

Goal and Scope Report

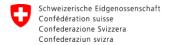
Deliverable 5.1





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Executive Summary

This deliverable, which is drafted in the framework of Work Package (WP) 5: Life Cycle Assessment (LCA), under Task 5.1: Goal & Scope, is developed for the purpose of design the research methods and alignment the approaches and system boundaries for LCA, economic and circularity assessment as important activities in the SOLARUP project. SOLARUP aims to analyse environmental impacts of thin film PV cells, comparing the Zinc Phosphide (Zn₃P₂) technology under development within SOLARUP with start-of-the art technologies Copper Indium Gallium Selenide (CIGS) and Cadmium Telluride (CdTe). The environmental analyses focuses greenhouse gas (GHG) emissions, use of resources (including energy, minerals, water and land), and the impacts on human health and ecosystems, as well as economic performance focussing on major cost drivers in production, use and recycling (e.g. material costs, production process, efficiency, lifetime and (by) product value. Additional (thermodynamic based) indicators to assess circularity will be explored and applied were relevant to help the development of circular end of life pathways (re-use, recycling). As the core technology under investigation is still embryonic and compared to mature Photovoltaic (PV) prospective elements will be included in the LCAs to account for the difference in technology readiness level and the moment of the assessment and the application of the technology.

The deliverable define the research approach to be used in the assessments during the project. It also contains a short description of the SOLARUP technology, the reference technology and some information on life cycle assessment in general.

The report is divided into the following sections:

Chapter 1 - Introduction: This chapter presents the objective and outline of this deliverable. Related tasks and work packages are also described.

Chapter 2 – Life cycle assessment: This chapter explains LCA in more detail including the different steps required. LCA is a well-established methodology for quantitatively assessing environmental impacts of a product or service.

Chapter 3 - Technology description: This chapter presents the novel Zn₃P₂, based solar cells to be developed in the SOLARUP project as well as the current state-of-the art thin film PV cells (CIGS and CdTe), which will serve as reference technologies.

Chapter 4 – Goal and scope definition: This chapter presents the approach to perform quantitative assessment of environmental and economic performance of the proposed future SOLARUP technology compared with reference technologies. The goal definition includes the intended application, method and impact category limitation, the rational for this study, intended audience and comparative assertion. The scope definition will provide insight into the object and functional unit, the system boundary, Life Cycle Inventory modelling, impacts and review.

Chapter 5 – Research approach and project planning: This chapter provides an outlook how all the activities under WP5 are linked and the planning until the end of the project is highly iterative and interactive with other WPs (1-4).



List abbreviations

CdTe Cadmium Telluride

CExD Cumulative Exergy Demand

CIGS Copper Indium Gallium Selenide

EoL End of Life

GaAs Gallium Arsenide

IoT Internet of Things

LCA Life Cycle Assessment

MCI Material Circularity Indicator

Mo Molybdenum

PV Photovoltaic

SOLARUP Name of this European project

TEA Technoeconomic Assessment

TCO Transparent Conductive Oxide

Zn₃P₂ Zinc Phosphide

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Advanced Strategies for Development of Sustainable Semiconductors for Scalable Solar Cell Applications

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1. Introduction

1.1. Description of the document and pursue

SOLARUP aims to demonstrate an ultra-thin nanostructure based on zinc phosphide (Zn₃P₂) solar cells with unprecedented conversion efficiencies. Zn₃P₂ is an earth-abundant, direct bandgap semiconductor with the potential to bridge the gap between efficiency, scalability and recyclability, providing a breakthrough technological solution that can revolutionise modern PV. This technology will be delivered together with a full life cycle strategy to ensure sustainability and recyclability at end of life (EOL). SOLARUP up is a European Horizon 2020 project financed under EIC pathfinder and runs over 4 years from October 2022 to September 2026. The consortium consists of 6 partners in 5 European countries amended by in-kind contributions from additional partners. An overview of the consortium partners and their roles is given in Appendix 1. This project is structured in 7 work packages that cover the whole value chain and is designed to and depends on a high level of interaction between the work packages and partners. The main strength is in bringing together key expertise that makes the project advancement towards the goal in a focused and directed manner. In this project, the expertise from four different disciplines: materials science (synthesis and characterization of materials), electrical engineering (solar panel design, fabrication and characterization), physics (theoretical simulations and basic semiconductor physics) and environmental engineering (life cycle assessment) will come together.

The main goal of work package (WP5) of the SOLARUP project is to quantitatively assess the environmental and economic performance of the proposed future SOLARUP technology compared with state-of-the-art thin film PV Copper Indium Gallium Selenide (CIGS) and Cadmium Telluride (CdTe). This WP goal aligns with objective 5 of the research proposal (see text box 1). This will include LCA from cradle to grave to guide the research and technological developments conducted during this project and design a system with optimized circularity.

Objective 5 will be achieved by analysing the impact of mining raw materials used in the device, following by understanding the materials synthesis and device fabrication processes. Understanding the efficiency prospects in solar cells we allow to judge the energy payback of the solar panel devices compared to commercial thin-film technologies, such as CIGS and CdTe. Lifetime of the devices will be quantified, and analysis on the options to ensure either a second life to the solar cells or for their optimal recycling will be performed. Evaluation of the use of these materials for other applications on a separate pathway, including budget electronics or economic optoelectronic

devices will be investigated. This will complete the full chain of the life cycle. All data and procedures developed here will be made widely available so that non - specialist can access and understand the methodology and thus participate in the LCA of other similar technologies. The feedback from the LCA analysis will be regularly communicated to other participants in the project, in order to ensure timely adjustment in material and process selection which will provide the lowest environmental impact and ensure circular economy approach.

Text box 1. Objective 5 from the SOLARUP proposal [1]



This report is the first deliverable (D5.1) of WP5 and describes the goal and scope for the life cycle assessment tasks. The deliverable outlines the sustainability assessment, the scope, benchmarks for the Zn_3P_2 panel and value chains, as well as the methodological choices to perform the assessments. Before detailing and goal and scope of the work in this work package, this report will give a short overview of the interrelation of this deliverable with other tasks and WPs, and the technologies and assessment methods included in the project. It concludes with an outline of the work intended.

1.2 WPs and Tasks related to the deliverable

For an innovative technology like (Zn₃P₂) solar cells to be scalable and contribute to climate mitigation, it must be competitive in terms of costs as well as environmental impacts. To achieve these goals, assessment of the performance of the technology in terms of both must be included from early design where results of (screening) assessments can still be used to improve technological design. Next to that, a life cycle and material resource efficiency perspective is needed to prevent unsustainable trade-offs and be in line with a circular economy. Therefore, it is important to consider end of life scenarios and waste prevention in the design stage. Due to many uncertainties related to future developments, simple indicators are needed to guide this circular design. Therefore, the research in WP5 makes use of a combination of methods to address environmental, cost and circularity performance. These methods are environmental life cycle assessment (LCA) on a screening, comprehensive and prospective level, economic assessment, exploration of different circularity indicators, and literature research into end of life pathways. WP 5 is organized in 5 tasks (see table 1 in Appendix 2). While TNO will lead WP5, two-way feedback with other WPs (1-4) will be crucial for WP5's execution. To facilitate this two-way feedback and to allow the partners to include insights on environmental effects in further technology design, WP5 will start with a screening or quick scan LCA and a workshop to introduce the consortium partners to the principles of LCA. The screening assessment will be performed using estimates provided by the partners, literature and publicly available data. The screening will provide the first impact scan and show environmental and cost hotspots. Over the project duration the screening LCA will be updated to include feedback and updates by the consortium partners (WP 1-4). This process cumulates in a detailed and comprehensive LCA to be presented at the end of the project.

For the circularity assessment, the aim is to assess established indicators such as the Material Circularity Indicator (MCI) and thermodynamics based indicators such as Cumulative Exergy Demand (CExD). Since circular systems come at the cost of energy consumption and sometimes other materials, it is important to use an indicator that considers both consistently which is not the case of MCI. Most circularity indicators commonly used are based on mass balances only, hence, to overcome this limitation, CExD and other thermodynamics concepts will be considered for indicating circularity in this study.

Economic feasibility is also fundamental to enable the commercialization and upscaling of the solar panel production, therefore TNO will collect cost data with project partners regarding the production of the solar panel, material costs, efficiency, lifetime and (by)product value and to estimate the economic and circularity performance of the SOLARUP technology. Thus, the successful execution of WP5 is to a large extent dependent on the inputs coming from the partners.



2 Life cycle assessment

LCA is a well-established methodology for quantitatively assessing environmental impacts of a product or service. It is generally performed in four interrelated steps (see Figure 1): 1. Goal and scope definition, 1. Inventory analysis where the data on emissions and resources uses over the life cycle are gathered, 3. Impact analysis where these data are related to environmental problem categories or damages to areas of protection and 4. Interpretation where results are interpretated with respect to the goal and uncertainties. A brief description of the topics and steps for each part is given below.

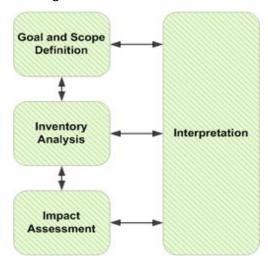


Figure 1 The four phases of an LCA study and the iterative process represented by arrows pointing back and forth, indicating the iterative nature of LCA studies [2]

The goal and scope definition serve to clarify the purpose and audience of the study and identify what is to be investigated and how. An overview of the aspects to be covered is given in Table 1 and Table 2. The inventory modelling is often the most time and resource consuming part of an LCA as all the data gathering (and updating) takes place in this stage. An overview of the steps is given in Table 3 based on the International Reference Life Cycle Data (ILCD) handbook [3] and [4].

Table 1: Goal definition: description of the required items (compiled by [5])

| Intended applications of the results | This step should clearly and unambiguously define the intended application of the study (e.g., comparing social/environmental impacts of several products or identifying parts in the life cycle where impacts are most significant = "hot spot identification") |
|---|---|
| Limitations due to methodological choices | Since methodological choices (e.g., impact categories, functional unit, system boundaries) can affect the LCA outcomes, it is necessary to state how that limits the interpretation of the results. |
| Decision context and reasons for carrying out the study | First, the rationale behind a study should be comprehended. This rationality should be directly related to the intended application of the study. It needs to be defined what the impact will be on the outcomes of the LCA. Generally, three different types of decision contexts can be recognized: |



| Comparative studies to be disclosed to the public Commissioner of the study and other influ- | This step should clearly define whether the LCA is characterized by a comparative nature and whether the results will be disclosed to the public. If this is the situation, the ISO standards specify extra requirements to deal with these potential consequences. Since involved parties during the research might influence the study, it needs to be stated which parties are involved and which may |
|---|---|
| Target audience | Since the target audience may affect the level of detail that can be provided in the documentation, it is important to define this group. |
| | (3) Situation C – in which the study is entirely descriptive and is not intended to support any decision. |
| | (2) Situation B – in which the study intends to support a decision, leading to structural modifications; and |
| | (1) Situation A – in which the LCA results tend to support a decision but won't result in structural modifications; |

¹As this study is part of a larger project, this is not addressed separately in the next chapter.

Table 2: Scope definition: description of required items (compiled by [5])

| Deliverables ¹ | In which the type of deliverable should be specified and should directly represent the intended applications. | |
|---|--|--|
| Object of the assessment | In which the object and its function should be defined, as well as the functional unit. | |
| LCI modeling framework and handling of multi-functional processes | | |
| System boundaries and completeness requirements | Specifying the system boundaries determines the unit processes which are included from which the social and environmental impacts are determined. Furthermore, the extent to which the impacts are captured in this study should be discussed. | |
| Representativeness of LCI data ² | Although LCAs intend to represent reality, not all physical phenomena of the considered system can be included. Therefore this item seeks to conclude which LCI data can reflect reality. | |
| Preparation of the basis for the impact assessment | Although LCAs intend to represent reality, not all physical phenomena of the considered system can be included. Therefore this item seeks to conclude which LCI data can reflect reality. | |
| Special requirement for system comparisons ³ | A requirements is proposed by the ILCD to prevent misleading LCA interpretations when comparing LCA studies. | |



| Needs for critical review ³ | A critical review of the LCA can contribute to ensuring the quality and credibility of the study. Therefore, in the scope definition it should be decided whether such a critical review will be incorporated. |
|--|---|
| Planning the reporting of results | Typically, three reporting levels can be recognized: (1) internal use; (2) external use by the third party; and (3) comparative studies to be disclosed to the public. The choice for selecting a specific reporting level should be clarified. |

¹Deliverables are described in the project plan and chapter 5, therefore they are not repeated in the next chapter; 2 merged with the system boundaries in the next chapter; 3 these aspects are also merged in the next chapter

Table 3: Steps in life cycle inventory analysis based on based on ILCD Handbook [3] and [4].

| Identifying processes | Gathering of all processes and interaction between them related to the product's value chain, e.g. by means of a flow chart |
|---|--|
| Planning data collec- tion | Identify data suitable for each process, e.g. primary (measured) data, secondary data from grey or peer-reviewed literature, data from databases |
| Data collection | Collect all resource demands and emissions over the products life cycle, either directly by compiling all material and energy inputs and relating them to databases, quantify the relation of all processes to the functional unit |
| Quality checking | Evaluate completeness and accuracy, e.g. by defining technological, temporal and spatial representativeness and data sources |
| Constructing LCI model | Implementing processes and connecting flows in a modelling software |
| Preparing uncertainty management and sensitivity analysis | By reporting assumptions and uncertainties, scenarios relevant for sensitivity analysis can be identified |
| Reporting | All data and approaches transparently |

The next calculation step is impact assessment where all the resource demand and emissions, jointly termed interventions, are translated into environmental areas of concern (so-called impact categories). The first two steps to achieve this are classification and characterisation (allocating the interventions to an impact category and translating it to a common measure of their relative contribution, i.e. 'equivalents' to that midpoint impact category). This way all interventions contributing to the same impact category can be summed. These steps are included in available life cycle impact assessment methods, such as ReCiPe, ILCD, CML and LC-Impact. Life cycle assessment indicators can be distinguished between midpoint and endpoint indicators depending on their place at the environmental cause effect chain. Midpoint indicators are relatively close to the interventions, resulting in many indicators with relatively low uncertainty. Endpoint indicators on the other hand model damage pathways to so-called areas of protection, commonly human health, biodiversity and resource availability (see Figure 2). These are much more intuitive to interpret, but also come at the cost of



higher uncertainties. Some methods (e.g. CML) restrict themselves to midpoints, others like ReCiPe provide both options.

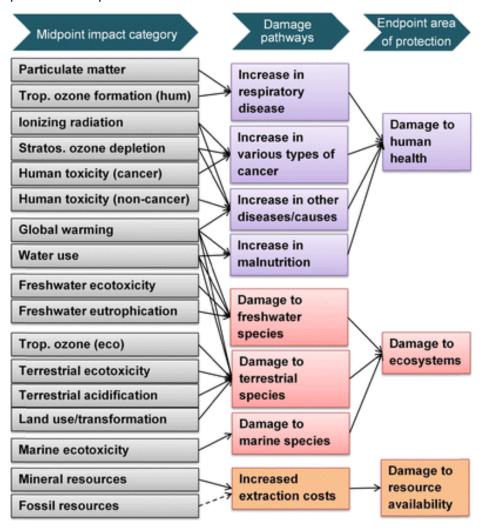


Figure 2: ReCiPe indicators [6]

Standards and guidelines have been developed on how to conduct an LCA. The most prominent ones are the ISO 14040 and 14044 standards. Next to that the International Reference Life Cycle Data (ILCD) handbook provides guidance on conduction LCA [3]. Guidelines specific to the PV sector aimed to enhance comparability of different LCA studies by standardized methodological choices like system boundaries, allocation riles and impact categories. Such guidance is provided by PV-LCA specific guidelines issued by Task 12 of the International Energy Agency (IEA) elaborated within the PV Power systems (PVPS) program, JRC technical reports on the modelling of PV cells from the Product Environmental Footprint project (TS PEF Pilot PV 2018) [7], [8],[9]. All of these standards and guidelines will be taken into account as much as possible during this research. To ensure consistent and relevant cost results suitable to combine with the LCA results, LCA guidelines will be used for the cost assessment where relevant and possible.

"Conventional" LCA impact indicators are not equipped very well for identifying circularity – not only from a quantitative aspect (volume of closing the loop) but also a qualitative aspect (value of closing the loop). Therefore the value added by different possibilities to bridge the shortcomings of

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commonly used indicators will be explored. Possible indicators to be explored and compared are entropy, Circularity indicator from Ellen MacArthur Foundation and Cumulative Exergy Demand. Many of these indicators have been used and partly integrated in LCA studies. However, the mass balance performed to calculate the indicator does not cover irreversibilities that are intrinsic to the processing and beneficiation of raw materials, production of products, recycling etc. To bridge that gap thermodynamics based indicators will be studied to understand their limitations and opportunities as circularity indicators. Inclusion of these indicators will be exploratory and indicate whether these types of indicators could be effectively used for this purpose and how to interpret such results.





3. Technology description

3.1. SOLARUP technology and development

As described in great detail in Annex I, part B of the Grant Agreement Project 101046297 – SOLARUP [1], the SOLARUP PV cells' main component is Zn_3P_2 , which is abundantly available on earth crust. Therefore, the solar energy conversion technology of SOLARUP can help reducing the dependence on critical raw materials. The main innovation lies in nanoengineering Zn_3P_2 as an absorber and combining it with novel device architecture to reach a panel efficiency enhancement of up to 15%.

At the same time it may also overcome efficiency thresholds to unlock the future of flexible PV solar cells for mass deployment in smart buildings, soft robotics, wearable electronics, and other consumer products. This will be supported by a new system archetype and full life cycle material strategy. This will be done by combining the strengths of high-throughput experimentation with the design of a novel Zn_3P_2 based solar panel architecture while assessing and improving its environmental, resource, health and circularity performance throughout development. The main innovation pillars of this project are shown in Figure 3.

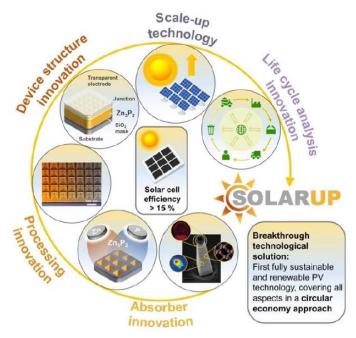


Figure 3: Innovation pillars of SOLARUP [1]

SOLARUP is expected to go beyond state-of-the-art in photovoltaics in various aspects as seen Figure 3. The following measurable indicators can be the contribution of the science towards technology breakthrough expected out of this project:

- All materials classified as critical raw materials (CRM) are eliminated from the cost-effective thin film PV technologies through development and use of earth abundant, low-cost semiconductors.



- A synthesis technology is developed to bypass the material/substrate mismatch and enable growth of high crystal-quality Zn₃P₂ thin-films, advancing state-of-the-art production of solar cells by allowing engineering of material properties at the atomic scale.
- A prototype Zn₃P₂-based solar panel device is demonstrated and collaborations are initiated for further optimization of the technology and transfer to industry.

3.2. Reference technology

Thin film solar panel market have a long history with continuous technological developments and its global market has increased significantly in the recent years and expected to increase due to increasing demand of electricity, growing use of renewable energy, rising solar PV installed capacity, declining solar prices, integration of thin-film PV cells in electric vehicles, associated technological advancements, etc. The current value chains for thin film PV cells are used to compare the novel SO-LARUP technology to. Copper Indium Gallium Selenide (CIGS) and Cadmium Telluride (CdTe) will be used as benchmark technologies. Figure 4 shows a simplified exemplary diagram of the layers of both cell types based on [10]. The main features of both technologies derived with a preliminary literature scan of previous LCAs for CdTe and based in a thorough literature review from a masted thesis for LCA of CIGS are summarized in Table 4.

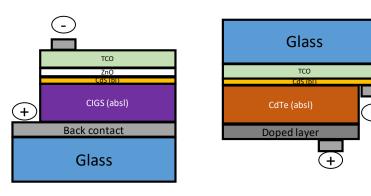


Figure 4: Simplified, exemplary diagram of PV cells with CIGS (left) and CdTe (right) semiconductor layers, TCO: transparent conductive layer, ZnO: zinc oxide, absl: absorber layer, CdS (yellow): Cadmium Sulfide, bl: buffer layer, small grey boxes: front (and back for CdTe) contact [10].

Table 4: Showing main characteristic of CdTe and CIGS technologies.

| | CIGS | CdTe |
|---------------------|------------------------------------|------------------|
| Efficiency | 10-22% | 8-19% |
| Lifetime | 20-30 years | 15-30 years |
| Carbon footprint | 7-110 gCO₂/kWh 1-86 kg CO₂eq/m² | 6- 66 gCO₂ / kWh |
| Energy payback time | 1-4 years | 0.57 – 1.3 years |
| References | De Witto, 2022 | [11] and [12] |

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Cadmium is abundant and is in fact produced as a by-product of industrial metals (zinc for example) but tellurium is extremely rare element (even though it is a by-product of copper mining). The draw-back is correlated to the toxicity of cadmium: it is known as the most toxic materials known to man [13].





Goal and scope definition

The goal and scope definition follows LCA guidelines, but the cost assessment will be aligned to the same rules as much as possible and where appropriate. If other assessments require other decisions this is mentioned separately.

4.1. Goal of the study

The objective of the study is to gain insights in the (prospective) environmental, economic and circularity performance of (Zn_3P_2) PV cells and benchmark these against current thin film PV technologies. By providing these insights to technology developers in the SOLARUP consortium, these assessment contribute to developing future technologies that are more sustainable than current commercial ones.

4.1.1. Intended application

The results of the LCA analysis will be shared with other participants in the project to allow the timely adjustment in material and process selection to help achieving the lowest environmental impacts and cost and support design for circularity. The study will identify environmental and economic hotspots at a screening level and compare processing, material and end of life alternatives throughout the project. Life cycle data will be updated throughout the project with increasing knowledge. Development of end of life circular options will be supported by literature research. To account for the emerging nature of the Zn_3P_2 technology, prospective elements such as scaling, learning and different background scenarios will also be included iteratively within the project. Results will be benchmarked against existing thin film technologies.

4.1.2. Method and impact category limitations

The LCA will include all core flows of the system with particular attention to the ones that distinguish in comparison between systems. However, several steps of the study such as the screening LCA and the investigation of thermodynamic indicators is exploratory in nature and intended for application within the project, not so much for wider comparisons. Likewise, cost estimations are influenced by current market prices and cannot be directly extrapolated to the future. For benchmarking, comparisons will be made with CdTe and CIGS solar applications, system boundaries of these studies will be aligned. Comparison to other studies should, however, be done with care. To extend the LCA application to include several aspects of circular economy additional indicators and pathways will be explored.

4.1.3. Reasons for carrying out the study

Zn₃P₂ is a potential new PV technology that includes no critical raw materials in its composition thereby making it suitable for large-scale deployment without risk of running out of material supply. However, renewable electricity generation technologies should also fit into a circular economy and be cost-competitive without generating pressures on other environmental and health areas of



concern. Guaranteeing these benefits requires systematic assessment from the outset of the development.

By providing these assessments WP5 contributes within SOLARUP:

- SOLARUP proposes simple, scalable and low-cost PV technology, which reduces large-scale deployment costs.
- For PV, important factors include low efficiencies and high embodied CO₂ footprints from component manufacture. A LCA study will build-in consideration of a broad spectrum of environmental impacts throughout the project and ensure a positive environmental impact.
- WP5 will contribute towards PV systems that are more efficient, have a longer lifetime, and are
 more reliable by assessing GHG emissions, and other sustainability impacts, to improve the
 overall understanding of the carbon impact.

4.1.4. Intended audience

The approach and results of this study are intended to be used within SOLARUP by all partners involved in the technology development. Next to that it is intended to disseminate methods and results in conferences and peer reviewed publications to professionals and scientist.

4.1.5. Comparative assertion

 Zn_3P_2 cells will be compared with CIGS and CdTe as benchmark. The results will be disseminated as stipulated in the Grant Agreement. The ISO guidelines for comparative assertion available to the public will be followed [2].

4.2 Scope of the study

Some general stages over a products life cycle can be described: Raw material extraction, pre-manufacturing, manufacturing, use phase and end-of-life are included in the system boundaries of the study as presented in Figure 5.



Figure 5: Life cycle stages.

More specifically for PV, The following life cycle stages and processes within the PV life cycle are recommended to be included in the system boundaries of LCA studies by Task 12 of the International Energy Agency (IEA) PV Power systems (PVPS) program [7]. In this study we expect to deviate from the guidelines to solely include the stages that may differ among the three different PV cells in the study: CIGS, CdTe and Zn_3P_2 .



Production stage (Modules A1 to A3):

- Raw material and energy supply;
- Manufacture of the cells;
- Manufacture of the panel; (to be decided with consortium partners)
- Manufacture of the mounting system;
- Manufacture of the cabling;
- Manufacture of the inverters;
- Manufacture of the further components needed to produce electricity and supply it to the grid (e.g. transformers for utility-scale PV).

Construction stage (Modules A4 and A5):

- Transport to the PV power plant site;
- Construction and installation, including foundation, supporting structures and fencing.

Use stage (Module B)

- Auxiliary electricity demand;
- Cleaning of panels;
- Maintenance; (to be decided with consortium partners)
- Repair and replacements, if any.

End of life stage (Module C)

- Deconstruction, dismantling;
- Transport;
- Waste processing;
- Recycling and reuse;
- Disposal.

An LCA study only including the raw material, production and construction stages is generally referred to as a cradle-to-gate analysis. Whereas a cradle-to-grave LCA includes all stages. LCAs studies for PV often focus on the production as the most impactful phase, several have also included the use phase, but excluded the end of life, often due to a lack of data, other focussed in end of life specifically to explore future options [14], [15]. In this study the system boundary extends during the course of the project. The screening LCA and cost assessment will focus on a cradle-to-gate, but will be extended to cradle-to-grave once the circularity assessment and exploration of end of life pathways have been performed.

4.21. Object and functional unit

The objective of the study is a Zn_3P_2 solar cell capable of generating electricity compared to other thin film technologies. The functional unit is the quantified performance of a product system for use as a reference unit in LCA and allows comparison of different products or technologies under study for the same function. The functional unit is defined as 1kWp solar panel for the screening level studies and will be extended to include (sensitivity scenario's for) generation of 1 kWh. Relations between Wp and m^2 of cells will be reported structurally to allow comparison to other studies and data sources.



4.22 Systemboundary

An overview of the Zn_3P_2 life cycle over the stages A, B, C/D as used above is system is given in Figure 5. For all parts in the system energy and material input as well as emissions and wastes have to be gathered. No cut-off criteria have been defined at this stage of the study, except for the ones already defined for common life cycle inventory databases. Cut-off between different life cycle stages will be addressed in the next section. For the screening LCA, a coverage of at least 80% of the impacts is aimed for, ambitions are higher for the full LCA. The following Figure 6, Figure 7, Figure 8 and Figure 9 contain a more detailed representation of the system boundaries applied to this study.

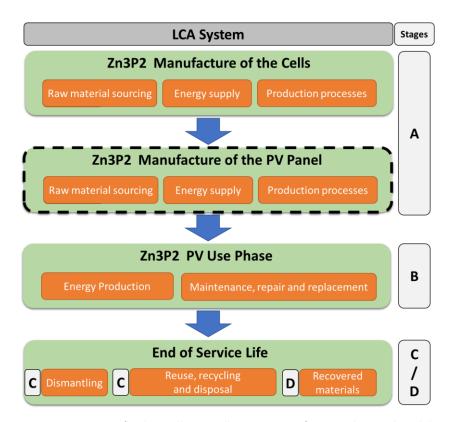


Figure 6: LCA system for the cradle-to-cradle assessment of Zn3P2 solar panels and the corresponding life cycle stages according to task 12 (IEA)[16].



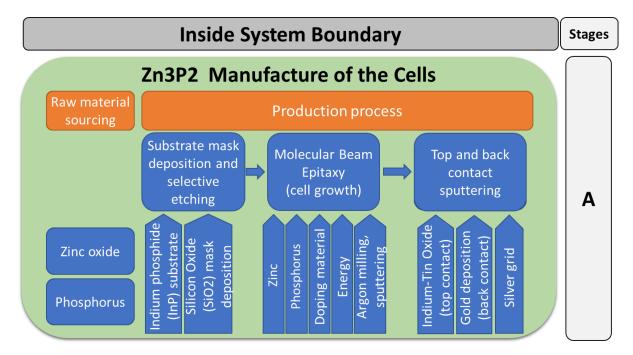


Figure 7: System boundaries, materials and production processes for the manufacture of the PV cells.

The manufacturing of the solar cells is referred to as stage A in task 12 of IEA work group.[16]

Figure 7 shows the system boundaries and an overview of the main materials and processes during the manufacture of the solar cells. It includes all the materials needed to produce the cells themselves and the materials needed for the processing steps, such as the Indium phosphide substrate. Data input from consortium partners is needed to quantify the electricity, other energy inputs needed, material masses and which other processing steps are needed to prepare the cell for PV module manufacturing.

Information from consortium partners will be the input for the model regarding what Zinc and Phosphorus precursors are necessary for growing the cells, how the Indium phosphide plate is produced, the origin of the silicon oxide for the mask, the materials and steps needed for the etching process. Apart from that, information on alternative materials and processes should also be provided to allow the modelling of different scenarios and finding the most sustainable solution among those scenarios.

Materials that are recovered after the production process and the process to recover them are also part of the study and included in the boundaries.



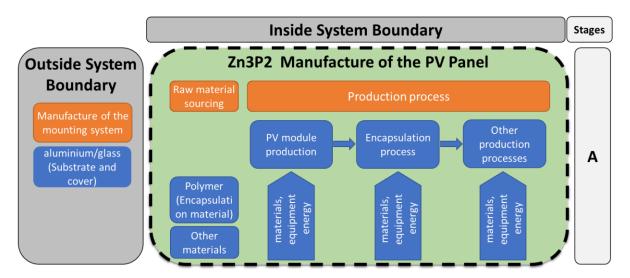


Figure 8: System boundaries, materials and production processes for the manufacture of the PV panel.

The manufacturing of the PV cells is referred to as stage A in task 12 of IEA work group [16].

Figure 8 shows the system boundaries and an overview of the main materials and processes during the manufacture of the solar panels. This study focuses on the Zn_3P_2 cell production, however it may be extended to include module and panel production in case the consortium is expanded to include in situ testing of the solar panels produced with Zn_3P_2 cells. Hence the dashed line surrounding the figure, that will also cover panel production in that case.

Manufacture of the mounting system, frames and supporting structures as well as glass covering the panels is excluded of the system boundaries as these will remain the same for any of the PV technologies included in the study, namely Zn_3P_2 as well as CdTe and CIGS solar panels.

Data for modelling the panel production shall be provided by the consortium partners for the materials needed and process used for encapsulation and other materials needed for producing the module such as cell interconnection material. Moreover, material amounts in mass and energy requirements per energy carrier for every production step also need to be provided.

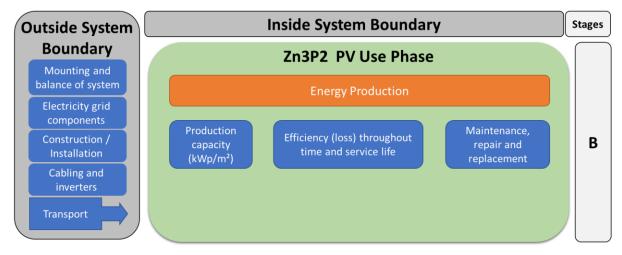


Figure 9: System boundaries, production capacity and other aspects of the technology and other processes that belong to the use phase of the solar panel.



The use phase of the PV cells is referred to as stage B in task 12 of IEA work group[16][17].

Figure 9 shows the system boundaries and an overview of the main aspects modelled in the use phase of the solar cells and which components and processes are excluded. Construction, installation, mounting, balance of system, cabling and inverters are not likely to change with the eventual introduction of the Zn_3P_2 technology in the PV market, therefore they are excluded of the system boundaries of this study. The transport from the production plant to the place where the panel gets installed is also excluded due to the uncertainty related to where production would take place and the places that would implement this type of solar panel as soon as it reaches the market.

The use phase includes the energy produced by the solar cells, the efficiency loss that happens during their service life, repair and/or replacements necessary. These aspects are also included in the comparative assessment with CdTe and CIGS.

Data on the estimated efficiency, efficiency loss, expected service life, maintenance, repair and replacements should be provided by the consortium partners. When that is not possible, literature will be used and assumptions based on the aspects and performance of similar PV technologies will be made.

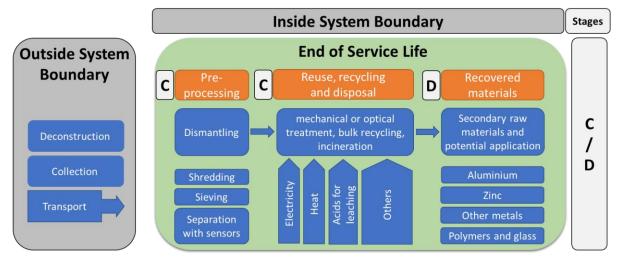


Figure 10: System boundaries for the end of service life assessment of the solar panels. As the exact process is not defined yet, the figure displays a mix of potential processing steps and necessary inputs.

The end of the service life of the PV panel is referred to as stage C and the recovery of materials including its benefit Is referred to as stage D in task 12 of IEA work group.

Figure 10 shows the main focus of the circularity study and the system boundaries for the end of the service life of the solar panel. Deconstruction and collection remain outside the system boundaries as they are common to all PV technologies in the study. The circularity study will research the pathways and technologies available to repair, reuse, recycle and recover solar cells and which of them are applicable to the SolarUp technology. Hence, it is not clear which circular strategies and processing steps throughout recycling will be applicable to this system. Therefore, the picture displays a mix of the potential processes the solar panel may undergo at the end of its service life. The pathways chosen to integrate the Zn_3P_2 PV technology system may cover and include re-use, closed-loop and open-loop recycling. The recycling strategies chosen should aim to recover majority of the



elements from Zn₃P₂ and apply it in products at the highest value, preferably in new PV production (closed loop recycling).

4.23. LCI modelling type and allocation

This study focusses on a micro-level decision support as defined by the ILCD [3] as they relate to a specific product and are not expected to induce structural changes, e.g. available production capacity outside the decisions scope. Therefore, attributional life cycle inventory modelling will be applied. In case of multifunctionality, we will strive to subdivide processes, use system expansion and as a last resort allocation based on energy content (with costs as a sensitivity scenario). For the end of life or secondary life cycle, roughly two modelling approaches can be distinguished (e.g. PV task 12) cut-off and other end of life modelling approaches like allocation at the point of substitution (APOS). In the cut-off, chains are modelled until the point of lowest value (usually before recycling) and all further steps are allocated to the second life cycle. In the end of life approach (APOS) further treatment and processing are also included up to the point where another product can be substituted. The screening LCA will make use of the cut-off as it focusses on the production stage. However, for the full LCA end of life modelling will also be explored. The LCI models will also be extended to include future supply chains by making use of scenarios available within the prospective LCA community [18].

4.24. Included Impacts

The assessments conducted in WP 5 will include the following impacts and performance measures:

- Environmental impacts: greenhouse gas (GHG) emissions, use of resources (incl. energy, minerals, water and land), and the impacts on human health and ecosystems. These will be quantified using the widely used and state of the art impact assessment method ReCiPe [6].
- Economic feasibility of the Zn₃P₂ PV solar panel and the recycling process for the whole life cycle of the solar panel by assessing major cost drivers such as material costs, production process, efficiency, device lifetime and (by)product value.
- Circularity potential: Cumulative Exergy Demand and other indicators

4.2.5. Review

All results reported in SOLARUP deliverables will be reviewed internally by TNO and by consortium partners. In case, results get published to a broader audience, additional review will be added (scientific e.g. peer-review).



5. Research approach and project planning

The overall approach of WP5 (relation between deliverables and activities in-between) is shown in Figure 11. Two-way feedback and data exchange with the consortium partners is crucial for successfully conducting the research. Necessary interaction moments are therefore indicated in the figure.

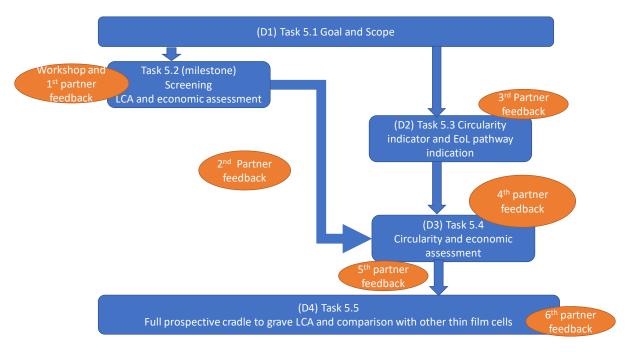


Figure 11: Research approach WP 5

A planning of all the tasks, deliverables, milestones as well as the workshop is illustrated in Figure 12. After the goal and scope definition (this deliverable) the next step will be to perform a screening LCA and cost assessment, largely based on literature and publicly available data, and to prepare a workshop to familiarize project partners with the basic principles of LCA. This workshop is planned to take place earlier in the project around month 9 (June 2023) instead of the original plan for the workshop taking place in month 34 (July 2025). The purpose of the life cycle scan will be to point out the hotspots and hence making a list of data required for the detailed LCA. These will also be shared with the partners during the workshop so that the screening LCA and cost assessment can be improved based in project specific data, possibly making use of a parameterized tool that can be shared within the consortium (task 5.2 and WS 1).

Next, the thermodynamics based indicators that could be used to indicate the circularity of technologies under development will be reviewed, selected, shared with the consortium partners, and applied to the screening LCA and cost assessment, thereby giving insights into which materials should have spatial attention in design for circularity (task 5.3). A screening of possible recycling routes and technologies for Zn₃P₂ technology will connect task 5.3 with the next: circularity and economic assessment that will assess these pathways in relation to the life cycle to support development of a circular technology either via re-use, closed or open-loop recycling. The identified routes will be verified with WP1-4.



In parallel an LCA will be built for CIGS and CdTe cells based on literature [11] and in-house data [19] following the goal and scope definition in this report. Additionally, to account for the fact that environmental impacts of diverse technologies might be different in the future due to ongoing transitions in the economy (such as increased use of low carbon energy sources) scenarios will be selected to take these developments into account [18].

To allow for a fair comparison with the more mature benchmark technologies, possible process changes, size scaling of the product or production equipment and synergies when producing in an industrial plant as well as industrial learning will be taken into account for the emerging Zn₃P₂ [19]. This modelling will be aligned and regularly updated with developments within the consortium during the project, cumulating in a full prospective LCA towards the end of the project. In that LCA independent changes in the supply chain will also be taken into account in the same way as for the benchmarks. For the full LCA use stage and the afore developed end of life scenarios will be taken into account.

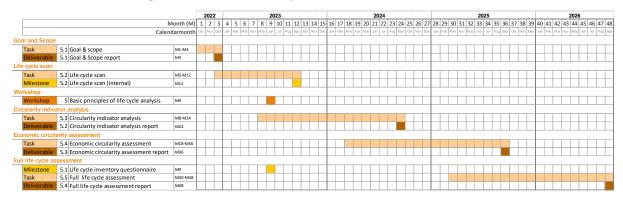


Figure 12: Project Plan for Workpackage 5

SOLARUP

Advanced Strategies for Development of Sustainable Semiconductors for Scalable Solar Cell Applications

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Appendix 1 - The SOLARUP Consortium



 ${\it Figure~13: SOLARUP~Consortium~partners~and~focus~areas~within~project~[1].}$



Table 5: SOLARUP consortium partners [20]

LIST OF PARTICIPANTS

| PARTICIPANTS Grant Preparation (Beneficiaries screen) — Enter the info. | | | | | |
|--|------|------------|---|---------|-----------|
| Number | Role | Short name | Legal name | Country | PIC |
| 1 | COO | ICN2 | FUNDACIO INSTITUT CATALA DE NANOCIENCIA I NANOTECNOLOGIA | ES | 999606923 |
| 2 | BEN | NWO-I | STICHTING NEDERLANDSE WETENSCHAPPELIJK ONDERZOEK INSTITUTEN | NL | 999624092 |
| 3 | BEN | FSU | FRIEDRICH-SCHILLER-UNIVERSITAT JENA | DE | 999868726 |
| 4 | BEN | TNO | NEDERLANDSE ORGANISATIE VOOR TOEGEPAST NATUURWETENSCHAPPELIJK ONDERZOEK TNO | NL | 999988909 |
| 5 | BEN | ULUND | LUNDS UNIVERSITET | SE | 999901318 |
| 6 | AP | EPFL | ECOLE POLYTECHNIQUE FEDERALE DE LAUSANNE | СН | 999973971 |

The project is divided into 8 WPs (shown in **Error! Reference source not found.**) which will be developed in following 48 months by all six consortium partners.

Table 6: List of WPs and lead beneficiary [20]

LIST OF WORK PACKAGES

| Work packag | es | | | | | | | |
|--|---|------------------|-------------------------------|----------------|--------------|--|--|--|
| Grant Preparation (Work Packages screen) — Enter the info. | | | | | | | | |
| Work Package No | Work Package name | Lead Beneficiary | Effort (Person- Months) | Start Month | End Month | Deliverable No(s) | | |
| WP1 | Lateral epitaxy of zinc phosphide | 6 - EPFL | 76.00 | 1 | 48 | D1.2, D1.3, D1.4, D1.1 | | |
| WP2 | Scaling of zinc phosphide growth | 5 - ULUND | 54.00 | 12 | 48 | D2.4, D2.3, D2.1, D2.2 | | |
| WP3 | Doping of zinc phosphide | 3 - FSU | 68.00 | 4 | 48 | D3.2, D3.5, D3.3, D3.4, D3.1 | | |
| WP4 | Device design | 2 - NWO-I | 76.00 | 4 | 48 | D4.2, D4.5, D4.3, D4.4, D4.1 | | |
| WP5 | Life cycle assessment | 4 - TNO | 25.00 | 1 | 48 | D5.1, D5.2, D5.4, D5.3 | | |
| WP6 | Communication, Dissemination and Exploitation | 1 - ICN2 | 24.00 | 1 | 48 | D6.4, D6.5, D6.2, D6.3, D6.1 | | |
| WP7 | Project Management and Coordination | 1 - ICN2 | 47.00 | 1 | 48 | D7.11, D7.10, D7.6, D7.3, D7.1, D7.7, D7.8, D7.2, D7.9, D7.4, D7.5 | | |
| WP8 | Ethics requirements | 1 - ICN2 | 0.00 | 1 | 48 | D8.1 | | |





Appendix 2 - Tasks and deliverables of WP 5

Table 7: Overview of task and deliverables of WP 5 as described in the SOLARUP proposal

| Task | Product | Description Work Plan | | | |
|--|---|---|--|--|--|
| 5.1 Goal & Scope | D5.1 Goal and scope report | set-up the goal and scope, system design, functional unit and impact assessment methods for the life cycle assessment. | | | |
| 5.2 Life cycle scan | Milestone WS5 Basic principles of life cycle assess- ment | LCA of SOLARUP technology compared with the current benchmark to identify the most important environmental impacts, economic costs and benefits in relation to processes and drivers in the complete life cycle. Major cost drivers will be covered, e.g. material costs, production process, efficiency, lifetime and (by)product value. Environmental impacts will include greenhouse gas (GHG) emissions, use of resources (including energy, minerals such as CRM and water and land), and the impacts on human health and on ecosystems. | | | |
| 5.3 Thermodynamics based circularity indicator | D5.2 Thermodynamics based circularity indicator report* | explore the value added of a new indicator, i.e. thermodynamics based indicator, as a fundamental unit for circularity, comparing with existing units (from e.g. Circularity indicator from Ellen MacArthur Foundation, Cumulative Exergy Demand, thermos-economic indicator by Helmholtz etc.) and applying it in SOLARUP. | | | |
| 5.4 Economic circularity assessment | D5.3 Economic circularity assessment | Analyze pathways for making SOLARUP technology circular, e.g. by re-use, closed-loop and open-loop recycling. Here, the entropy indicator should lead the way to circular and environmentally benign pathways, which are economically feasible. Different physical and chemical routes will be explored based on the literature. The proposed recycling strategy should aim to recover majority of the elements from Zn3P2 and apply it in products at the highest value, preferably in PV (closed loop recycling). Here, | | | |



| | | also technology scalability and learning will be of key importance, also for the comparison of embryonic innovations with current mature state-of-the-art technology. |
|--------------------------------|---------------------------------|--|
| 5.5 Full life cycle assessment | D5.5 Full life cycle assessment | integrate the insights of the previous tasks but above all the technological developments reached in the other WPs on the SOLARUP technology in a full LCA to demonstrate the environmental performance and economic prospects over the whole life cycle including a sensitivity analysis that addresses the major uncertainties and key factors for this young technological development. |

D = Deliverable, WS = workshop

^{*}The indicators for this deliverable have been updated in the project proposal, hence the deliverable title has been updated accordingly in this table.



Appendix 3 - System boundaries

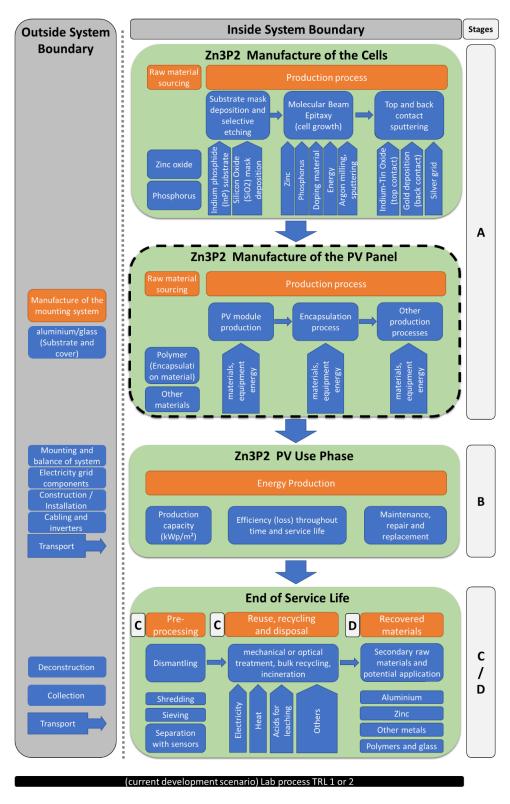


Figure 14: System boundaries