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METHODS ARTICLE

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

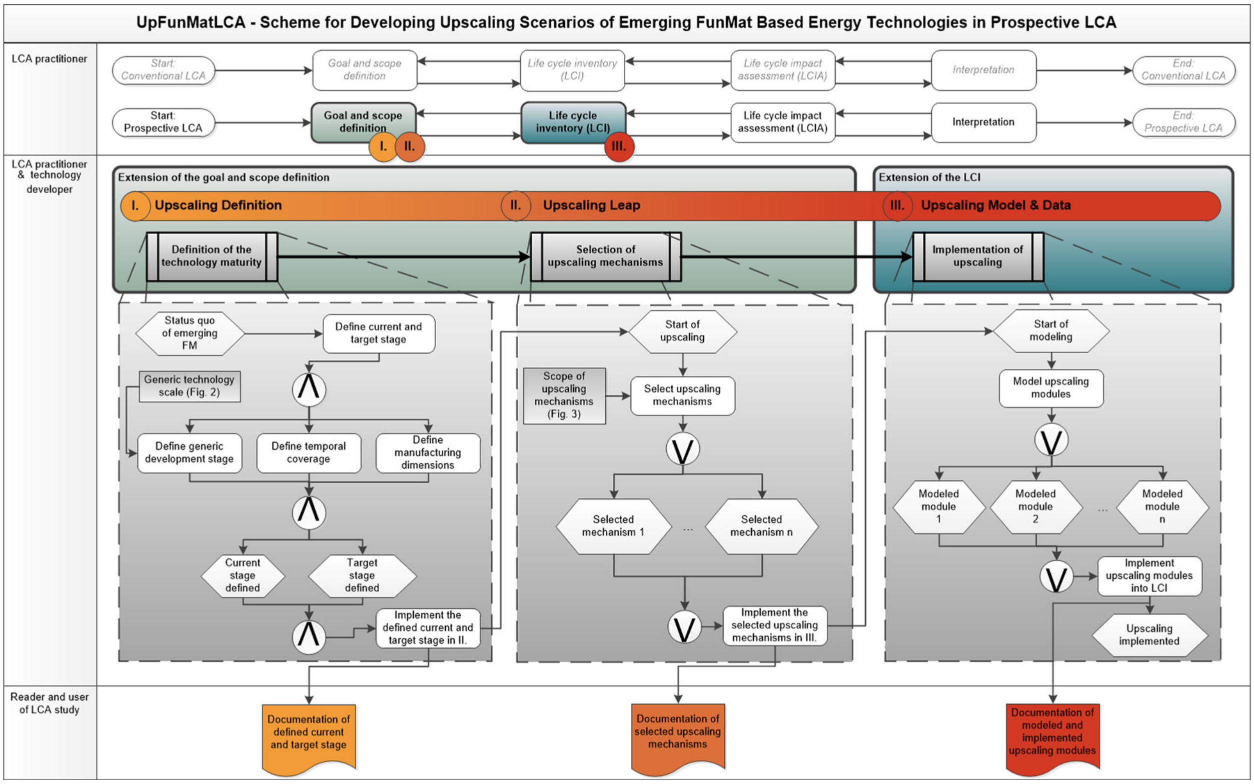


FIGURE 1 Workflow of the UpFunMatLCA with the three upscaling Steps I–III (marked with orange circles) as extensions to the four life cycle assessment (LCA) phases in prospective LCAs and the division of the three user groups—LCA practitioner, cooperation with technology developer, and user of prospective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

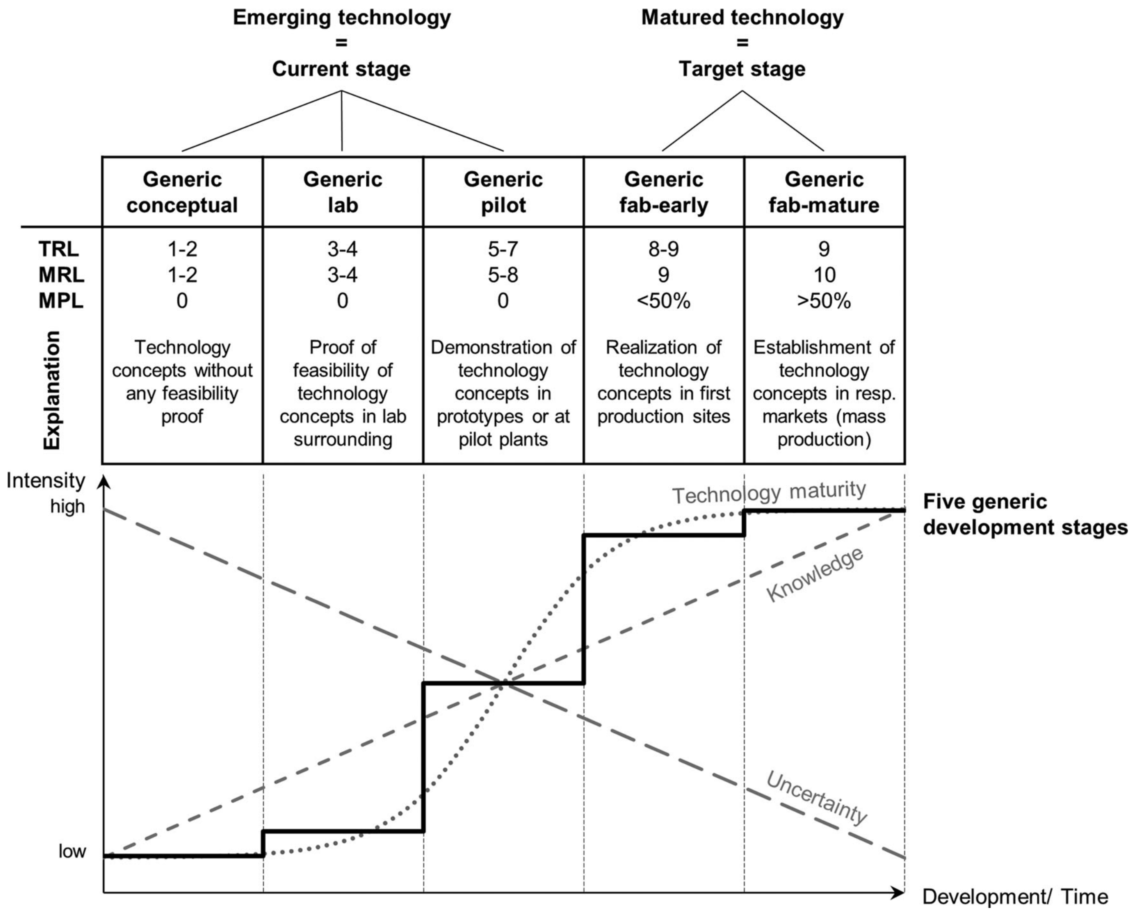


FIGURE 2 Generic technology scale for the definition of the modeled development stages illustrating the schematic dependency of the intensity of technology maturity, knowledge, and uncertainty on the five generic development stages (as summary and extension of Arvidsson et al., 2017; Bergerson et al., 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).

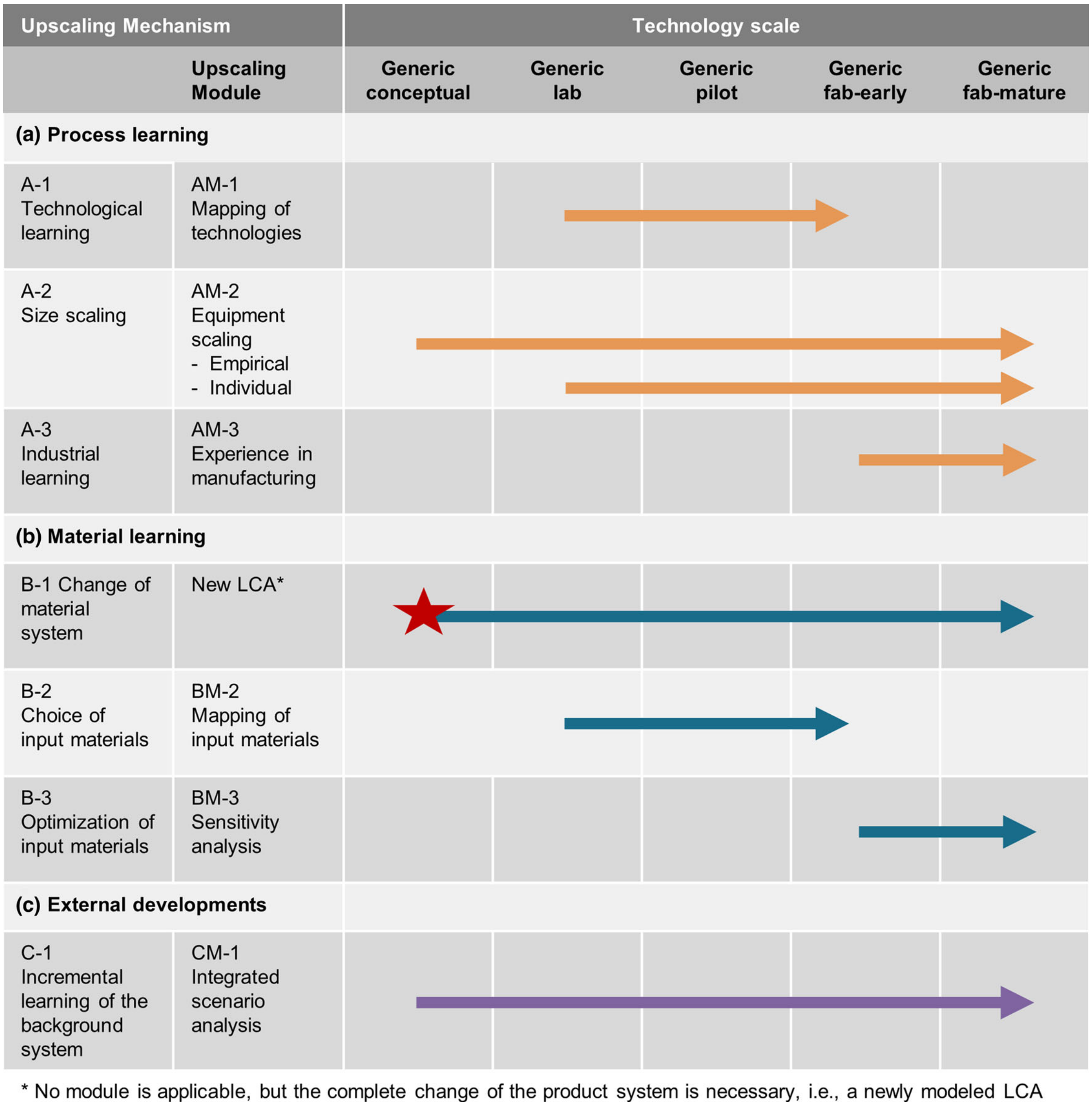


FIGURE 3 Schematic illustration of the scope of the upscaling mechanisms concerning a specific "leap" from one to another generic development stage for the upscaling of emerging FunMat-based technologies. Legend: orange arrows, possible leap of the process learning modules; blue arrows, possible leap 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.

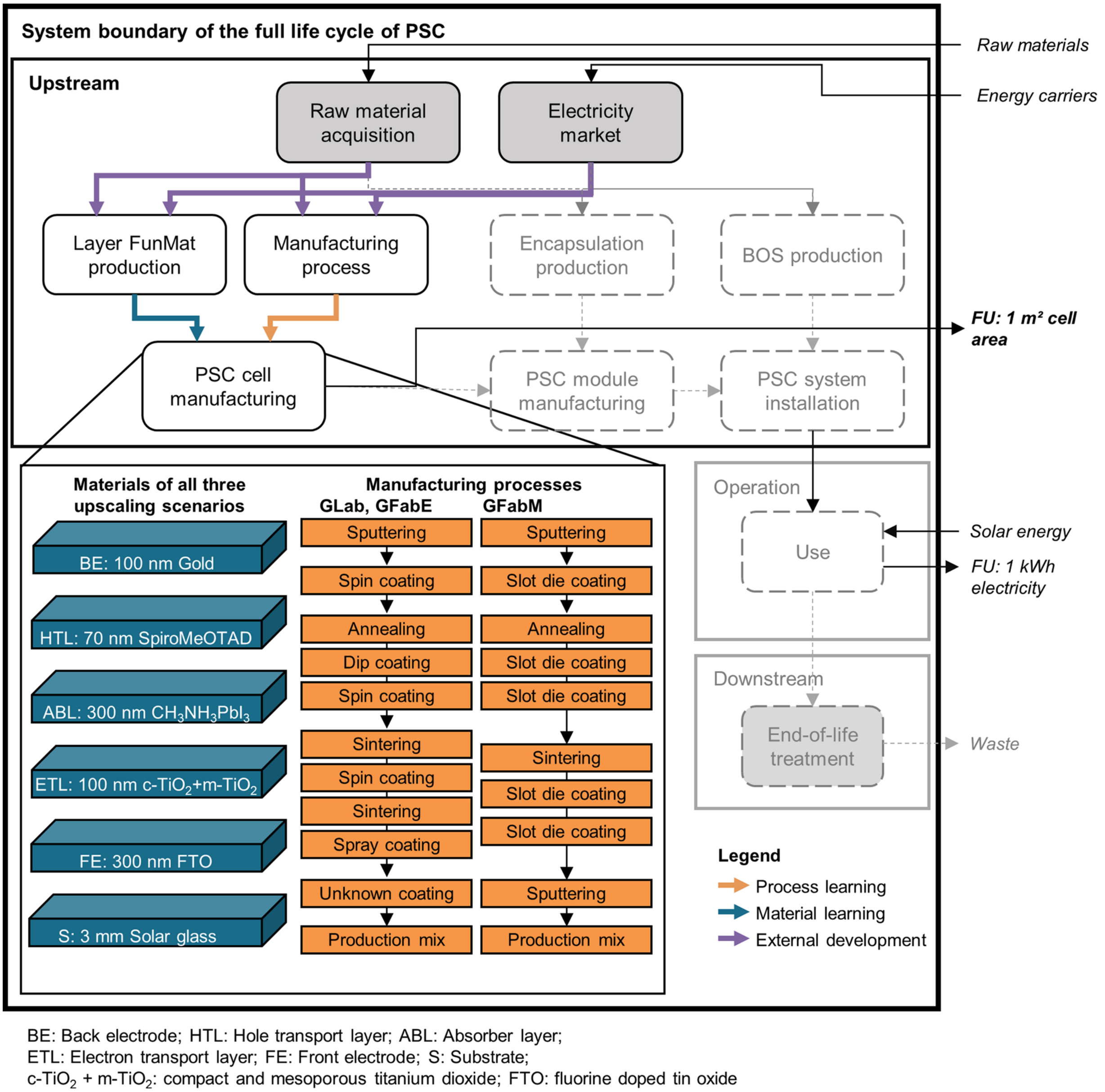


FIGURE 4 Product system of the selected perovskite solar cell samples at the status quo (extended from Weyand et al., 2019), differentiated into (1) foreground (white filled boxes) and background processes (grey filled boxes), (2) considered (black border) and unconsidered (grey dashed border) upstream, 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

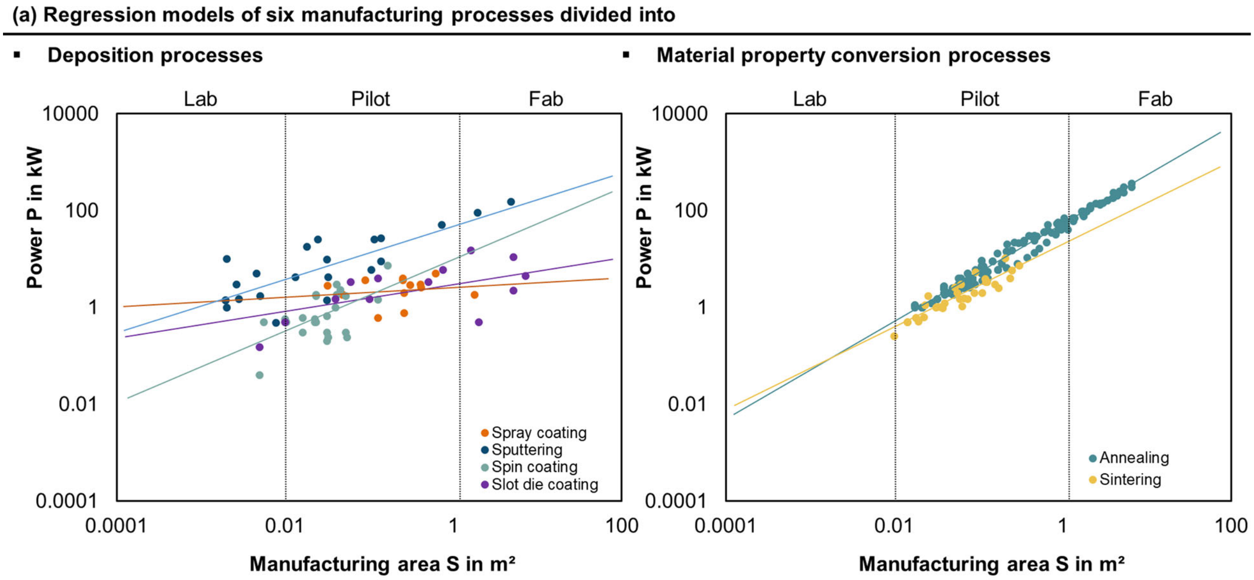
I. Over 250 empirical data sets to derive regression models of the six manufacturing processes (Table 1) for applying both the empirical (Model 1, Equation 1) and individual scaling (Model 2, Equation 2);
II. LCI data of the status quo for the individual scaling (Model 2, Equation 2).

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)



(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; R^2: 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

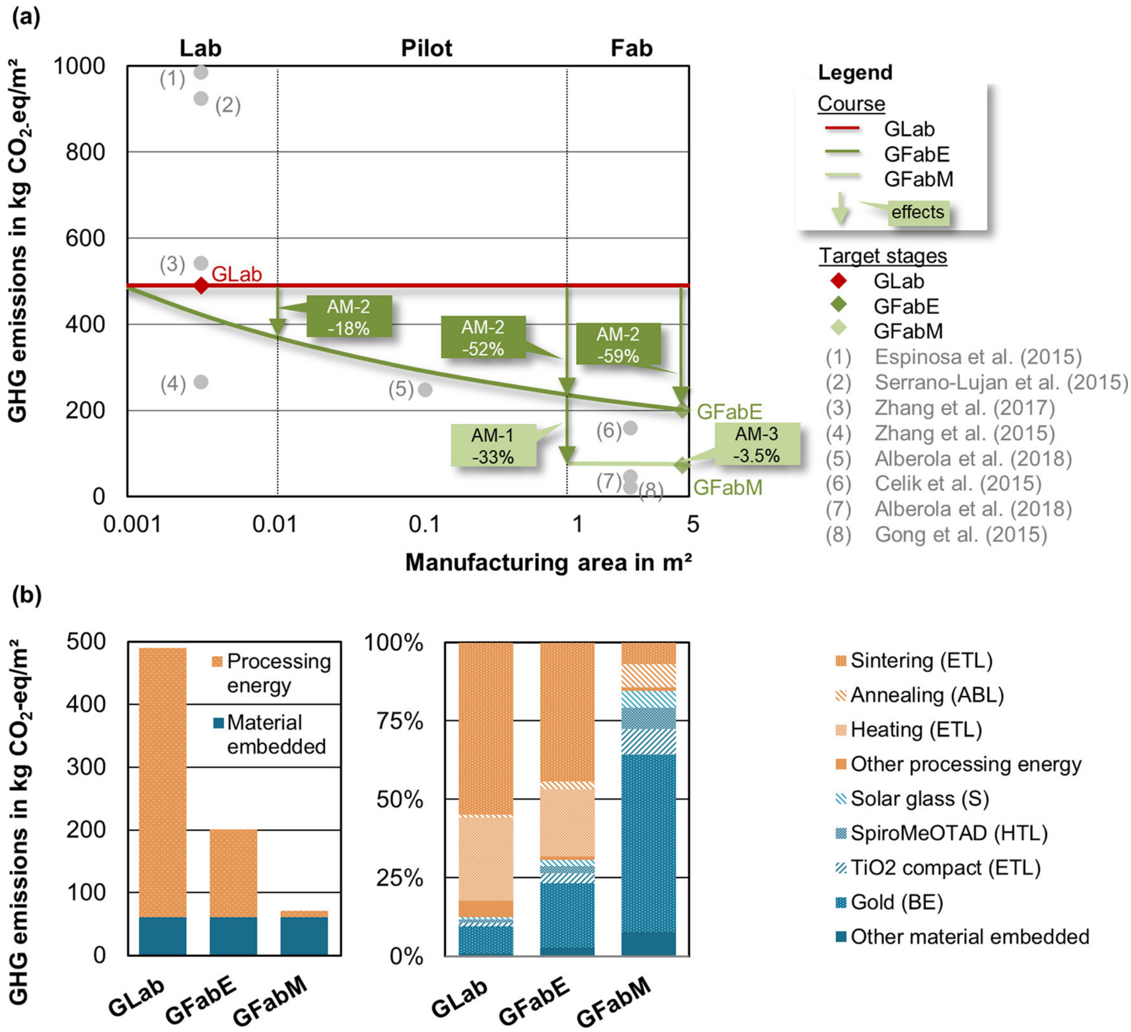


FIGURE 6 Projection of the upstream greenhouse gas emissions of the selected perovskite solar cell samples from lab to fab (a) course of the greenhouse gas (GHG) emissions per manufactured m^2 of the status quo and the two upscaled scenarios, compared with harmonized literature results averaged per study 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.

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