred to as KEYIs, are the impact category indicators selected for a comprehensive description of the potential environmental impacts of the assessed PSC case study according to Weyand et al. (2019).[1] The selected KEYIs to assess environmental sustainability are explained below.

LCA description for technology developer only

LCA is a method standardized in the ISO 14040/14044[2,3] for the evaluation of a full range of environmental impacts throughout the life cycle of products and services: It is also applied widely to technologies based on FunMat.[4] The integration of LCA in the early stages of the maturation process has several advantages: LCA integrates environmental and sustainability indicators into technology development, enables the identification of unintended consequences, and gives environmental-friendly guidance before costly investments and resources are made. Technology developers can thus take actions to eliminate these consequences while supporting the prioritization of research activities.[4] To this end, the following four LCA phases are applied according to the standards (ISO 14040 2006; ISO 14044 2006):

1) The **goal and scope definition (G&S)** encompasses the framework conditions such as the G&S of the LCA, the so-called functional unit as a reference unit, system boundaries, and the so-called product system. The product system represents the modeled life cycle. It is differentiated into upstream, encompassing processes from the raw material extraction to the manufacturing stage, operation, corresponding to the use phase, and downstream processes, referring to the recycling and end-of-life treatment of materials at the end of the product life cycle.

2) **Life cycle inventory (LCI)**: In this phase, extensive data collection occurs. To this end, the product system is divided into a foreground and background system. Generic or secondary data from LCA databases such as ecoinvent (ecoinvent 2020), IDEA (National Institute of Advanced Industrial Science and Technology 2018), or GaBi Databases (Sphera Solutions Inc. 2020) is usually used for the background system; the foreground system corresponds to case study-specific data preferably from primary sources. For example, for emerging FunMat, the primary data on material inventories and processing energies are collected either from or together with technology developers during their investigations.

3) In **life cycle impact assessment (LCIA)**, the environmental impacts are quantified per impact category indicator. The considered indicators are selected depending on the G&S of the LCA study and the potential environmental impacts resulting from the assessed technology. For example, regarding climate-friendliness, LCIA focuses on energy-related

impacts or other impacts involving GHG emissions rather than on impacts corresponding to materials like resource depletion or release of toxic substances during the extraction of raw materials.

4) In the **interpretation** phase as the last phase, the LCA results are processed as a basis for recommendations and decision-making, addressing uncertainty issues.

Material and methods

Case study description

The PSC samples selected and assessed in this study were manufactured in lab as part of the material development of the Surface Science Group of the Technical University of Darmstadt. The interest of this material development lies in the fundamental understanding of the interplay of each layer or semiconductor band alignment[5,6] to achieve high efficiencies and to find optimal layer combinations and manufacturing processes[7–10]. The selected samples are intended to represent a typical PSC material with layer materials and manufacturing methods commonly used in many research laboratories.[11,12]

One selected sample have solar cell dimension of 32,5 mm^2 and a mini-module substrate dimension of 4 cm^2. The detailed experimental procedure is explained in the following subsection.

1.1.1 Experimental procedure (taken from Weyand et al., 2023 [13])

Front electrode with substrate (S) and front electrode (FE) (Glass coated with fluorine doped tin oxide (FTO): Pilkington NSG TEC15 FTO glass substrates have been used, cut as 2 cm x 2 cm squares, with a sheet resistance of 12-14 Ω/sq. and a glass thickness of 2.2 mm. The substrates are cleaned with isopropanol, soap, tap water, distilled water and blown dry with a nitrogen gun.

Electron transport layer (ETL) (compact and mesoporous titanium dioxide (c- and m-TiO_2)): The c-TiO_2 layer is produced by spray pyrolysis on the glass/FTO substrates. 500 µL of titanium diisopropoxide bis(acetylacetonate), 75 wt. % in isopropanol (TIAA) from Merck is mixed with 18 mL reaction grade Ethanol. This solution is sprayed using oxygen carrier gas onto the glass/FTO substrates, that have been treated for 5 min. in an oxygen plasma oven and heated to 450°C for 25 min. prior to deposition. After the spraying process, the glass/FTO/c-TiO_2 substrates are annealed for 30 min. at 450°C in atmospheric conditions.

The m-TiO_2 layer is deposited by spin coating 100 µL of a 1:7 weight ratio solution of 18NR-T Titania (TiO_2) paste from Greatcell Solar and reaction grade ethanol onto each glass/FTO/c-TiO_2 substrates in atmospheric conditions. The solution is dropped on a substrate, before spinning at 83 rps (revolutions per second) for 45 s. After drying for 10 min. at 70°C, an additional sintering step takes place for 45 min. at 450°C on a hot plate, in atmospheric conditions.

Absorber layer (ABL) (PbI_2- and CH_3NH_3I-precursor): Prior to the deposition of the lead(II)iodide layer, the glass/FTO/c-TiO_2/m-TiO_2 substrates are treated in a UV/ozone oven for 15 min. The deposition takes place in a nitrogen (N_2) filled glovebox. After each substrate has been heated for 2 min. at 80°C on a hotplate, 100 µL of a 555 mg PbI_2 (Alfa Aesar 99.9985%, metal base) in 1 mL DMF (N,N-Dimethylformamide, Merck, 99.8%, anhydrous) solution, that has been stirred for at least half an hour at 80°C is dropped onto the hot substrates, then spun at 108 rps for 90 s. Each substrate is subsequently dried for 10 min. at 80°C.

In a nitrogen glovebox, a solution of 400 mg methylammonium iodide (MAI, Greatcell Solar) and 40 mL anhydrous 2-propanol (99.5%, Merck) is stirred at 70°C until dissolved. After reaching room temperature, the solution is added to a Petri dish containing the glass/FTO/c-TiO_2/m-TiO_2/PbI_2 substrates. After 2 min., each substrate is rinsed in a clean 2-propanol bath of excess MAI and immediately blown dry with a pen blower. After additional drying on a hot plate for 15 min. at 50°C in the glovebox, the substrates are annealed in a tube furnace, in atmospheric air for 20 min. at 120°C.

Hole transport layer (HTL) (Spiro-MeOTAD): The deposition of the spiro-MeOTAD layer takes place on the glass/FTO/c-TiO_2/m-TiO_2/MAPI substrates, in a nitrogen glovebox. 80 mg spiro-MeOTAD (Borun New Material, 99.9%) is mixed in 1 mL chlorobenzene (Merck, anhydrous, 99.8%) with 28.5 µL 4-tert-butylpyridine (Merck, 98%) and with 17.5 µL of a solution made from 260 mg Li-TFSI (bis(trifluoromethane)sulfonimide lithium salt, Merck, >99%) and 0.5 mL acetonitrile (Merck, anhydrous 99.8%). 100 µL of the resulted spiro-MeOTAD solution is dropped on a glass/FTO/c-TiO_2/m-TiO_2/MAPI substrate. After a pause of 20 s, it is spun at 23 rps for 30 s and left to dry at room temperature in the glovebox.

Back contact with back electrode (BE) (Gold layer): The gold (Au) layer is deposited by argon sputtering on top to the spiro-MeOTAD layer, in a Quorum Technologies Q300TD machine with 30 mA current for 120 s, using a steel mask for defining the contacts.

Estimation of the worldwide PV potential

Kawajiri et al. (2011) estimate a worldwide PV potential of ground-mounted PV systems consisting of multi- and monocrystalline silicon PV modules according to Eq. S1. The estimation includes the effects of country-specific irradiation and temperature effect on the PV performance.

$$Y_{py} = \frac{E_{py}}{P_{AS}} = \frac{K'}{G_S}\sum_{m=1}^{12}\left\{1 + \alpha_{Pmax}\left(T_{Am} + \Delta T - 25\right)\right\} H_{Am} \qquad \textbf{Eq. S1}$$

With:

Y_{py}: Annual PV potential in kWh/kW

E_{py}: Annual energy generation in kWh

P_{AS}: Nominal power of the PV module at standard test conditions in kW

K': Design factor

G_s: Solar irradiance at STC = 1 kW/m² (IEC 61724 [14])

H_{Am}: Monthly total solar irradiation [kWh/m²]

α_{Pmax}: Maximum power temperature coefficient of PV modules

T_{Am}: Ambient temperature profile averaged over a month

ΔT: Weighted average of module temperature annual increase for PV systems mounted on platforms = 18.4°C [15]

Prospective LCA

Goal and scope definition – upscaling definition and leap

The general product system of PSC modules with the defined system boundaries, foreground, and background system, and the considered processes is summarized in the Figure S1. Figure S1 illustrates the three upscaling mechanisms recommended for PSC upscaling using UpFunMatLCA.[13] The detailed documentation of the generated upscaling scenarios are summarized in Table S1.

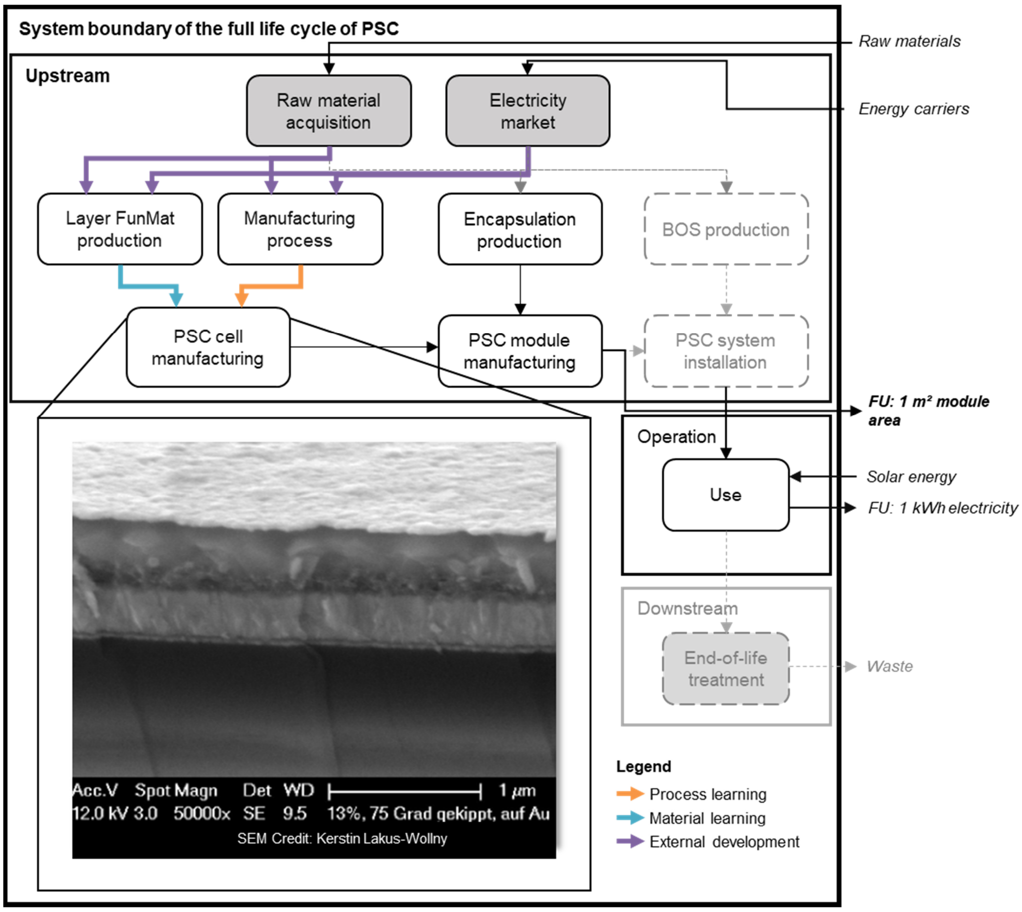

Figure S1 Illustrating the life cycle as product system of the assessed PSC samples applied as PV modules (adjusted from Weyand et al. (2023)[13], with system boundaries, including the considered (black border) and unconsidered (grey dashed border) upstream, operation, and downstream processes, with foreground (white filled boxes) and background processes (grey filled boxes), and with involved upscaling mechanisms (colored arrows). Elementary flows and functional units are marked by italic font.

Table S1 Key characteristics of the three generated upscaling scenarios using UpFunMatLCA

	Current stage	Target stage	Further upscaling scenarios		
Step I - Upscaling Definition					
Name	GLab (Baseline)	GFabM	GLab+ED	GFabM+ML	GFabM+ML+ED
General description (PSC configurations with layer materials and manufacturing processes are summarized in the study, Table 1)	Status quo: PSC samples manufactured with a size of 20 x 20 mm² in lab surroundings; primary data was collected during lab manufacturing of 20 PSC samples in total over the period from 2016 to 2020.	Prospective: Aims for the evaluation of the prospective environmental impacts of the selected PSC samples upscaled and integrated into a PV module as an alternative to today's electricity mix based on the hypothetical assumption that PSC would have been manufactured in mass production sites with manufacturing sizes of 10m² and MPL >50% in 2020.	Prospective: considering only simplified external development: PSC samples manufactured with a size of 20 x 20 mm² in lab surroundings; primary data was collected during lab manufacturing of 20 PSC samples in total over the period from 2016 to 2020. Here, it was assessed what happens if PSC modules were manufactured using electricity from PVs. The limitation is that we use ecoinvent 3.7.1 instead of prospective LCI data.	Prospective: Aims for the evaluation of the prospective environmental impacts of the selected PSC samples upscaled and integrated into a PV module as an alternative to today's electricity mix based on the hypothetical assumption that PSC would have been manufactured in mass production sites with manufacturing sizes of 10m² and MPL >50% in 2020. In addition, the material learning of the back electrode from Au to C was assessed.	Prospective: Aims for the evaluation of the prospective environmental impacts of the selected PSC samples upscaled and integrated into a PV module as an alternative to today's electricity mix based on the hypothetical assumption that PSC would have been manufactured in mass production sites with manufacturing sizes of 10m² and MPL >50% in 2020. In addition, the material learning of the back electrode from Au to C was assessed and the electricity provided electricity from PV. The limitation is that we use ecoinvent 3.7.1 instead of prospective LCI data.
Generic development stage	Lab	Fab (mature)	Lab	Fab (mature)	Fab (mature)
Temporal coverage	2020	2020	2020	2020	2020
Manufacturing dimensions	20 x 20 mm²	10 m²	20 x 20 mm²	10 m²	10 m²
Step II - Upscaling Leap					
Selected upscaling mechanisms (details to preselection are shown in Figure S4, Supporting Information S1)	None	A-1 Technological learning A-2 Size scaling A-3 Industrial learning	C-1 Incremental learning of the background system (only change of electricity supply process)	A-1 Technological learning A-2 Size scaling A-3 Industrial learning B-2 Choice of input materials (only BE material changed)	A-1 Technological learning A-2 Size scaling A-3 Industrial learning B-2 Choice of input materials (only BE material changed) C-1 Incremental learning of the background system (only change of electricity supply process)

Step III - Upscaling Data and Model					
Modeled modules (description see below)	None	AM-1 Mapping of technologies (Figure 4, Table 2) AM-2 Equipment scaling – empirical (Figure 5) AM-3 Experience in manufacturing	CM-1 Electricity supply changed from mix to PV generated electricity (ecoinvent 3.7.1)	AM-1 Mapping of technologies (Figure 4, Table 2) AM-2 Equipment scaling – empirical (Figure 5) AM-3 Experience in manufacturing BM-2 Mapping of input materials (Gold substituted by Carbon)	AM-1 Mapping of technologies (Figure 4, Table 2) AM-2 Equipment scaling – empirical (Figure 5) AM-3 Experience in manufacturing BM-2 Mapping of input materials (Gold substituted by Carbon) CM-1 Electricity supply changed from mix to PV generated electricity (ecoinvent 3.7.1)

Life cycle inventory (LCI) – upscaling model and data

Current stage

The material inventory and its data source are summarized in Table S2. The process-specific energy inputs of each manufacturing step were measured with the Gossen Metrawatt test instrument SECUTEST 0701/0702S and outlined in Table S3.

Table S2 Status quo inventory of the material inputs collected during manufacturing of 0.0004 m² sized PSC (GLab)

Layer	Material	Amount	Unit	Comment
BE	Gold	1.31E-07	kg	Mass of gold in kg (average of leaching tests) (only embedded material on sample included, no loss considered)
HTL	SpiroMeOTAD	1.00E-07	m³	Volume of spiroMeOTAD mixture per spin-coated substrate of 4 cm² (embedded material and material loss included)
ACT	MAI mixture	4.00E-05	m³	Volume methylammonium mixture useable for chemical bath coating of a maximum number of 50 substrates (embedded material and material loss included)
	PbI2 mixture	1.00E-07	m³	Volume of lead (ii) iodide mixture per spin-coated substrate of 4cm² (embedded material and material loss included)
EBL	TiO2 mesoporous mixture	1.00E-07	m³	Volume of TiO2 mesoporous mixture per spin-coated substrate of 4cm² (embedded material and material loss included)
	TiO2 compact mixture	1.85E-05	m³	Volume of TiO2 compact mixture in filled in the spray coater head (embedded material and material loss included)
FE	Fluorine	1.28E-11	kg	Mass of fluorine according to [4]
	Tin	4.16E-10	kg	Mass of tin according to [4]
S	Glass	0.001428	kg	Mass of the lab substrate

Table S3 Status quo inventory of the processing energy collected during manufacturing of 0.0004 m² sized PSC (GLab); Data is either measured (m), calculated (c) or taken as rated power (r).

Layer	Manufacturing processes	Manufacturing steps	Manufacturing equipment	Power input P_0 [kW]		Processing time t_0 [h]	Energy input E_0 [kWh/4 cm²]	
BE	Sputtering	Sputter coater operation	Sputter coater	1.40E+00	r	3.30E-02	7.78E-03	c
		Vacuum pump operation	Vacuum pump	3.70E-01	r	1.10E-01	6.68E-03	c
HTL	Spin coating	Spin coater operation	Spin coater	2.50E-03	m	8.30E-03	2.08E-05	c
ACT	Annealing	Hot oven operation	Hot oven	8.40E-02	c	2.50E-01	3.50E-03	m
	Dip coating	Hot plate operation	Hot plate	4.00E-03	c	2.50E-01	1.67E-04	m
	Spin coating	Spin coater operation	Spin coater	2.50E-03	m	2.50E-02	6.25E-05	c
		Hot plate operation	Hot plate	4.90E-02	c	4.20E-01	3.00E-03	m
EBL	Sintering	Hot plate operation	Hot plate	6.70E-01	c	7.50E-01	8.33E-02	m
	Spin coating	Spin coater operation	Spin coater	2.50E-03	m	1.30E-02	3.13E-05	c
		Hot plate operation	Hot plate	1.20E-02	c	1.70E-01	3.33E-04	m
	Sintering	Hot plate operation	Hot plate	1.40E+00	c	5.00E-01	1.15E-01	m

	Spray coating	Spray coater operation	Spray coater	2.20E+00	c	2.80E-03	1.00E-03	m
		Hot plate operation	Hot plate	1.40E+00	c	4.20E-01	9.58E-02	m
FE	*Unknown coating*	*N/A*	*N/A*	*N/A*		*N/A*	*N/A*	
S	*Market for solar glass, low iron (ecoinvent)*	*N/A*	*N/A*	*N/A*		*N/A*	*N/A*	
Total							**3.17E-01**	**c**

Target stage

No upscaling modules from current to the target stage were considered for the material inputs. Consequently, the material inputs were linearly upscaled. The above-mentioned upscaling modules modeled the process-specific energy inputs at the target stage. In addition, we differentiate between the original measured energy inputs per total manufacturing size and the optimized energy inputs. For the optimized energy inputs, we consider the full utilization per equipment, i.e., the maximum number of samples per hot plate is determined, and the measured energy inputs of six manufactured samples are allocated to this maximum number. The processing energy of the target stage is derived from the implementation of the following upscaling modules into the inventory of the current stage. The inventory of the processing energy per manufacturing process and applied upscaling module are summarized in Table S4. Upscaled inventory of the processing energy inputs per manufacturing process in kWh/m² (GFabM, GFabM+ML); for a maximum manufactured substrate area of 10 m².

Table S4 Upscaled inventory of the processing energy inputs per manufacturing process in kWh/m² (GFabM, GFabM+ML); for a maximum manufactured substrate area of 10 m²

Manufacturing process	Target stage		
	linear	empirical	individual
Sputtering (Sputter coater: Quorum)	19.4	0.8	0.2
Sputtering (Vacuum pump)	16.7	0.0	0.0
Annealing (Hot oven)	8.8	12.7	2.4
Spin coating (Spin coater)	0.1	0.1	0.01
Spray coating (Spray coater)	2.5	0.002	0.0003
Sintering (Hot plate)	245.1	8.5	7.1
Heating (Hot plate)	2.9	4.2	0.1
Slot die coating (Slot die coater)	N/A	0.001	N/A

Life cycle impact assessment – explanation of the selected KEYIs

Climate-friendliness can be assessed by a high net energy gain, indicated by a high energy potential to be harvested, low cumulative energy demand as expended energy, and low GHG emissions. Besides these energy-related key indicators (KEYIs), trade-offs to other potential environmental impacts are described by the so-called material-related KEYIs. According to Weyand et al. (2019), three material-related KEYIs were recommended for a comprehensive description of the potential environmental impacts of photovoltaic technologies and their trade-offs[1]:

- ILCD midpoints 2011, resource depletion – mineral and fossil,
- ILCD midpoints 2011, human toxicity,
- ILCD midpoints 2011, freshwater ecotoxicity.[16,17]

The ILCD midpoints 2011 were updated to the Environmental Footprint Methods in 2021.[18] Therefore, three become the following four categories:

- EF method 2021, Resource use, mineral and metals,
- EF method 2021, Resource use, energy carriers,
- EF method 2021, Cancer human health effects,
- EF method 2021, Ecotoxicity freshwater.

We assess the climate-friendliness and resource-efficiency, and we leave the toxicity assessment for future research for the following reasons:

- Our upscaling focuses on the manufacturing stage. The main toxicity impacts are expected in the end-of-life phase.
- Toxicity indicators require regionlized assessment[19] and detailed knowledge of direct and indirect heavy metal emissions during the life cycle as shown in Fthenakis et al. (2008)[20].
- Other possible risky materials such as nanomaterials can not adequately assessed with LCA and a combination with risk assessment is recommended. [21,22]

Interpretation - Break-even comparisons for the assessment of the environmental-friendliness

The framework of Glogic et al. (2019) includes a break-even comparison to find the point when an OPV charger's environmental impact equals the impact of charging a phone with the country-specific electricity mix using Eq. S2 [23]. These calculated break-even charges enable a more realistic interpretation of how environmentally friendly an OPV charger is or how often an OPV charger has to be used to be more environmentally friendly than the existing country-specific electricity mix. Together with the irradiation model developed there, a more realistic statement on the environmental-friendly use of OPV chargers can be made for respective countries. The environmental impacts are taken from an LCA study.

$$\boldsymbol{break-even\ OPV\ charges} = \frac{\boldsymbol{env.impact\ of\ production\ and\ disposal\ of\ OPV\ charger}}{\boldsymbol{env.impact\ of\ single\ grid\ charge\ \cdot lifetime\ of\ OPV\ charger}} \quad \textbf{Eq. S2}$$

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Appendix IV

Appendix IV contains the PSC LCI Database (openLCA model, openLCA results and monte carlo simulations).

Supporting information S1: S1 includes the openLCA results (XLSX) and monte carlo simulations (XLSX) and is available at: https://tudatalib.ulb.tu-darmstadt.de/handle/tudatalib/3924 or use QR code.

Supporting information S2: S2 contains the PSC LCI Database (ZOLCA) and is limited accessible at: https://tudatalib.ulb.tu-darmstadt.de/handle/tudatalib/3925 or use QR code.