Life cycle analysis of perovskite solar cells for production in Europe

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TU Delft

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by

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Abstract

The photovoltaic (PV) technology plays a significant role in the global energy transition and perovskite solar cells (PSC) have been experiencing rapid development in the past few years. The life cycle analysis (LCA) method evaluates the possible environmental impacts during each life stage of one product, and applying this method to the production processes of perovskite solar cells can assess the environmental implications in each phase of the PSC life cycle, from the initial raw material extraction to manufacturing, operation, and end-of-life stages.

This thesis mainly focuses on the cradle-to-gate stages of LCA, more specifically in raw material extraction and manufacturing of one perovskite PV module. This work selects a perovskite solar module with a mesoporous TiO_2 scaffold as the studied module, then defines the goal and scope, including the definition of the research goal, functional unit and system boundaries of this LCA study. Followed by the selection of Ecoinvent V3.8 and Idemat 2023 databases, a new life cycle inventory (LCI) is created both in material and energy aspects. Based on the existing literature inventory, some changes and improvements are made to specialize the life cycle inventory data. Due to the limitation of existing databases, the missing materials and data are collected, self-calculated or replaced to complete the LCI. After calculating and integrating the LCI data by mass allocation, three impact categories are chosen to conduct the life cycle impact assessment (LCIA), which are separately climate change, human health and resource use (fossil). Next, the thesis compares the LCIA results in three different perovskite PV modules, one is the studied perovskite PV module with a silver cathode, one is the same studied module but with a gold cathode, and the other is the literature's perovskite PV module (with a gold cathode). This thesis compares the environmental impact results in material, energy consumption and total three perspectives, simultaneously analysing the different LCIA performances between the metal gold and silver. This thesis also compares the LCA results of the selected perovskite solar module with the other two c-Si modules. Finally this work exerts the contribution analysis on three life cycle impact categories, explains the LCIA results of three different perovskite solar modules and proposes further research advice.

The LCIA results illustrate that compared to the literature's module, the studied perovskite PV module with silver cathode has the lowest life cycle environmental impacts in all three impact categories. More specifically, 46% in climate change, 12% in human health and 34% in resource use (fossil) compared to the literature. Furthermore, the metal gold has the highest contribution in all three categories, FTO and energy contribute the second and third both in climate change and resource use (fossil), and silver takes the second occupation in human toxicity. Compared to c-Si modules, the LCA performance of this thesis's perovskite module shows lower environmental impacts in CO_2 emissions.

Acknowledgement

This thesis is the final work of my MSc Sustainable Energy Technology program at Delft University of Technology (TU Delft), it's the result of the project in the last nine months. This thesis has been done with the help of the Photovoltaic Material and Devices (PVMD) research group, and I want to thank everyone in the PVMD group for all the support and help I received.

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Furthermore, I am grateful to my parents far away in China. In spite of the long distance and six-hour time zones, they keep supporting me spiritually and economically. The initial decision to study abroad was not easy for you, I can still remember the arguments, tears-shedding moments we had. when it comes to the end of my master program, I sincerely thank you for loving me and supporting me as always.

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Nomenclature

Abbreviations

Abbreviation	Definition
AC	Alternating Current
AP	Acidification Potential
BL	Blocking Layer
CML	Centre of Environmental Science of Leiden University
$CaTiO_3$	Calcium Titanate
CVD	Chemical Vapor Deposition
CoO	Cobalt Oxide
C-Si	Crystalline Silicon
DC	Direct Current
DR	Degradation Rate
EP	Eutrophication Potential
ETL	Electron Transport Layer
FTO	Fluorine-doped Tin Oxide
GHG	Greenhouse Gas
GWP	Global Warming Potential
H_2S	Hydrogen Sulfide
HI	Hydriodic Acid
HTL	Hole Transport Layer
HTM	Hole Transport Material
IDEMAT	Industrial Design and Engineering Materials
IEA	International Energy Agency
ILCD	International Life Cycle Data
ISO	International Organization for Standardization
ITO	Indium Tin Oxide
KOH	Potassium Hydroxide
LCA	Life Cycle Analysis (Assessment)
LCI	Life Cycle Inventory
LCIA	Life Cycle Impact Assessment
C_6H_5Cl	Chlorobenzene
CH_3NH_3I	Methylammonium Iodide
NaCl	Sodium Chloride
$NaNO_2$	Sodium Nitrite
ODP	Ozone Depletion Potential
OPV	Organic Photovoltaic
PbI_2	Lead Iodide
PERC	Passivated Emitter and Rear Contact
PSC	Perovskite Solar Cell
PV	Photovoltaic
RVIM	Dutch National Institute for Public Health and the Environment
S	Sulphur

Abbreviation	Definition
SIMF	Sustainable Impact Metrics Foundation
TCO	Transparent Conductive Oxide
Tg	Transition Temperature
TiO_2	Titanium Oxide

Symbols

Symbol	Definition	Unit
A	Equivalent Operation Area of the PV module	[m^2]
FF	Fill Factor	[]
J_{mpp}	Maximum Power Point Current Density	[A/cm^2]
J_{sc}	Short-circuit Current Density	[A/cm^2]
PCE	Power Conversion Efficiency	[%]
P_{in}	Incident Power Irradiance	[W/m^2]
P_{max}	Maximum Power	[W]
PR	Active Area Ratio	[%]
T	Lifetime of PV module	[yr]
V_{oc}	Open-circuit Voltage	[V]
V_{mpp}	Maximum Power Point Voltage	[V]
ε	Electricity generated by PV module	[kWh]
η	Module Efficiency	[%]

1 Introduction

Sustainable energy technologies play an irreplaceable role in global warming and climate change. Photovoltaic technology (PV), one of the most significant renewable energies, has increased rapidly during the last two decades. According to the latest report of the International Energy Agency (IEA) [1], installed solar PV generation has exceeded 1000 TWh in 2021, and solar PV is responsible for 3.6 % of global electricity generation, which means it is the world's third-largest renewable energy technology. From a policy perspective, many countries and regions are promoting positive decarbonization policies and goals. China is promoting its 14th Five-Year plan in 2022, which indicates the goal that 33% of electricity generated will come from renewable energy by 2025, including 18% from wind and solar energy [2]. The United States introduced the Inflation Reduction Act law to support the development of renewable energy in the next 10 years [3]. The European Commission launched the REPowerEU Plan to increase the 2030 renewable energy target up to 45%, which requires 600 GW of solar PV [4].

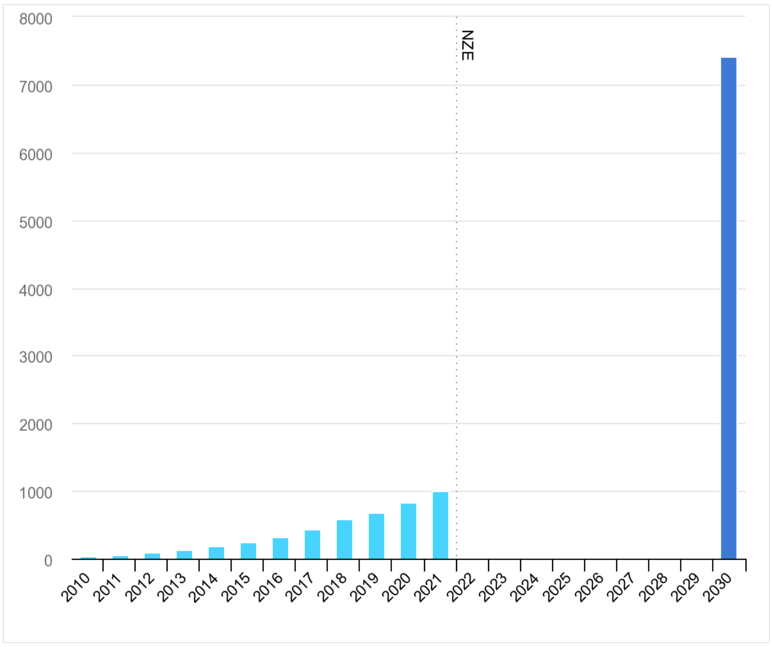

Figure 1.1: Solar PV power generation in the Net Zero Scenario, 2010-2030 [5]

The increasing installation of PV panels accelerates the energy transition and decarbonization, however, this process also causes a series of environmental problems, for instance, the manufacturing of silicon materials and encapsulation of solar cells can lead to greenhouse gas (GHG) emissions. So evaluation of the environmental impacts of solar cells is necessary to be quantified, which can be assessed by life cycle analysis (LCA) method.

1.1. Photovoltaic technology

Photovoltaic technology directly converts sunlight's irradiation into electrical energy. The solar cell works based on photovoltaic effects, which is the absorption of photons to form the potential at the junctions of two different materials to generate direct current electricity. In 1839, this phenomenon was first discovered and then commercially applied by scientists from Bell Laboratories, opening the prelude of the first solar silicon solar cell [6].

The working principle of a solar cell can be generally described as follows:

- The difference between the conduction band and valence band in a semiconductor forms the bandgap
- Electron-hole pairs are generated by the absorption of light, and electricity is generated
- The separation of charge carriers of opposite types and the separate extraction of those carries causes an external circuit [7]

There are various types of solar cells, and each of them has different characteristics on optical or electrical performance. Currently the most widely used is crystalline silicon solar cells, with the advantages of high efficiency and a mature commercialization chain. Thin-film solar cells are produced by depositing thin film layer(s) on glass or metal plastics with its high flexibility and low manufacturing cost [8]. One of the thin film layers is the perovskite solar cell, which has easy assembly and similar high efficiency close to crystalline silicon. Another type of solar technology, organic PV, consists of organic carbon-rich compounds and plays a significant cost-effective role in high volumes production. In this thesis, researches and results relevant to LCA method are mainly focused on perovskite solar cells in Europe specifically.

1.2. Perovskite solar cell

As an advanced type of solar cells, perovskite solar cells are embedded with special absorber materials which are halide perovskites. The original mineral perovskite, which is calcium titanium oxide ($CaTiO_3$), has a distinctive crystal configuration. Perovskite structure is derived from the ABX3 crystal structure of the absorber materials, where A = organic cation, B = metallic cation and X = halide anion [9]. Perovskite solar cell (PSC) applies a perovskite-structured compound, typical perovskite solar cells consist of an absorber layer (for example $CH_3NH_3PbX_3$), which is inserted between the electron-transport layer (ETL) and hole-transport layer (HTL).

There are different types of perovskite solar cells applied in the market, for instance, four commonly used types of perovskite solar cells are introduced as follows:

1.2.1. Mesoporous structure

Mesoporous structure cells usually consist of a transparent conductive oxide (TCO), a compact layer, a mesoporous Titanium Oxide(TiO_2) or Al_2O_3 scaffold, a perovskite absorber, an HTL and metal electrode. With a solid-state hole transport material (HTM), the perovskite solar cells can be commercialized with high efficiency, cost and stability. For example, one of the downsides of TiO_2-based perovskite solar cells is the poor electron mobility of TiO_2 [10].

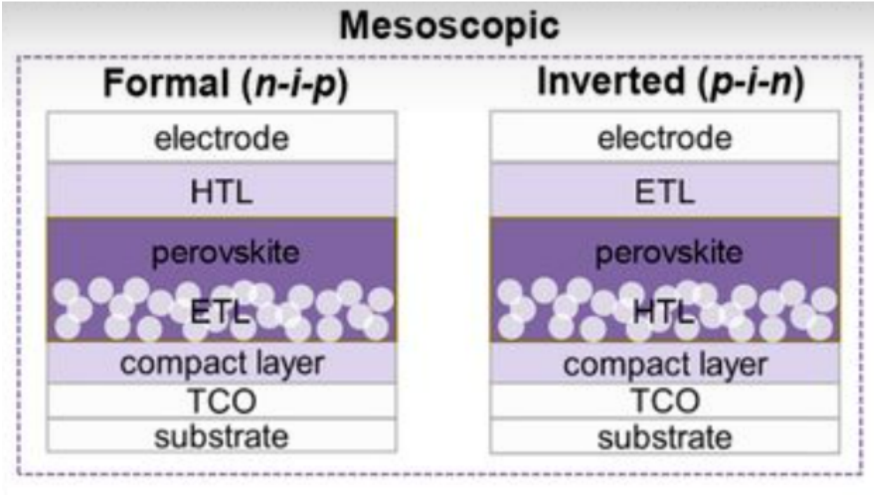

Figure 1.2: Mesoscopic structure solar cell [10]

1.2.2. Planar n-i-p and p-i-n structure

There are two basic types of planar solar cells, one is n-i-p and the other is p-i-n structure. The difference between the p-i-n structure and the n-i-p structure is the relative location of charge transport layers. For the n-i-p structure, the HTL is on top of the perovskite layer; for the p-i-n structure, the HTL is on top of the transparent conducting substrate [11].

Due to the charge diffusion length of mesoporous structure perovskite solar cells less than 20 nm, which is mostly too short for the real case, the planar structure has a feasible charge diffusion length more than 100 nm [12]. The mesoporous TiO_2 layer can be eliminated so that the processing temperature of solar cells is able to be under 150 degrees Celsius.

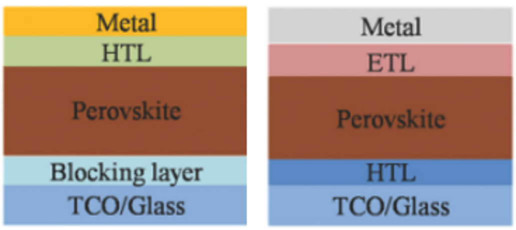

Figure 1.3: Planar n-i-p and p-i-n structure solar cell [11]

1.2.3. Cells with a carbon electrode

The structure of cells with a carbon electrode can be described in figure 1.4. Nanoporous TiO_2, ZrO_2, and carbon black/graphite electrodes are printed sequentially on TiO_2-coated FTO glass, then the perovskite precursor solution is dropped onto the carbon electrode, and it infiltrated through the carbon electrode to reach TiO_2 and ZrO_2 [11]. In this case, perovskite solar cells with a carbon electrode can operate without HTL, thus the device fabrication doesn't need vacuum evaporation that can reduce fabrication costs [11].

Figure 1.4a and figure 1.4b below show the structure of fully printable mesoporous perovskite solar cells and its energy band diagram, and figure 1.4c indicates a typical crystal structure of $CH_3NH_3PbI_3$. Figure 1.4d and 1.4e show the J-V curve of printable solar cells and stability test for a $(5-AVA)x(MA)1–xPbI_3$ solar cell.

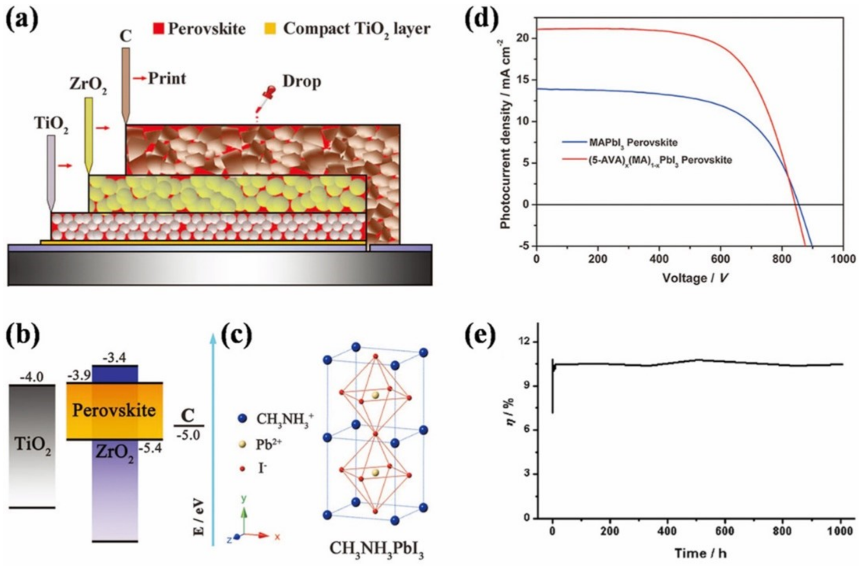

Figure 1.4: Structure and performance of cells with a carbon electrode [11]

1.2.4. Tandem cells

Tandem cells are assembled by combining a wide bandgap solar cell with a narrow bandgap solar cell in series. For a single junction cell, the V_{oc} is not high because of the narrow bandgap, but tandem cells can absorb a broad range of solar spectrum and provide a high V_{oc} which is the sum of the V_{oc}s of the sub-cells. Meanwhile, tandem cells can reduce the thermalization of the excess energy of high-energy photons and transparency to low-energy photons [13]. Generally, there are two commonly commercialized tandem cells, 4-terminal tandem cells and 2-terminal tandem cells separately. There exist some disadvantages of tandem cells, for instance, the photocurrent generated by the two sub-cells should be balanced because the photocurrent exported from the tandem cell is limited by the sub-cell with the smaller photocurrent [11].

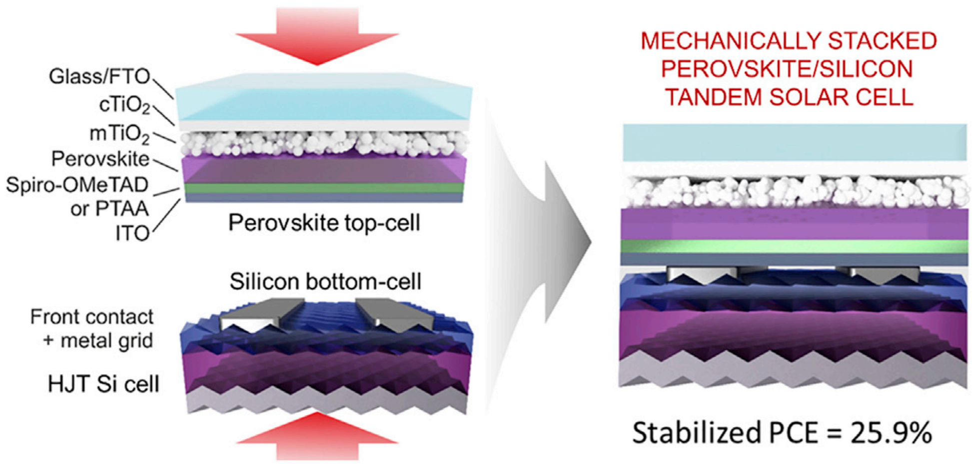

Figure 1.5: Mechanically stacked perovskite/silicon tandem solar cell[14]

1.3. Life cycle analysis

Life cycle analysis (LCA) or assessment is a method to evaluate the environmental impacts of a product or system throughout its life cycle. Typically LCA is referred to as "cradle-to-grave", it consists of classical five steps as follows:

- Raw material extraction
- Manufacture
- Distribution and transport
- Operation and maintenance
- End of life

By quantifying the environmental impacts of a product or system, LCA benefits the stakeholders to understand and improve the LCA method can be applied to different research or social fields, such as energy generation, food delivery, GHG emissions, etc [15]. For renewable energy, LCA can be used to quantify and assess the materials, energy flows and their relevant emissions to measure global warming, pollution like air, water and soil, ecotoxicity and so on, in order to estimate the potential of renewable energy in the future.

There are some limitations of the current LCA method, for instance, currently there is not a single, standardized or acceptable LCA method and each LCA methodology has its own imperfections in several points [16]. Besides, LCA highly depends on the inventory data, so the availability and accuracy of databases is always an issue that needs to consider.

1.4. Research questions and objectives

This thesis aims to deeply research on the life cycle analysis of perovskite solar cells in Europe. To realize the final goal of this thesis, a necessary academic question needs to be asked:

- ***What are the environmental impacts on the manufacturing of perovskite solar cells?***

There are some knowledge gaps between the theories and practice. Most life cycle analysis of perovskite solar cells is on the basis of generic assumptions about the environmental impact of raw material extraction, but one application in practice may vary by specific location, unique technology or other constraints. Besides, due to the characteristics of the LCA method, the database of perovskite solar cells needs to be accurate, representative and persuasive. To answer these questions and overcome the knowledge gap, the following objectives require to be achieved:

- **Objective I**: Deep understanding and learning of the manufacturing process of perovskite solar cells, LCA method and relevant theories
- **Objective II**: Create a new database for the selected PSC, operate the whole LCA study on the production of the selected PSC applied with chosen LCA method
- **Objective III**: Technical analysis and comparison of the life cycle environmental impact results, explain the reasons behind the scenery and possible advice on the future

2

Literature review

In this chapter, the relevant knowledge and theoretical background of this thesis is introduced and explained. Section 2.1 analyzes the current development state of photovoltaic technologies, section 2.2 introduces the perovskite solar cells from a technical scope. Section 2.3 describes the manufacturing process of perovskite solar cells.

2.1. Photovoltaic technologies

Photovoltaic (PV) technology is a form of solar energy conversion that directly converts sunlight into electrical energy, this phenomenon is named as photovoltaic effect. It involves the use of photovoltaic cells, also known as solar cells, which are semiconductor devices that generate an electric current when exposed to light.

2.1.1. Photovoltaic performance

Solar radiation is essentially the radiant energy emitted by the sun due to nuclear fusion processes. The solar radiation spectrum refers to the distribution of solar radiation within a range of wavelengths. It extends roughly from 100 nanometers (nm) to 1 millimeter (mm), covering the ultraviolet, visible, and infrared regions of the electromagnetic spectrum. The spectral composition of sunlight at the Earth's surface changes throughout the day, depending on factors like the sun's position in the sky and atmospheric conditions. More than 95% of the energy flux emitted by the sun is in the spectral region of 0.15-4 µm, with around 50% in the visible light region of 0.4-0.7 µm [17]. As shown in figure 2.1, the standard spectrum for space applications is referred to as AM 0 with an integrated power of 1366.1 W/m^2. The AM 1.5 Global spectrum is defined for flat plate modules and has an integrated power of 1000 W/m^2 (100 W/m^2) [18]. The AM 1.5 Direct (+circumsolar) spectrum is defined for solar concentrator work, which includes the direct beam from the sun and the circumsolar component in a disk 2.5 degrees around the sun. The direct and circumsolar spectrum has an integrated power density of 900 W/m^2 [18].

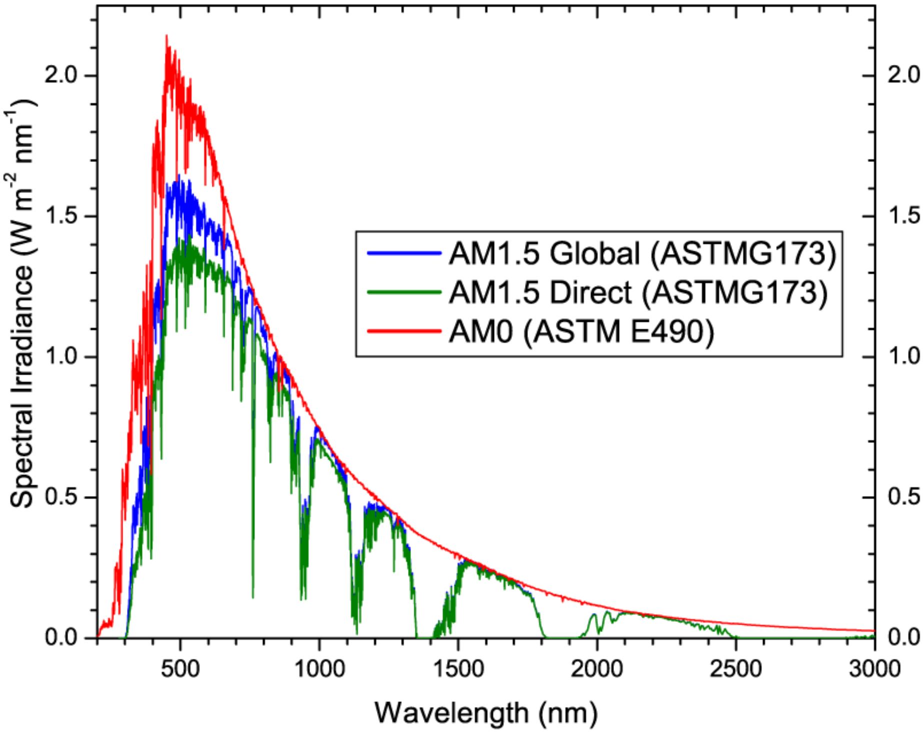

Figure 2.1: Solar radiation spectrum [18]

When the sunlight consists of protons is absorbed, The basic working principle of PV technology can be described as the following seven steps:

- **Photon absorption:** When the sunlight consists of photons absorbed, the surface of a photovoltaic cell is penetrated, and the energy is transferred from photons to electrons.
- **Electron excitation:** The absorbed energy causes some of the electrons in the semiconductor material to gain enough energy to break free from their atomic bonds, creating free electrons and leaving behind positively charged "holes" in the material [19].
- **Charge separation:** Due to the presence of a built-in electric field at the p-n junction (formed by the doping of the semiconductor), the free electrons are pushed toward the n-side, while the positively charged holes are pushed toward the p-side of the cell. This separation of charges generates a voltage potential across the cell [20].
- **Current generation:** The separated charges create an imbalance of electrons, resulting in an electric current that flows through an external circuit connected to the cell. This flow of electrons constitutes the usable electricity generated by the photovoltaic cell [19].
- **Direct current (DC) conversion:** The electricity produced by the PV cell is in the form of direct current, which is the same type of electricity used by most electronic devices. However, for many practical applications, such as powering household appliances or feeding the electrical grid, the DC output needs to be converted into alternating current (AC) using an inverter.
- **Power utilization or storage:** The generated electricity can be utilised directly to power devices or stored in batteries for later use when sunlight is unavailable. In grid-connected systems, excess electricity can be fed back into the electrical grid, allowing net metering or selling electricity back to the utility company.

2.1.2. Electrical performance

The electrical performance of solar cells is illustrated based on a number of parameters obtained from the current-voltage (I-V) characteristics under illumination, for instance, open-circuit voltage (V_{oc}), short-circuit current density (J_{sc}), fill factor (FF) and power conversion efficiency (PCE). Among them, PCE is a key parameter measuring the quality of one solar cell's photovoltaic performance, which can be calculated as:

$$PCE = \frac{J_{sc}V_{oc}FF}{P_{in}} \tag{2.1}$$

Where P_{in} represents the incident power irradiance. J_{sc}, V_{oc} and FF can all be measured directly from an I-V curve measurement of solar cells. The fill factor is the ratio between the maximum power ($P_{max} = J_{mpp}V_{mpp}$) generated by a solar cell and the product of V_{oc} with J_{sc}. The calculation formula of FF is:

$$FF = \frac{J_{mpp}V_{mpp}}{J_{sc}V_{oc}} \tag{2.2}$$

Where J_{mpp} and V_{mpp} represent the maximum power point current density and maximum power point voltage respectively [21].

2.2. Perovskite solar cells

The material perovskite is a calcium titanium oxide mineral composed of calcium titanate ($CaTiO_3$), first discovered by Gustav Rose in the Russian Ural Mountains in 1839, named after Russian mineralogist Lev Perovski, and the classical Cubic crystallographic ABX3 structure of perovskite is shown in figure 2.2 [22]. A represents an organic cation, B is a metal cation and X is a halide anion. Perovskites have been particularly studied for their applications in photovoltaic technology, as well as in many other areas such as LED lights, lasers, and memory devices.

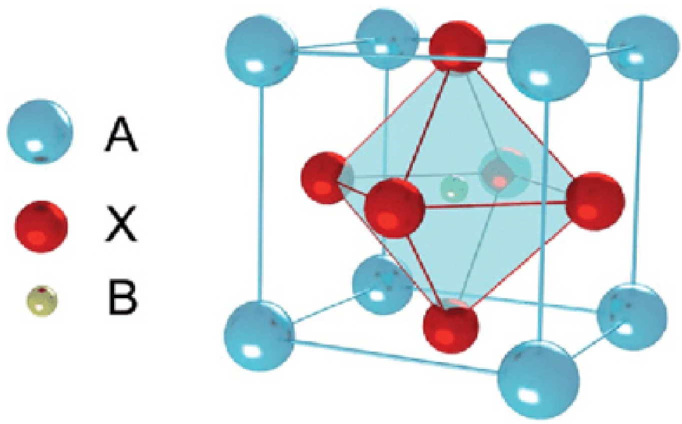

Figure 2.2: Structure of perovskite [23]

When implementing perovskite material in solar cells, perovskite solar cells have gained significant attention in the field of photovoltaics due to their excellent light-harvesting properties, tunable band gap, and comparatively low production costs. The general structure of a perovskite solar cell and how the perovskite material is implemented can be described as follows:

- **Transparent electrode:** The solar cell structure begins with a transparent electrode or substrate, usually made from a material like Fluorine-doped Tin Oxide (FTO)/ Indium Tin Oxide (ITO) glass or plastic, which allows the light channel of sunlight.

- **Electron transport layer (ETL):** Above the transparent electrode, an electron transport layer is added, often made of materials like titanium dioxide (TiO_2). The primary role of the ETL is to transport electrons from the perovskite layer to the electrode while blocking holes (positive charges) from doing the same [23].
- **Perovskite layer:** The perovskite layer acts as the light absorber, which excites the electrons from the valence band to the conduction band, thus creating electron-hole pairs. This perovskite layer's bandgap can be changed by different compositions of the perovskite, which allows for the absorption of light over a wide range of the solar spectrum.
- **Hole transport layer (HTL):** On top of the perovskite layer, a hole transport layer is used to extract positive charges. Materials like spiro-OMeTAD are commonly used for this layer. The purpose of the HTL is to transport holes from the perovskite layer to the other electrode while simultaneously preventing electrons from transporting in the same direction [24].
- **Back electrode:** The back electrode also known as the top electrode, is generally situated on top of the hole transport layer (HTL) and is responsible for collecting the positive charges that migrate through the HTL from the perovskite layer [19]. Gold and silver are often chosen for their excellent conductivity and chemical stability to be the material of the back electrode. The back electrode also provides a physical barrier to protect the underlying layers from environmental factors such as moisture, air, and light exposure which could otherwise cause degradation of the solar cell.

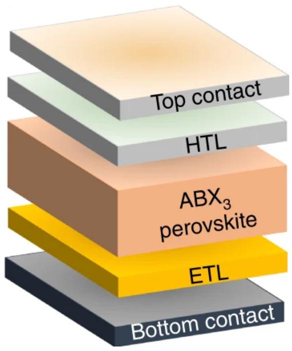

Figure 2.3: Typical structure of a perovskite solar cell [25]

2.3. Manufacturing technologies for PSCs

After being introduced in section 2.2, it's necessary to learn more about different manufacturing technologies of PSCs. Since the manufacturing process of PSCs has not been commercialized and scaled, when it comes to scaling the dimensions of PV modules, there are still some difficulties to be overcome, for instance, control of the morphology of a large-area perovskite layer is one of the biggest challenges [26].

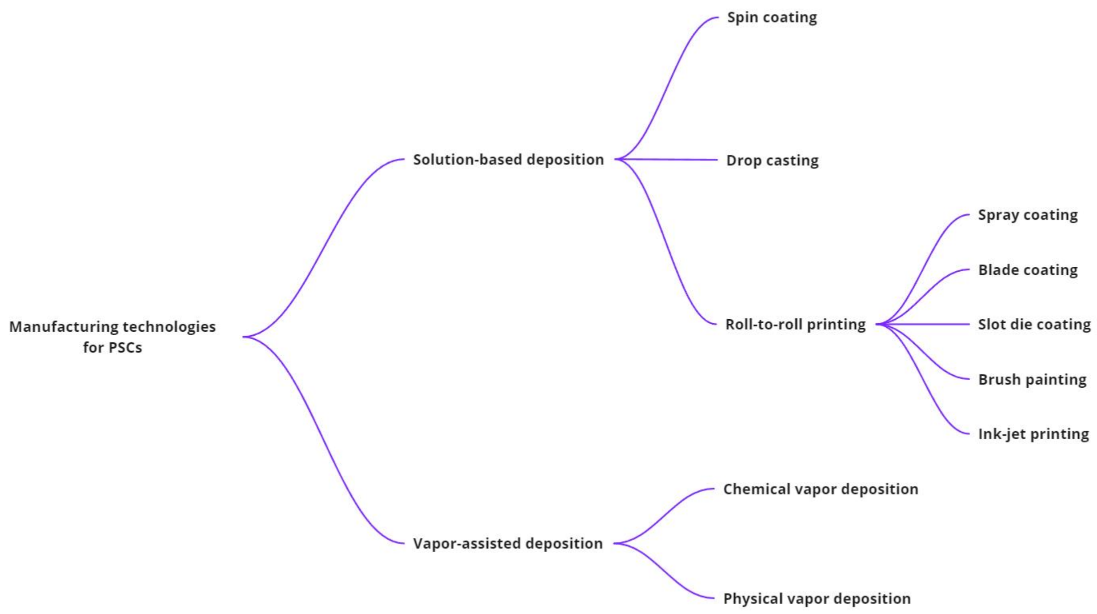

Figure 2.4: PSC manufacturing techniques [26]

Basically scalable manufacturing techniques for PSCs can be divided into two types, which are solution-based deposition and vapor-assisted deposition techniques respectively. The solution-based deposition currently is the most widely used technology of perovskite thin films, including spin coating, drop casting and roll-to-roll printing technologies. Vapor-assisted deposition approach with better film uniformity is further classified into two main categories, i.e., physical-based and chemical-based techniques, as illustrated in figure 2.4. In this section, spin coating, spray coating and chemical vapor deposition (CVD) technologies are mainly introduced due to their common usage.

2.3.1. Spin coating

As the most simplified and lowest costly solution-processed technique, spin coating is widely used for uniform deposition of the perovskite layers during the manufacturing of PSCs. Following the spin coating process, the film is baked to form crystallized layers of perovskite. The baking stage leads to strong adhesion and bonding between metal cations and halogen anions [27]. The film's thickness and quality can be optimized by adjusting the spin speed, acceleration or time of spin coating [26]. Unfortunately this technology is still constrained in the small scale of solar cells, as well as the uniformity of the film. Due to slow processing and material waste, spin coating is not appropriate for manufacturing large-scale PSCs [28]. Appling spin coating in the two-step deposition of perovskite can be explained in figure 2.5.

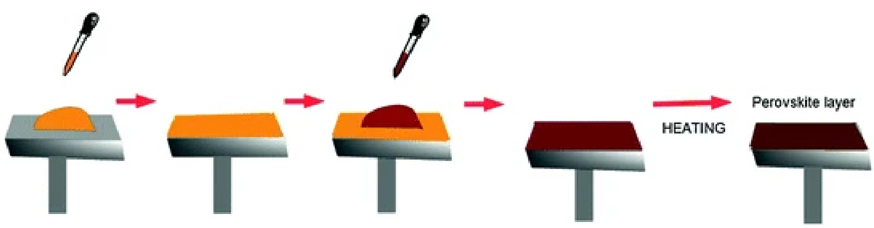

Figure 2.5: Sequential steps of spin-coating process [27]

2.3.2. Spray coating

Spray coating is one of the most efficient and fast solution-based deposition approaches for producing flexible solar cells. In spray coating, a solution containing perovskite precursors is atomized into a fine mist, and this mist is then directed towards a heated substrate, where the droplets land and spread, forming a thin film. Compared to spin coating, spray coating is highly scalable with higher thermal stability and better Photoelectric properties, due to better charge transfer capability and higher minority carrier lifetime [29]. Spray coating also allows for the deposition of perovskite layers onto flexible substrates, leading to the potential development of flexible perovskite solar cells [29].

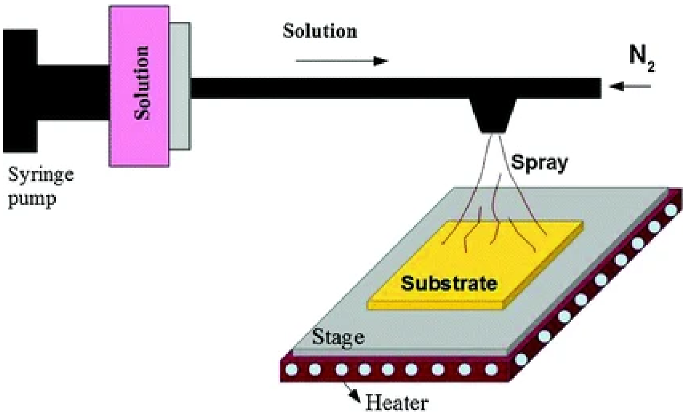

Figure 2.6: Schematic diagram of ultrasonic spray-coating process [30]

2.3.3. Chemical vapor deposition (CVD)

Compared to classical solution-based deposition, vapor-assisted deposition approach can be performed more uniformly. For instance, CVD is one of the promising vapor deposition techniques for large-scale production of highly scalable and uniform pinhole-free perovskite thin films [26]. CVD spares the disadvantages of other vapor deposition methods, such as low material utilization, and poor control of flux deposition [31]. High material yield ratio and scalability make CVD an exceptional technology for depositing perovskite layers [31]. The CVD approach operates in a vacuum environment resulting in highly pure uniform films but also makes it expensive and slower. The schematic of perovskite layer deposition by CVD approach is shown in figure 2.7. With argon gas injected in the first zone, perovskite layers are deposited at a high temperature and then transferred to a preheated substrate to form uniform and pinhole-free films with larger size [32].

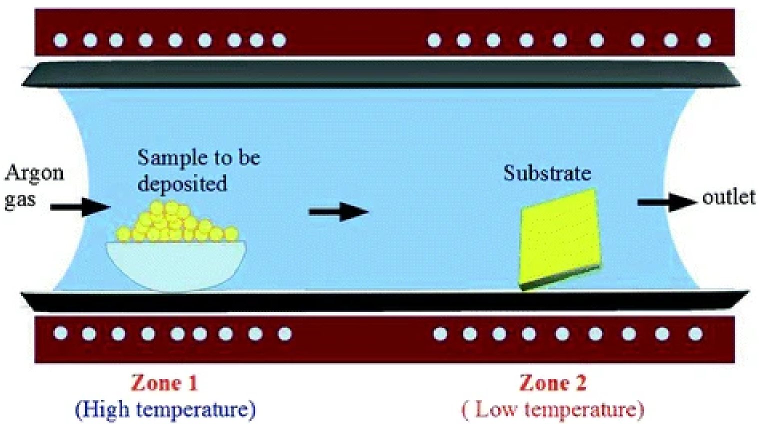

Figure 2.7: Schematic diagram of perovskite film fabrication applying CVD [32]

3
Life Cycle Analysis (LCA)

In this chapter, the methodology of life cycle analysis is introduced. Life cycle assessment is one of the most common methodologies for quantifying sustainability. According to International Organization for Standardization (ISO) 14040 and 14044 [33], LCA study consists of four phases: goal and scope definition, inventory analysis, impact assessment, and interpretation. Section 3.1 includes the definition of functional unit and system boundaries. Section 3.2 is the second phase of LCA study, the life cycle inventory analysis, which involves collecting data to create a life cycle inventory (LCI) of the inputs (energy and materials) and outputs (environmental emissions and waste) associated with each stage of the life cycle. The translation from LCI data into potential environmental impacts can be seen in section 3.3. The final explanation can be found in section 3.4.

3.1. Goal and Scope

Before conducting an LCA study, it's crucial to specify the LCA's goal properly. Generally the goal definition should set out the background of the study and interpret how and whom the results are to be communicated. The ISO 14040 standard [33] states that the goal of the study should define:

- The intended application and the reason for carrying out the study
- The intended audience, i.e. to whom the results are intended to be communicated
- Whether the result is intended to be used in comparative assertions disclosed to the public [33]

The goals should also be defined with the study commissioner, and it is recommended that a detailed explanation be obtained from the commissioner as to why the study is being conducted [34].

After setting the goal of the LCA study, the scope must be determined by specifying the qualitative and quantitative data contained. The definition of scope describes the detail and depth of the study and demonstrates that the goal can be achieved within the stated limitations [35]. According to the ISO LCA Standard guidelines, the scope of a study should explicate the functional unit and system boundaries.

3.1.1. Functional unit

In the framework of LCA, the functional unit is an essential starting point for a comprehensive and comparative analysis of goods or services. It's a quantified description of a product, good, service, or system under study for which the LCA is carried out. The functional unit facilitates comparisons by standardizing the varied inputs and outputs associated with producing a product or delivering a service [35]. It enables the scaling of environmental impacts in relation to the function performed by the product system, effectively converting complex data into information that can be compared on an 'apples to apples' basis. Defining a functional unit involves quantifying the performance of a product system. The attributes encapsulated in a functional unit can vary broadly and may include aspects such as quality, durability, and functionality.

For example, in assessing a lighting system, the functional unit could be defined as 'providing 20,000 hours of lighting at a luminosity of 800 lumens'. This approach allows for the comparison of different lighting technologies (like incandescent, LED, or CFL) on a common basis.

3.1.2. System boundaries

In an LCA, system boundaries determine the scope of research by defining which processes are included or excluded. When defining the system boundaries, it should include all processes that significantly contribute to the total environmental impact and also include all processes directly related to the functional unit. Meanwhile, the definition of system boundaries should comply with the goal and scope definition of the LCA study.

For some specific research, it's necessary to consider both temporal and spatial aspects. The temporal boundaries refer to the timeframe over which impacts are considered, while spatial boundaries refer to the geographical scope of the study. System boundaries can be categorized into two main types: process boundaries and environmental boundaries. Process boundaries define which steps in the life cycle are considered, which could range from raw material acquisition, transportation, production, usage, to waste management. Environmental boundaries are concerned with the types of environmental impacts considered in the study. This could include categories such as global warming potential, eutrophication potential, human toxicity, acidification potential, etc.

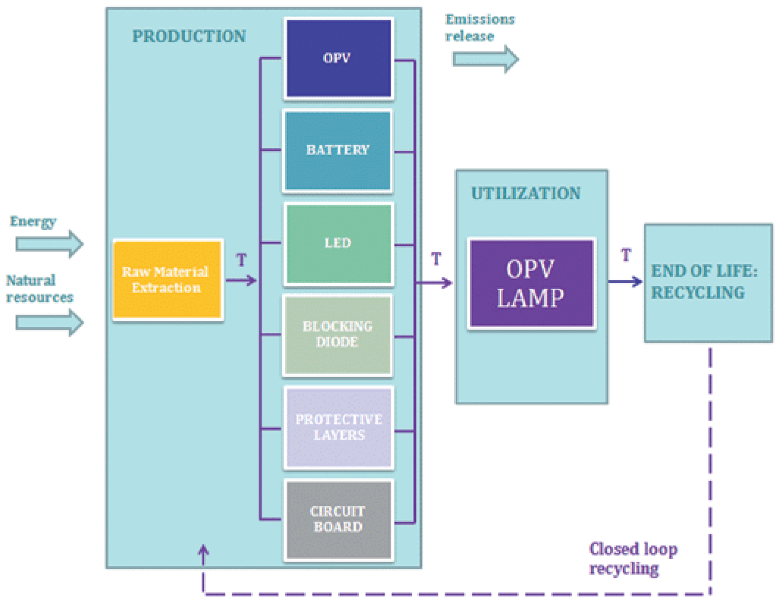

Figure 3.1: System boundaries of the OPV lamp life-cycle assessment [36]

Take a streamlined life cycle assessment of the production of organic photovoltaic (OPV) as an example, three main phases of OPV are illustrated in figure 3.1. The upstream phase is the fabrication of the organic solar module and OPV lamp, the second phase is the utilization of the OPV lamp and the downstream steps of the OPV lamp recycling life cycle are based on end-of-life scenarios [36].

3.2. Life cycle inventory (LCI)

Life cycle inventory is a crucial phase in the Life Cycle Assessment process. In an LCA context, an inventory analysis involves quantifying energy and raw material inputs and environmental releases (emissions to air, water, and land) associated with each stage of a product's life cycle. According to ISO 14044 standard [37], the LCI should follow the procedures below:

- **1. Data collection based on goal and scope:** This is the first step in the LCI phase, where data concerning all inputs and outputs of a product's life cycle are collected. This can be a challenging process, as it involves the collection of primary data directly from operations (e.g., manufacturing processes) and the collection of secondary data from databases and literature for upstream and downstream processes.
- **2. Data validation:** Data quality refers to aspects such as reliability, completeness, precision, and temporal, geographical, and technological representativeness. Validation of the data is important for understanding the reliability and validity of the LCI and, ultimately, the LCA results [38].
- **3. Flow modelling and data management:** The collected data are sorted and organized in a meaningful way to model material and energy flows. This process involves converting the raw data into a standardized format that can be manipulated and analyzed. The modelling and managing of data should be consistent with the definition of the functional unit and the system boundaries established previously.
- **4. Relating data to the unit process:** This step involves mapping all the gathered input and output data to each specific process within the system under study, according to its contribution to the defined functional unit. This allows a standardized and comparative assessment of environmental impacts across the product's entire life cycle [38].
- **5. Relating data to the functional unit:** The data gathered needs to be related back to the functional unit defined in the goal and scope phase. This is necessary to ensure that the inventory reflects all the inputs and outputs required to fulfill the function of the product or system under study.
- **6. Data aggregation:** At the end of the LCI phase, a complete list of inputs and outputs per functional unit should be available. The LCI provides a comprehensive account of the energy used, materials consumed, and emissions and waste generated at each life cycle stage of a product or service.

To sum up, the basic principle of Life Cycle Inventory is collecting and managing data by sorting data from the existing databases or creating new databases or combing them together. The LCI phase is a rigorous, data-intensive process that provides a detailed account of the environmental flows associated with a product's life cycle. The quality and reliability of the LCI significantly influence the validity of the subsequent life cycle impact assessment and the overall LCA results.

3.3. Life Cycle Impact Assessment (LCIA)

Once the life cycle inventory phase is completed, Life Cycle Impact Assessment (LCIA) is followed to study product systems to get information about their environmental issues. The aim of LCIA is to evaluate the potential environmental and human health impacts resulting from the elementary flows determined in the LCI [34]. As outlined in the ISO 14040 and ISO

14044 standards, LCIA involves several three key steps, which separately are the selection of impact categories, category indicators, and characterization models, classification of inventory results and characterization. Apart from this, there are also other optional steps including normalization, grouping of LCIA results and weighting of impact categories [34].

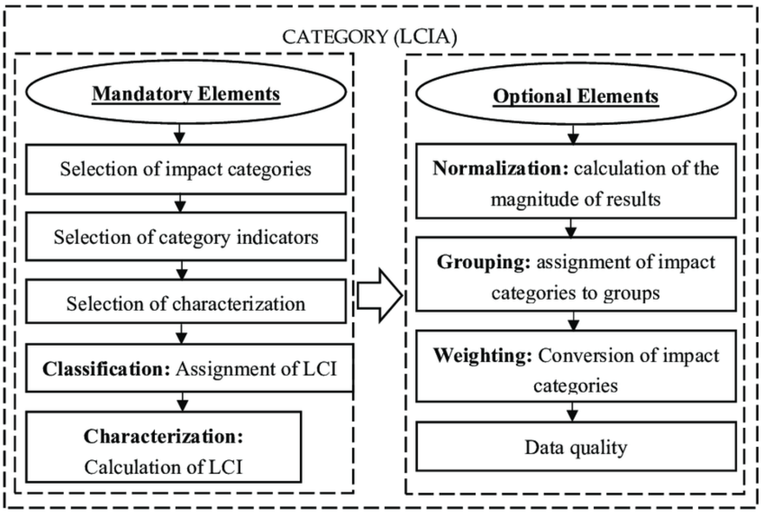

Figure 3.2: Structure of the life cycle impact assessment (LCIA) phase [39]

3.3.1. Selection

The selection of impact categories, category indicators and characterization models plays an essential role in Life Cycle Impact Assessment. Impact categories are environmental themes under which environmental impacts are classified (e.g., global warming potential, human toxicity). All the impacts should be associated with the geographic area under study, and the rationale for each selected impact should be discussed. Category indicators quantify the impacts within each category. Characterization models establish relationships between LCI results and their potential environmental impacts.

The selection of impact categories must be aligned with the target of the LCA study and is completed during the scope definition phase before the collection of inventory data to make sure that the latter focus on what will be assessed in the end [40]. According to ISO 14044, the impact categories must assure that they are complete, enable traceability, and do not lead to double counting or disguise significant impacts [37]. There are also some criteria based on fundamental requirements for impact categories, for instance, the scientific criteria in ISO 14044 describe the completeness of scope, environmental relevance, scientific robustness and certainty, documentation, transparency and reproducibility and applicability [37].

The selection of category indicators is a critical step in the LCIA, common examples of impact category indicators include global warming potential (GWP), ozone depletion potential (ODP), acidification potential (AP), eutrophication potential (EP), human toxicity and others [37]. Typically the impact category indicators can be divided into two types, which are midpoints and endpoints respectively. When utilizing midpoint impact indicators within an impact assessment, the classification step assembles the data derived from the inventory into subsets of substance flows. Each subset shares the potential to influence identical environmental repercussions. This collection process paves the way for a nuanced analysis of the potential impacts from environmental interactions, deploying specifically tailored characterisation factors pertinent to the respective impact category under consideration. The conversion from midpoints to endpoints is used to simplify the interpretation of the LCIA results.

Take the results of Rosenbaum et al. as an example, there are 12 midpoints and 3 endpoints applied in the framework of the International Reference Life Cycle Data System (ILCD) characterisation, as shown in figure 3.3 below.

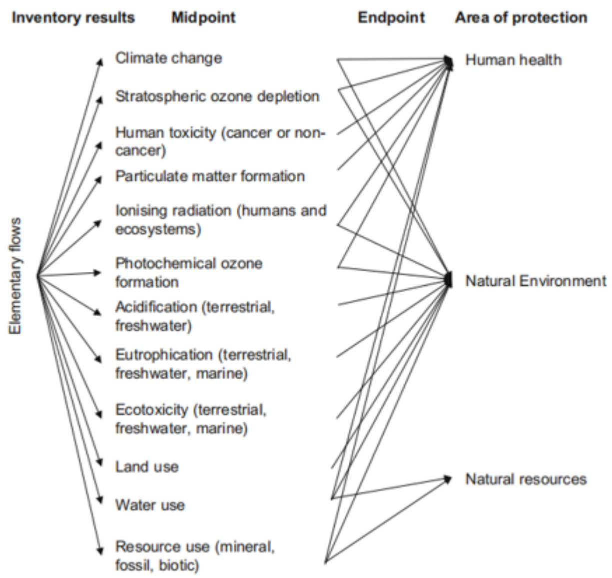

Figure 3.3: Framework of the ILCD characterisation [40]

3.3.2. Classification of inventory results

In this step, the inventory data from the LCI is assigned to the selected impact categories. Each input or output identified in the LCI phase is linked to one or more impact categories, based on the potential environmental effects they might cause [37]. For instance, carbon dioxide emissions would be classified under the 'global warming potential' category, due to its contribution to greenhouse gas emissions. The classification of inventory results also lays the groundwork for the subsequent characterization stage.

3.3.3. Characterization

Characterization within LCIA involves using characterization factors to transform the inventory data within each impact category into common units, thereby enabling an evaluation of the potential impact. These characterization factors are scientifically derived values that represent the potential impact per unit of inventory flow (e.g., the potential for a kilogram of carbon dioxide to contribute to global warming). The following procedure involves multiplying the quantity of each inventory flow by its respective characterization factor. The result is an estimate of the potential contribution of each inventory flow to the environmental impact in each impact category [34]. The whole process translates the LCI data, which is a collection of emissions and resource consumption data, into potential environmental impact data.

It's important to note that characterization inherently includes necessary assumptions and approximations due to scientific uncertainties or gaps in LCI data. Therefore, it's crucial to record the process transparently, stating the characterization factors applied, their original sources, and all the assumptions made. This enhances the credibility and reliability of the LCA study.

3.3.4. Other Optional Elements

Apart from the LCIA processes mentioned above, normalization, grouping of LCIA results and weighting of impact categories are the three other optional operations possibly conducted during LCIA. These three elements can provide informative or practical benefits to LCIA study. In this thesis, these optional elements are not studied due to the limitation of time and depth.

3.4. Interpretation

Interpretation is the final phase in the Life Cycle Assessment process. The interpretation stage of the life cycle embodies a structured method for identifying, quantifying, verifying, and assessing data derived from the life cycle inventory and/or life cycle impact assessment. A summary of the results obtained from the inventory analysis and the impact assessment is performed during this phase. The ultimate deliverable from the interpretation phase includes a collection of conclusions and recommendations pertinent to the study. As explained in ISO 14043 [41], the interpretation should contain the following:

- Identifying significant issues according to LCI and LCIA results
- Evaluation of the reliability, sensitivity and consistency
- Conclusions, recommendations, and constraints

4

LCA of perovskite PV module

As discussed in the third chapter, the theoretical method of life cycle assessment is introduced in detail, and LCA method can be implemented in many fields of marketing, agriculture, supply chain and industry. This report focuses on applying the LCA method to PV technology, more specifically to the production of perovskite solar cells in Europe. When applying the LCA method to create a new system model, some changes are necessary to be made in order to make this study more balanced and practical. For instance, as explained in the third chapter, generally Life Cycle Assessment includes the cradle-to-grave 5 steps, however, due to the limitation of time, the immature PSC technologies and limited scales, this thesis only focuses on the cradle-to-gate steps, which are raw material extraction, manufacturing & processing and distribution separately. Since the topic of this study is the production of PSCs in Europe, mostly concentrating on the manufacturing process of solar cells, so the distribution consideration will not be discussed specifically.

In this chapter, section 4.1 demonstrates the selection type of PSCs used in this project and provides an explanation for the reasons behind it. Section 4.2 introduces the functional unit and system boundaries of the model. In section 4.3, the life cycle inventory of this model is illustrated with more details on databases. The LCI of the manufacturing process of PSCs consists of material inventory and energy inventory. Last but not least, the LCIA of the perovskite PV module is described in section 4.4, including the selection of life cycle impact categories and midpoint indicators, designed model calculations on environmental impacts and classification of inventory results.

4.1. Selection of perovskite solar cells

As introduced in the section 1.2, there are different types of perovskite solar cells currently designed and used. Compared to existing Crystalline Silicon (c-Si) cells like Passivated Emitter and Rear Contact (PERC) solar cells, most perovskite solar cells are still within the development phase and have not been in large-scale commercial production. However, due to the rapid development of technology, advanced perovskite solar cell has already reached a power-conversion efficiency of 26.08 % in 2023 [42].

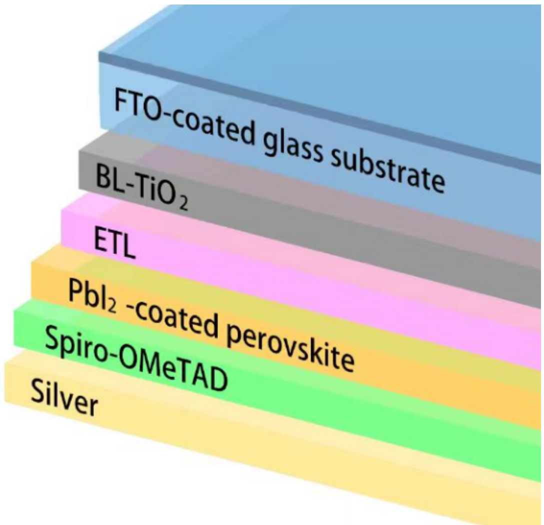

Figure 4.1: Structure of studied TiO_2 perovskite solar cell

Among all the possible choices possibly acquired, this study takes a perovskite solar module with a mesoporous titanium oxide (TiO_2) scaffold into account. More specifically as shown in figure 4.1, the TiO_2 solar module's structure displays in FTO-coated glass, a blocking layer of TiO_2 (BL-TiO_2), nanocrystalline (nc)-TiO_2 electron transport layer (ETL), lead iodide (PbI_2) spin-coated perovskite layer, spiro-OMeTAD hole transport layer (HTL) and silver cathode. There are several considerations and explanations of the choice made:

- TiO_2 is commonly used as an ETL of regular-structure PSCs, the presence of TiO2 nanoparticles in the perovskite film could improve the electron extraction, and promote the formation of a compact perovskite layer with large grains [43]. TiO_2 has good optical and chemical stability, nontoxicity, corrosion resistance and a simple manufacturing process etc [44].
- Currently spiro-OMeTAD is still the most popular hole transporting material (HTM) for high-performing PSCs, which works effectively in combination with some additives, such as Li-TFSI and t-BP [45]. Amorphous organic materials including spiro-OMeTAD have good conductivity, morphological stability, and high glass transition temperature (Tg) are essential parameters of a reliable HTM for PV solar cells.
- Using silver as cathode indicates a decrease in material costs, compared to the usage of gold. Although under standard AM1.5 illumination, gold shows a slightly better power conversion efficiency than silver, the environmental impacts of primary gold metal are significantly higher than that of silver, which can also be seen in the following chapter 5.
- Due to the restrictions on the accessibility to the original material data, for instance, the experimental data with accurate and of most universities, institutions or solar cell manufacturing companies are confidential, which leads to the existing accessible solutions of perovskite solar cells are limited. At the beginning of this project, necessary contacts were made with some institutions, unfortunately, the outcomes of all the contacts turned out to be not positive. By literature research, also combining the previous considerations, finally the selection of PSC is determined.

4.2. Goal and scope of LCA

This section describes the definition of the research goal, functional unit and system boundaries of this model. As discussed in the previous section 3.1, the system boundaries clearly define the research scale of the LCA study and consolidate the goal of this project, with a more systematic, visualized model.

4.2.1. Research goal

The research goal of this study is to assess the potential life cycle impacts on the manufacturing process of different perovskite PV modules: one is a perovskite solar module with a mesoporous TiO_2 scaffold whose original data is from the literature's result [46], one is the selected perovskite PV module with a silver cathode and the other one is the same type of perovskite PV module but with a gold cathode. The difference between the selected PV module and the perovskite module from the literature will be explained later in section 4.3. After the calculation of the environmental impacts of these different modules, comparisons, analysis and discussion of the results are conducted to tell the reasons and explanations of the different performances of modules, for instance, identify which components of the PV module contribute the highest environmental impact thus analyze the potential reasons behind. Besides, the thesis also compares the environmental impacts of perovskite solar modules with single-crystalline silicon (sc-Si) modules.

4.2.2. Functional unit of LCA

As introduced in subsection 3.1.1, the functional unit is an important starting point for a comprehensive and comparative analysis of goods or services. In the existing LCA studies on perovskite solar cells, the functional unit of a PV module is usually considered to be 1 m^2 of PV perovskite module or 1 kWh of electricity generated by perovskite module. In this study, the functional unit is defined as 1 kWh of electricity generated by perovskite solar cells (modules) that are frequently used in LCA studies of PV. This aims to realize the functional unit conversion from area to electricity, which is more convenient to analyse environmental impact results from a normalization perspective. The functional unit is not chosen as the unit of area to prevent inter-external considerations such as efficiency difference, for example, solar cells with higher efficiency require less area to produce one kWh [47]. Some recent literature uses area as the functional unit, in order to simplify the calculations, unit conversion is crucial to be conducted.

$$\varepsilon = A \cdot r \cdot \eta \cdot PR \cdot T \tag{4.1}$$

Where ε represents the electricity generated by a PV module (kWh), A represents the total area (m^2) of the PV module, since the thesis chooses to convert the unit from per m^2 to per kWh, the value of A is set to be 1. r is the annual average solar radiation on modules (kWh $year^{-1}m^{-2}$), η is the module efficiency (%), PR is the performance ratio stated in percentage, which describes the ratio of the energy effectively produced (used), with respect to the energy which would be produced if the system was continuously working at its nominal STC efficiency. T equals the lifetime (year) of the PV module.

So the conversion from area-based (per m^2) to energy-based (per kWh) as the functional unit is:

$$\mu = \frac{A}{\varepsilon} = (r \cdot \eta \cdot PR \cdot T)^{-1} \tag{4.2}$$

Based on equation 4.1, coefficient μ (m^2/kWh)is defined as area divided by electricity to convert the unit to per kWh, which can be directly multiplied with the results originally calculated in per m^2. Take climate change as an example, by multiplying the coefficient μ, the results can be transferred from kg CO_2 eq/m^2 to kg CO_2 eq/kWh directly.

More assumptions are reasonable to be made during the set-up of the functional unit, for instance, the efficiency of selected TiO_2 modules keeps 9.10% the same as the literature [46], derived from the previous experimental result of mesoscopic PSC modules to make results comparisons more reasonable [48]. For the lifetime of perovskite solar cells, recently Princeton researchers made a breakthrough in the first perovskite solar cell with a commercially viable lifetime of around 30 years [49]. According to the U.S. Department of Energy Solar Energy Technologies Office (SETO), the operational lifetime of commercialized perovskite solar cells should be at least 20 years, preferably more than 30 years [50]. Since the development and commercialization of PSCs are not mature enough, in this thesis, the designed lifetime of the selected PV module is assumed to be 20 years. According to the methodology guidelines by IEA and the population-weighted average for Europe [51], the annual solar irradiation is assumed to be 1391 kWh $\mathrm{year}^{-1}\mathrm{m}^{-2}$ in this study. The performance ratio of the TiO_2 module is assumed to be 80% according to Fraunhofer's photovoltaics report in Germany [52].

4.2.3. System boundaries of LCA

The definition of system boundaries of this study is illustrated in figure 4.2. The life cycle can be divided into four different stages, which are elements production, module manufacturing, module use and disposal respectively. The operation and end-of-life phases provide more uncertainty than the production phase. In this study, the system boundaries are defined within the range of the first two stages as the grey dotted line shown in the figure due to the limitation of time and conditions. The first stage is the production of the elements, including the raw materials extraction and production of the first-stage materials, in order to prepare for the next fabricating step. The second stage is the manufacturing process of the PV module, which is related to different technologies. During the second stage, the PV module is constructed by depositing components onto the substrate to form all the layers. This manufacturing process not only consumes energy mainly in terms of heat and electricity but also generates emissions. Other disposal methods such as waste-cycling and incineration are not studied in this project, due to the lack of information and data on waste-cycling or combusting PSCs [46].

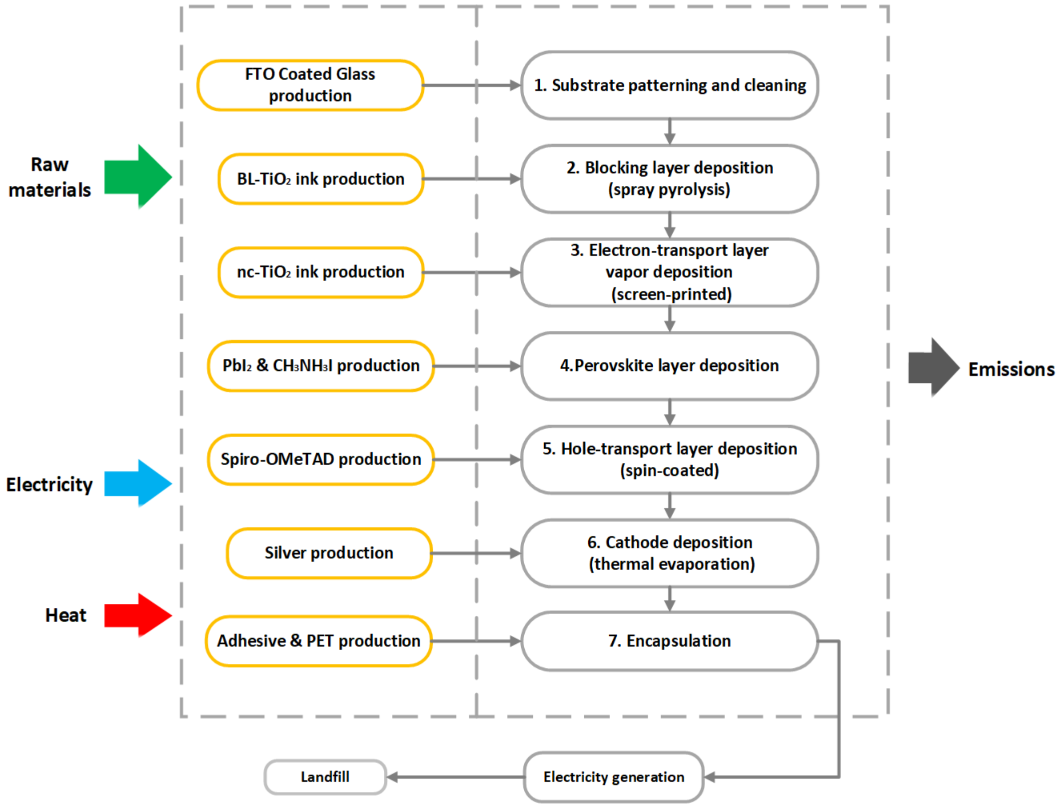

Figure 4.2: System boundaries of manufacturing studied perovskite solar module

Diving into the whole process of manufacturing, more information is depicted. As shown in figure 4.2, generally the manufacturing process of a perovskite module involves the following seven steps: The initial step is the patterning and cleaning of the substrate. The fluorine-doped tin oxide (FTO)-coated glass substrates are patterned by a raster scanning laser. The most commonly used method for patterning FTO is to chemically remove the FTO from specific areas on the substrate by chemical etching. The chemical etching involves the usage of zinc powder and 3 M Hydrochloric acid (HCl). Then the substrate is cleaned with 2% Hellmanex (AlOH) solution and washed with ethanol, deionised water, acetone, methanol, etc in an ultrasonic bath [53]. Afterwards on the interconnection area of cells, silver paste is screen-printed and finally a metallic mask is formed by sintering the substrates [46]. The second step describes the deposition of the blocking layer of TiO_2 (BL-TiO_2). The technology of spray pyrolysis, where a precursor solution is sprayed onto a heated substrate, is applied in the deposition of the blocking layer. During the third step of the manufacturing process, the ETL is deposited on the substrate. Before the substrates are sintered to create a mesoporous nanocrystalline TiO_2 layer (nc-TiO_2), a TiO2-scaffold layer is screen-printed, which directly uses the nc-TiO_2 ink during the production of elements stage. In the fourth step, the forming of a perovskite active layer is introduced by deposition as well. PbI_2 is spin-coated on the TiO_2 films via the cost-effective electrochemical deposition method named chemical vapor deposition (CVD). Subsequently, PbI_2 is immersed in in a CH_3NH_3Isopropanol solution to form a methylammonium lead triiodide ($CH_3NH_3IPbI_3$ or $MAPbI_3$) layer. The fifth step indicates the HTL's deposition on top of the perovskite layer. Experiments demonstrate that perovskite remains stable when interacting with a solid-state hole transporter like spiro-OMeTAD [54]. The perovskite and spiro-OMeTAD layers from the interconnection area are etched away using a green and cost-effective microchip Nd:YVO4 laser. When it comes to the sixth step, the deposition of the silver cathode is conducted by thermal evaporation. It's worth mentioning that replacing the original gold cathode in paper [46] with silver may cause a quantified difference in the environmental impacts, which can be seen later in chapter 5. Finally the seventh step shows the encapsulation of the module. Commonly used encapsulation methods are either depositing a clear film encapsulant or utilizing an edge sealant to sandwich the device between sheets of glass or polymer, and this study takes the former method.

4.3. Life cycle inventory of perovskite PV module

In this section, the life cycle inventory of perovskite solar cells for production is described as follows: Databases, Material inventory, Energy inventory and Life Cycle Impact Assessment of the model. To realize the life cycle inventory of the designed model, firstly the new database is essential to be built during the data collection and validation. Based on the functional unit, system boundaries and created database, a material inventory of selected perovskite PV module can be set up. Meanwhile, the energy inventory that demonstrates the energy consumption during the manufacturing process should be built regarding all the possible technologies and machines possibly implemented.

4.3.1. Databases

Database plays an integral role in LCA studies, providing a rich source of data necessary for these extensive analyses. For instance, databases offer comprehensive and reliable data that covers a broad range of aspects associated with products, services, and processes. This information includes raw material extraction, energy use, emissions, and waste generation, among others. Besides, the continuous updates and improvements in these databases represent LCA studies can stay relevant and reflect the current situation. For example, the Ecoinvent database has been updated to the latest version 3.9.1. This aspect is crucial as technology and processes constantly evolve, and having up-to-date data ensures the validity and relevance of the LCA studies.

There are different types of databases used for LCA study created by different institutions, such as Ecoinvent, USDA, GaBi, Idemat and so on. The most commonly used database in Europe is Ecoinvent, which consists of more than 18000 reliable life cycle inventory datasets in the industry, agriculture, nature, waste, etc [55]. Almost all the data in Ecoinvent is attributed to a geographic location, like RER (Europe) in Ecoinvent represents the location of Europe area. Unfortunately the direct accessibility to Ecoinvent database is limited during this LCA study, but some of the elements are able to be self-calculated from Ecoinvent V3.8 official website.

Activity	**MG-silicon**	*All columns past the first two for database and activity definitions are ignored in any case.*						
categories	Metal grade silicon production							
code								
comment								
filename								
location	CN							
production amount	1							
type	process							
unit	kilogram							
Exchanges								
name	**amount**	**unit**	**database**	**categories**	**location**	**type**	**uncertai**	**loc**
MG-silicon, at plant	**1**	**kg**	**IEA PV inventory**	Metal grade si	**CN**	**production**		
market group for electricity, medium voltage	0	kWh	ecoinvent 3.8_cutoff		CN	technosphere	1	
market for wood chips, dry, measured as dry mass	3.25E-3	kg	ecoinvent 3.8_cutoff		RER	technosphere	1	
market for hard coal briquettes	2.31E+1	MJ	ecoinvent 3.8_cutoff		RER	technosphere	1	
graphite production	1.00E-1	kg	ecoinvent 3.8_cutoff		RER	technosphere	1	
market for charcoal	1.70E-1	kg	ecoinvent 3.8_cutoff		GLO	technosphere	1	
market for petroleum coke	5.00E-1	kg	ecoinvent 3.8_cutoff		RER	technosphere	1	
silica sand production	2.70E+0	kg	ecoinvent 3.8_cutoff		DE	technosphere	1	
market for oxygen, liquid	2.00E-2	kg	ecoinvent 3.8_cutoff		RER	technosphere	1	
slag from metallurgical grade silicon production, inert mater	2.50E-2	kg	ecoinvent 3.8_cutoff		CH	technosphere	1	
market for silicone factory	1.00E-11	unit	ecoinvent 3.8_cutoff		RER	technosphere	1	
transport, freight, sea, container ship	2.55E+0	tkm	ecoinvent 3.8_cutoff		OCE	technosphere	1	
transport, freight, lorry, unspecified	1.56E-1	tkm	ecoinvent 3.8_cutoff		RER	technosphere	1	
transport, freight, train	6.90E-2	tkm	ecoinvent 3.8_cutoff		RER	technosphere	1	
Heat, waste	7.13E+1	MJ	biosphere3			biosphere	1	
Arsenic	9.42E-9	kg	biosphere3			biosphere	1	
Aluminium	1.55E-6	kg	biosphere3			biosphere	1	
Antimony	7.85E-9	kg	biosphere3			biosphere	1	
Boron	2.79E-7	kg	biosphere3			biosphere	1	
Cadmium	3.14E-10	kg	biosphere3			biosphere	1	
Calcium	7.75E-7	kg	biosphere3			biosphere	1	
Carbon monoxide, from soil or biomass stock	6.20E-4	kg	biosphere3			biosphere	1	

Figure 4.3: MG-silicon example in Ecoinvent V3.8 database

Idemat (Industrial Design & Engineering Materials database) is a compilation of LCI data of the Sustainable Impact Metrics Foundation (SIMF), a non-profit spin-off of the Delft University of Technology [56]. Idemat is designed for the needs of designers, engineers and architects in the manufacturing and building industry. After Ecoinvent Version 3 is introduced in 2014, there was growing dissatisfaction with the lack of sufficient transparency and the inaccuracies of data on e.g. electricity and transport, and the latest version of the Idemat database has been updated to Idemat 2023. Idemat data are based on peer-reviewed scientific papers, plus additional LCIs made by Delft University of Technology, and Plastics Europe [56]. Idemat climate change impact is built on IPCC 2013 GWP 100a method, in compliance with ISO 14040, 14044, EN15804, and the ILCD Handbook (General guide for Life Cycle Assessment Detailed guidance) with some special calculation rules, for example, the embodied fossil fuels are added to the LCIs for plastics, paints and inks at the gate of the production step, in line with the philosophy that it is an indicator for the plastic soup [56]. Compared to the Ecoinvent database, even if Ecoinvent provides more data on chemicals and chemical processes, Idemat database is more powerful in the field of product design and engineering. More specific features of Idemat contrasted to Ecoinvent are extra LCIs of alloys, a correction of the market mix data of metals, extra LCIs of wood types, more up-to-date LCIs for electricity, newer data on sea and road transport and others [56].

Product	Climate change (kg CO2 eq)	Human health (CTUh)	Resource use, fossil (MJ)
Boron	5.14E+01	8.94E-11	2.54E+02
Cobalt oxide (CoO)	5.02E+00	2.94E-09	6.60E+01
Graphite for batteries	9.26E+00	2.07E-06	1.20E+02
H_2O_2, 70% in H_2O	5.34E-01	8.25E-14	7.32E+00
Potassium hydroxide (KOH)	1.82E+00	4.71E-10	2.31E+01
Lime	6.10E-01	6.97E-10	6.71E+00
Manganese dioxide	7.02E-01	3.70E-09	1.56E+01
Ni in FerroNickel (27%)	4.51E+01	4.24E-11	1.18E+00
Ni in $NiSO_4$ (22%) for car batteries	2.46E+01	9.49E-11	1.18E+00
Silicagel	3.51E+00	9.41E-10	4.39E+01
Sodium cumene sulphonate	2.21E+00	2.65E-08	5.75E+01
Sodium silicate	1.33E+00	3.52E-10	1.65E+01
Sodium sulphate	3.52E+00	9.42E-10	4.39E+01
Sulphur (S)	0.00E+00	0.00E+00	0.00E+00
Titanium dioxide	7.68E+00	2.03E-09	9.57E+01
Urea (AdBlue)	5.38E+00	1.34E-08	6.74E+01
Vanadium pentoxide	1.78E+01	8.45E-06	2.07E+02
Zinc Oxide	3.04E+00	2.29E-07	3.82E+01

Table 4.1: Inorganic chemicals example in Idemat 2023 database

When it comes to this study, the strategy of the choosing database is combining Ecoinvent V3.8 and Idemat 2023 together to create a new database dedicated to LCA on the production of PSC in Europe. As discussed above, necessary significant self-calculations from Ecoinvent have to be operated when creating the new database, and there are some significant assumptions and changes to the original databases during the whole process, for instance, the replacement of one material, which is explained in the following contents.

4.3.2. Material inventory of perovskite PV module

In LCA research, material inventory clearly indicates all the material production processes of LCA, including the input and output of each flow or process of LCA. Some materials cannot be found in the existing Idemat 2023 database or Ecoinvent V3.8 database, so these unavailable raw materials require further study of their production process. In this project, the unavailable raw materials contain PbI_2, FTO glass, spiro-OMeTAD, methylammonium iodide (CH_3NH_3I), BL-TiO_2 ink, nc-TiO_2 ink and silver paste. The calculation rules of this LCA study's life cycle material inventory are explained in this report, and the manufacturing flow charts of PbI_2, FTO glass, spiro-OMeTAD, and CH_3NH_3I are shown to explain the production procedures of these unavailable materials. Compared to the literature's PV module, the updated module uses some different materials to replace or update, for instance, the studied module uses methanol to replace dimethylformamide due to their similar chemical properties. All the changes in materials can be found in the table 4.2 below.

Literature module's material	Updated module's material
Dimethylformamide	Methanol
Gold	Silver
Soda ash	Sodium silicate
Cullet	Glass bottles, recycled
Mineral oil	Crude oil EU General
Chromium/copper/tin/lead/nickel/zinc	Copper
Coal tar	Bituminous coal at mine US
Sodium nitrite ($NaNO_2$)	Sodium chloride (NaCl)
Acetone	EVA chemical upcycled
Marine aquatic ecotoxicity	MAETP

Table 4.2: Material changes between literature's module and updated module

Calculation rules

The first step of creating a new material inventory specific to perovskite PV modules is data collection. As introduced above, Idemat 2023 database and Ecoinvent V3.8 are the two original databases applied in this LCA study. Based on the existing literature [46], the new inventory uses Idemat 2023 as the main database to find the required material or energy inputs and outputs, then calculate the relative unit amount of these inputs and outputs according to the original values per unit in the database. With the unit and amount of each material given, calculate and add up the environmental impacts in midpoints to get the results of mid-materials, and iterate these mid-materials into the final material inventory. Finally all materials and energy inputs and outputs data are calculated per kWh of the selected perovskite PV module over its lifetime. Energy consumption of some material production happens in electricity and heat generated, which are all calculated in LCA values chosen as electricity EU-27 and industrial heat in Idemat 2023. When some raw materials cannot be found in Idemat 2023, the inventory asks for help from the Ecoinvent V3.8 database website to self-calculate all the data needed. Meanwhile, necessary improvements and changes are operated during the whole process, as shown and explained in the following subsections below. It's worth noting that this LCA only refers to the inventory of the literature instead of the database, because the literature chooses Ecoinvent V3.1, which is the older version of Ecoinvent, leading to the difference between the two more updated databases applied.

$$W = \sum_{i,j} (m_i \alpha_i + E_j \alpha_j) \tag{4.3}$$

From equation 4.3 above, W represents the total environmental impacts, and its unit depends on the impact category. i is the number of required materials, j is the number of energy consumption during manufacturing and α refers to the environmental impacts per kg material from the existing databases such as Idemat or Ecoinvent. m represents the mass (kg) of materials and E equals the required energy in MJ. The calculation principle of material inventory is based on mass allocation. Mass allocation involves distributing the environmental impacts of a process based on the mass (or weight) of the different products that come out of that process. Apart from heat and electricity calculated in MJ, all materials are calculated in mass units (kg). If there is no co-product during the whole process, the calculation of environmental impacts is conducted by adding up of each material's impact with respect to its mass. When there are co-products generated during the processes, it's necessary to apply mass allocation to the material inputs, product output and emissions. The mass allocation first determines the mass of each co-product generated per kg of the main product resulting from the process and generates an allocation factor representing the main product's proportion of all outputs except emissions, then calculates the environmental impacts of each material. The next step is multiplying the allocation factor with all the inputs and emissions, and summing up the environmental impacts which have been already multiplied to get the results of 1 kg of the main product needed. Last but not least, apply the same calculation methods into multi-processes and repeat the iteration processes until the production of the perovskite PV module.

PbI_2

As shown in this figure 4.4, the manufacturing process of PbI_2 material is illustrated. In the flowchart, the red broad arrow represents heat energy, the blue broad arrow represents electricity energy, the green thin arrow represents input materials, the purple thin arrow represents co-products, the black thin arrow represents product process and the black bold product represents the output wanted.

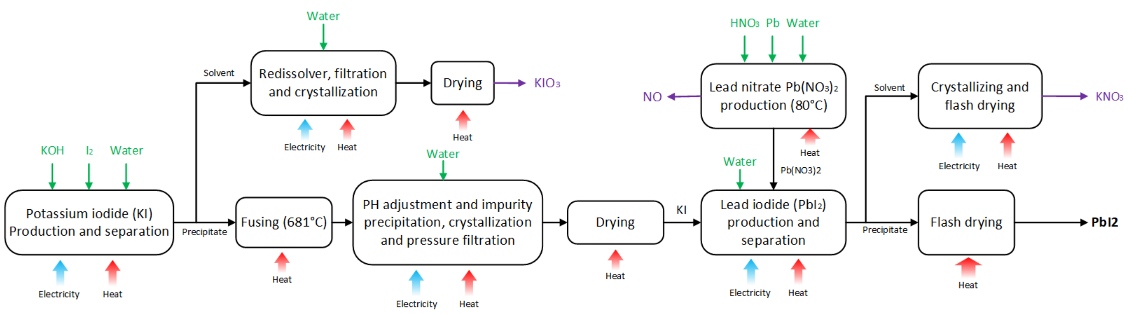

Figure 4.4: Manufacturing process of PbI_2

Although the inventory does not indicate water input or output, the relevant heat consumption for distilled water is taken into account when calculating the cumulative energy consumption in terms of heat [46]. The commercial production of potassium iodide and lead nitrate is predicated on the previous research [57][58]. The input materials are potassium hydroxide (KOH), water, and iodine(I_2), and the outputs are required PbI_2 product, a precipitate product mainly consisting of potassium iodate (KIO_3) and a solvent product mainly consisting of potassium iodide (KI) [58].

FTO Glass

The flowchart 4.5 demonstrates the production steps of FTO Glass, with chemical reactions and physical heating technologies. In the material inventory of FTO Glass, some reasonable replacement of materials is conducted to improve the manufacturing process. For instance, use sodium silicate to replace soda ash because sodium silicate has adhesive properties and can provide better protection against corrosion and is more controlled in pH than soda ash [59]. Glass bottles (recycled) are chosen to replace cullet due to the lower melting point of the raw material, which causes lower energy environmental-friendly [60].

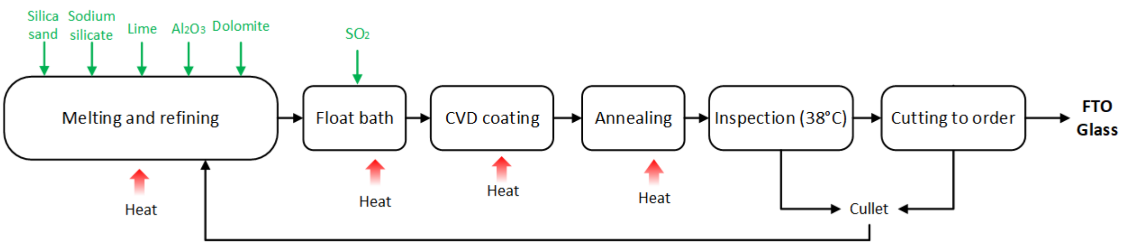

Figure 4.5: Manufacturing process of FTO Glass

Spiro-OMeTAD

The production of Spiro-OMeTAD can be divided into two stages. The first stage involves the production of 2,2′,7,7′-tetrabromo-9,9′-spirobifluorene as mid-product, and using the mid-product to generate Spiro-OMeTAD in the second stage. As shown in figure 4.6, the technical routes of production of Spiro-OMeTAD are based on Yuans thesis [61].

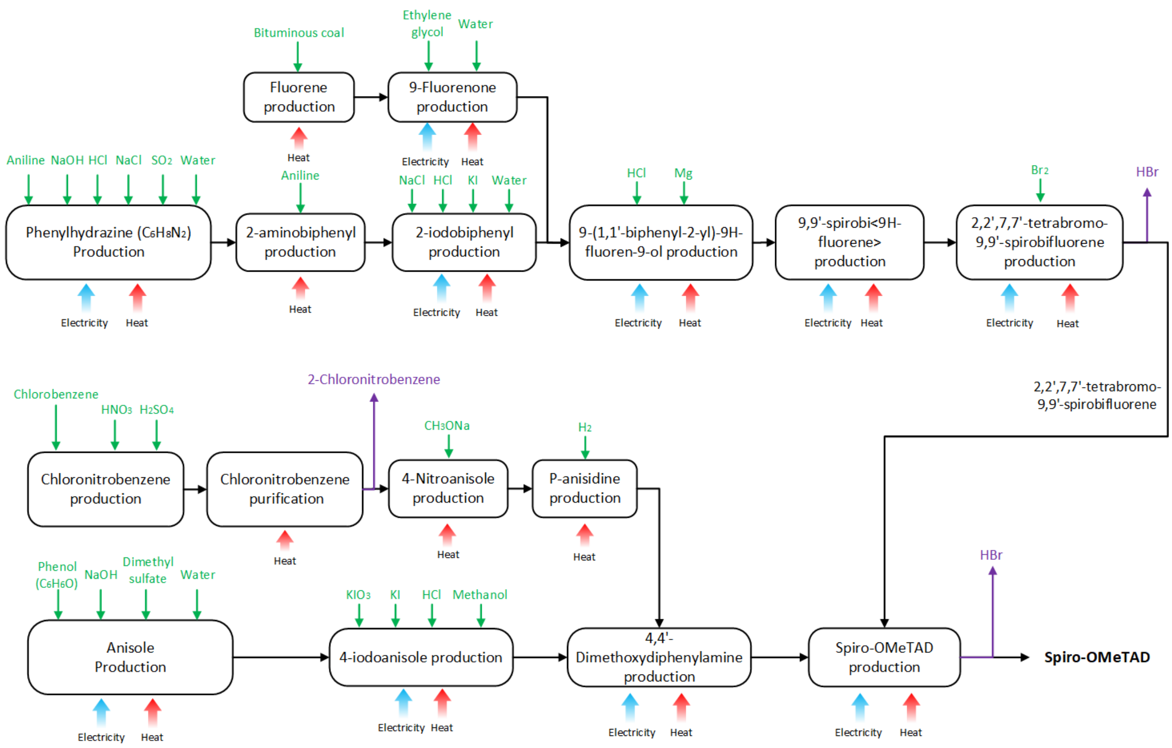

Figure 4.6: Manufacturing process of spiro-OMeTAD

In the material inventory of Spiro-OMeTAD, due to the lack of data of sodium nitrite ($NaNO_2$) in databases, the inventory considers replacing $NaNO_2$ with sodium chloride (NaCl), since NaCl is more cost-effective and has similar chemical properties to $NaNO_2$ [62]. The inventory data of KI is self-calculated based on the chemical reaction $3\,I_2 + 6\,KOH \longrightarrow 5\,KI + KIO_3 + 3\,H_2O$. Similar to PbI_2, the inventory does not include water input or output but the relevant heat consumption for distilled water [46].

CH_3NH_3I

The production of CH_3NH_3I material requires the production of 57% hydriodic acid (HI) as indicated in figure 4.7, iodine, hydrogen sulfide(H_2S) and water are used to generate hydriodic acid [63]. Meanwhile, co-product sulfur(S) is generated after the separation of solid sulfur. The life cycle impact assessment results are obtained by allocating the environmental effects of the manufacturing process based on the mass of the co-products. In the material inventory of $CH_3NH_3IPbI_3$, hydrogen sulfide, iodine and methylamine as input materials are self-calculated from Ecoinvent V3.8 database since they are not listed in the Idemat 2023 database. Both electricity and heat are considered as energy consumption during the manufacturing process, for example, evaporation to 50°C requires necessary heat energy [46].

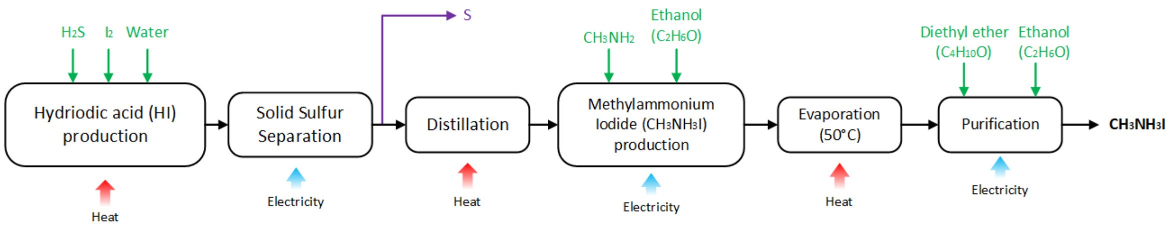

Figure 4.7: Manufacturing process of CH_3NH_3I

4.3.3. Energy inventory of perovskite PV module

Energy inventory describes the energy consumption of the manufacturing process of a PV module. To differentiate from the energy consumption in material inventory, energy inventory introduces the energy consumption of different manufacturing process steps, for instance, some machines require electricity to be operated. In this study, all the energy is described in terms of electricity or heat, and the whole process can be divided into seven steps specifically, as discussed in section 4.2.3. In the energy inventory of the studied perovskite PV module, all the processes are operated by electric equipment, which illustrates the power and time multiplied to evaluate the energy consumption, as shown in the table 4.3 below.

Manufacturing process	Power (W)	Time (s)	Energy (MJ)
1. Substrate patterning			
Ultrasonic cleaning	1450	1200	1.74
Screen printing	6420	6	0.04
Sintering	3050	1800	5.49
2. Blocking Layer (BL) deposition			
Spray pyrolysis	130	26.5	0.00
3. Electron-transport Layer (ETL) deposition			
Screen printing	6420	6	0.04
Sintering	3270	1800	5.89
4. Perovskite layer deposition			
PbI2 spin coating	20200	40	0.81
Sintering	355	3600	1.28
5. Hole-transport Layer (HTL) deposition			
Spiro-OMeTAD spin coating	26900	30	0.81
6. Cathode deposition			11.90
7. Encapsulation			0.01
Total			**28.00**

Table 4.3: Energy Inventory of the manufacturing process of the perovskite module [46]

The first step is substrate patterning and cleaning, including ultrasonic cleaning, screen printing and sintering procedures [46]. The second step is blocking Layer deposition, and the spray pyrolysis process takes up the energy consumption mostly in terms of heat. Next followed by Electron-transport Layer deposition, in which screen printing and sintering are operated again. Perovskite layer deposition is the fourth stage, which includes the PbI_2 spin coating technology and sintering [46]. The fifth step is Hole-transport Layer deposition consists of spiro-OMeTAD spin coating and thermal evaporation, which causes both electricity and heat consumption [46]. Cathode deposition and encapsulation are simplified to calculate only in the energy aspect, due to the uncertainty about data.

4.4. LCIA of the perovskite PV module

In the manufacturing stage of the perovskite PV module, as introduced previously, Life cycle impact assessment is carried out through three important phases, which are selecting impact categories, identifying category indicators, and undertaking characterization. The first phase, the selection of impact categories, in manufacturing primarily involves processes like material processing, module assembly, and transportation. This helps identify where significant environmental impacts may occur within the manufacturing stage. Secondly, category indicators are decided upon which allow us to quantify these impacts. Greenhouse gas emissions, waste generation, energy consumption, and water usage, among others, serve as key indicators for manufacturing impacts [39]. They offer quantifiable measures of the environmental burdens associated with the manufacturing processes. Lastly, the characterization step associates the collected data from each category indicator with its respective environmental impact. For example, CO2 emissions are linked to global warming potential, waste generation is tied to landfill impacts, and water usage is related to water scarcity. Through this stage, one can fully understand and interpret the environmental repercussions of the manufacturing process. By combing these three LCIA points, the PV module's manufacturing stage's environmental impact is thoroughly assessed, offering invaluable insights for improving environmental efficiency and mitigating impact in future iterations of the module.

4.4.1. Selection of impact categories in this study

There are different types of life cycle impact categories used in LCIA, these categories are related to different LCIA methods. Different techniques are used to assess different impact areas, based on the main goals of the study. Certain standards may ask for a specific LCIA method to be used or require that certain impact areas be reported on. Currently commonly used LCIA methods are CML (Centre of Environmental Science of Leiden University), Eco-Indicator 99, ReCiPe, ILCD (International Life Cycle Data), etc. Each LCIA has different measuring standards, perspectives and focuses.

Impact Category	**Abbreviation**	**Unit**
Global warming potential (GWP100a)	GWP	kg CO_2 eq.
Abiotic depletion	ADPe	kg Sb eq.
Abiotic depletion (fossil fuels)	ADPf	MJ
Acidification	AP	kg SO_2 eq.
Eutrophication	EP	kg PO_4 eq.
Ozone layer depletion	ODP	kg R-11 eq.
Photochemical oxidation	POCP	kg C_2H_4 eq.
Freshwater aquatic ecotoxicity	FAETP	kg 1,4-DB eq.
Human toxicity	HTP	kg 1,4-DB eq.
Marine aquatic ecotoxicity	MAETP	kg 1,4-DB eq.
Terrestrial ecotoxicity	TETP	kg 1,4-DB eq.

Table 4.4: Impact categories for CML-2001 [64]

Before making the decision of which LCIA method is appropriate, more information about these LCIA methods should be known. The CML method is based on a problem-oriented approach, which means it focuses on the existing environmental problems and assigns impact categories accordingly [64]. It includes numerous impact categories, including global warming potential, ozone depletion potential, human toxicity, and acidification. Although the research range of CML is wide, CML focuses more on specific environmental issues like global warming potential, ozone layer depletion, and acidification, which may be challenging to analyze the different products and environments in a comprehensive way. The Eco-Indicator 99 is an LCIA method developed by PRé Consultants in the Netherlands. As a damage-oriented method, it aggregates all potential environmental damages from raw material extraction to disposal into a single score [65]. This approach allows for a straightforward and easier comparison of products or processes' environmental impact, thus facilitating informed decision-making in design and policy [65]. Even if Eco-Indicator 99 is comprehensive and easy to compare, it can also conceal the nuances of different types of environmental impact, which may lead to oversights in specific areas.

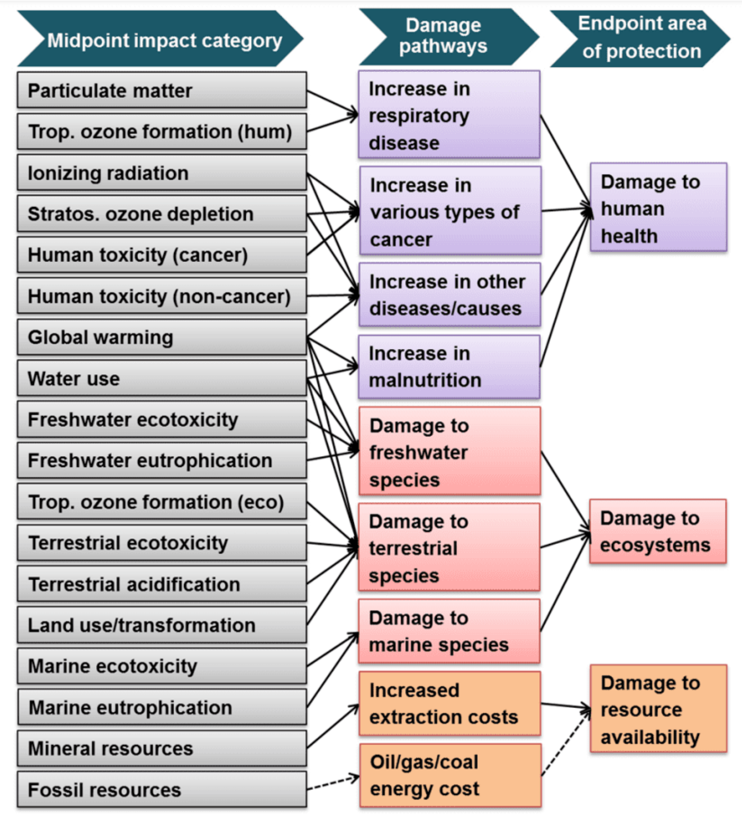

Figure 4.8: Impact categories for ReCiPe 2016 [66]

When the ReCiPe method is introduced, it is also created by PRé Consultants, the Dutch National Institute for Public Health and the Environment (RIVM) and Radboud University in the Netherlands [66]. ReCiPe combines and updates the CML and Eco-Indicator 99 methods and it provides users with the option to choose between midpoint and endpoint indicators, facilitating an adaptable analysis based on different perspectives, namely Hierarchist (H), Egalitarian (E), and Individualist (I) [66]. Currently the most updated ReCiPe model is ReCiPe 2016, as shown in figure 4.8. Compared to the originally released version of ReCiPe 2008, ReCiPe 2016 improves with more recent data, refined impact categories and updated characterization factors reflecting new scientific knowledge. Basically there are 18 midpoints, 9 damage ways and 3 endpoints, which highly aligns with the Idemat 2023 and Ecoinvent V3.8 databases.

Applied to this LCA study, the selection of life cycle environmental impact categories is combing CML-2001 and ReCiPe 2016 together, focusing on the three categories: Climate change, Human toxicity and Resource use (fossil). Among most of the impact categories, these three are all included in the LCIA method, which makes the selection more representative and persuasive. It is not practical to exert LCIA studies on each life cycle environmental category, due to the limitation of research time, so finally the three most essential categories are determined. It's worth noting that resource use has different kinds of categories in LCIA method, such as mineral and metals, fossil, and energy carriers, but only fossil takes MJ as the basic unit. For the manufacturing of perovskite solar cells, it's less complicated and more appropriate to choose resource used (fossil), to conduct the life cycle analysis on the environmental influence. More reasons why this study chooses these three impact categories are shown as follows:

- **Climate change:** This is a critical category due to the global significance of climate change and the high contribution of human activities to it. Various activities, such as burning fossil fuels for energy, deforestation, industrial processes, and waste disposal, emit greenhouse gases (GHGs), which increase the Earth's average temperature, leading to a multitude of negative impacts. The unit of climate change is kg CO_2 eq. Including climate change in an LCA can help identify the most significant sources of GHG emissions in a product's life cycle and inform strategies to reduce them. In this study, the manufacturing process of perovskite solar cells causes greenhouse gas emissions, for instance, the extraction and processing of raw materials necessary for perovskite solar cells could involve CO2 emissions, like lead and tin, which require energy-intensive mining and refining processes that often rely on fossil fuels.
- **Human toxicity:** This impact category relates to the release of substances that can harm human health, either through direct exposure (e.g., from air or water pollution) or indirectly (e.g., through the product chain) [67]. In some databases' categories, human toxicity is also indicated as non-cancer human health, like Ecoinvent V3.8. The production and use of many products involve the release of toxic substances, and an LCA can help identify the stages of the life cycle where these releases are most significant. This information can guide efforts to reduce these impacts, for instance, by substituting harmful substances with less harmful ones or improving waste management practices. In this study, human toxicity is calculated as a Non-cancer health category in databases. Take PbI_2 as an example, lead is a well-known toxic substance that can cause serious health problems, including neurological damage. The unit of human toxicity applied in the LCIA is CTUh, it's worth noting that the original unit used in the literature is kg 1,4-DCB-eq, so the unit conversion from kg 1,4-DCB-eq to CTHh is necessary to make, referring to [68].
- **Resource use (fossil):** Fossil fuels (coal, oil, natural gas) are finite resources that are heavily used for energy in many industries. They are linked not only to climate change but also to various environmental and social problems, such as air pollution, water pollution, habitat destruction, and conflicts over resource control. An LCA that includes this category can help identify opportunities to reduce fossil fuel use, for instance, through energy efficiency improvements or substitution with renewable energy sources, like improvements in perovskite photovoltaic modules. In this study, the resource use (fossil) can happen in the raw material extraction, the synthesis of perovskite and cell fabrication, etc, which are all indicated in MJ.

5 Results and Discussion

Previously section 4.3 introduces the process of how to create a life cycle inventory in this study. In this chapter, the results and comparisons of the selected perovskite solar modules are analyzed and discussed. Generally, the results are illustrated in three different types of PV modules: one is the selected perovskite PV module with silver cathode, one is the same type of selected perovskite PV module but with gold cathode, and the other one is the original perovskite module designed by the literature [46]. At the beginning of this thesis report, one question was raised:

What are the environmental impacts on the manufacturing of perovskite solar cells?

The descriptions and explanations on implementing the LCA method in the production of PSCs can be found in Chapter 3 and Chapter 4. To answer the environmental impact question, this chapter analyzes the results of LCA inventory and LCIA and compares the life cycle environmental impacts with different material cathodes and the literature's result in section 5.1. The results and figures are introduced by material inventory, energy inventory and the total impacts. In section 5.2, based on the different life cycle performance between modules with gold cathode and silver cathode, it's crucial to dive into the sceneries behind. Section 5.3 explores the materials and energy consumption by contribution analysis, displayed in three categories studied respectively. Besides, in section 5.4 the thesis also compares the perovskite solar module with different types of c-Si solar modules, which are separately framed back-sheet (G-BS) modules and frameless glass-glass (G-G) modules, and see how the perovskite solar module performs in LCA compared to other modules. Finally, section 5.5 lists some research implications and future advice.

5.1. Comparison of total life cycle impact

This section describes the LCIA results in material inventory, energy inventory and total life cycle (material + energy) inventory. In this section, the comparison between three different modules is operated in percentage. To make this study's results more intuitive and comparable, for the material and total impacts, the literature's results are all set to be 100% in climate change, human toxicity and resource use (fossil), and for the energy consumption during the manufacturing process of perovskite module, the results are shown in absolute value (MJ). All the calculations and figures shown are based on the functional unit.

5.1.1. Material environmental impact analysis

As introduced before, the main difference between this study's TiO_2 PV module turns out in the material inventory. Subsection 4.3.2 clearly indicates the changes of materials in the life cycle material inventory. Now focus on the material inventory, the environmental impacts (%) for manufacturing a 20-year lifetime perovskite module when generating 1 kWh electricity as the functional unit is shown in figure 5.1.

Compared to the literature's results, the environmental impacts of PV module with gold cathode in material performs relatively high, which can be explained in two aspects. First, The difference between different databases is the main reason for the comparison. Furthermore, the literature chooses Ecoinvent V3.1 as the database, an older version of Ecoinvent database. During the last several years, Ecoinvent V3.8 kept on adding changes to update the older versions. Meanwhile, this study combines the Ecoinvent V3.8 and Idemat 2023 together to create the life cycle inventory, and Idemat 2023 also has a statistics gap with Ecoinvent database series, more details have already been introduced in subsection 4.3.1. Take climate change as an example, the LCA value of 1 kg gold in Idemat 2023 is 1.79 E04 kg CO_2 eq, but in Ecoinvent V3.1 this value is 5.46 E03 kg CO_2 equivalent. Second, during updating the module and creating the own inventory, the replacements or improvements to the literature module caused the difference between the perovskite PV modules from this study and the literature, even though they both select gold metal as cathode.

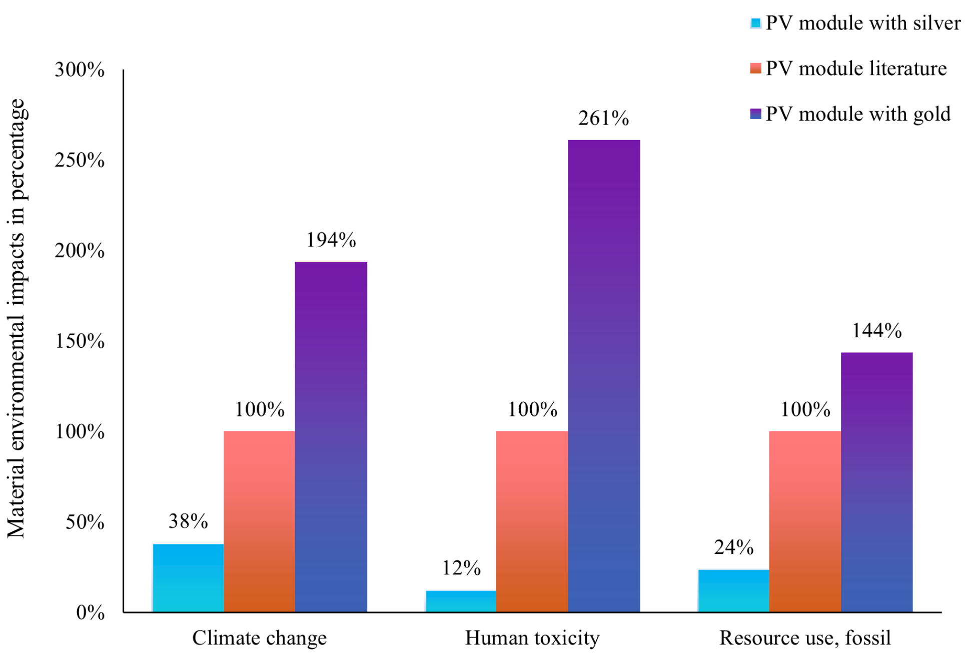

Figure 5.1: Material use related environmental impacts (%) of three perovskite modules relative to the literature reference

According to the figure 5.1 above, it's clearly illustrated that the perovskite PV module (with silver cathode) shares the lowest life cycle material impacts in all three impact categories. Compared to the literature's 100%, the selected module with silver cathode shares 38%, 12% and 24% of the climate change, human health and resource use (fossil) respectively. From the absolute value's perspective, the perovskite module shows 3.57E-03 kg CO_2 equivalent in climate change, 1.14 E-10 CTUh in human toxicity and 4.09 E-02 MJ in fossil use, which are all less than half of the literature's value. This means the changes and improvements to the original literature's life cycle inventory turn out to be positive generally. However, compared to the result of the PV module with silver cathode, the selected perovskite PV module (with gold cathode) takes up the highest proportion, for instance, the gold-cathode perovskite module has 194% in climate change and 261% in human toxicity, which indicates the large difference between these two modules both with a gold cathode. Based on the material inventory, the only difference between these two modules is the metal of cathodes, so the reason for the large difference in LCA results should only focus on the difference of cathodes. The reason can be explained by the difference LCA values between material gold and silver. Specifically, in Idemat 2023, the LCA values of silver (1 kg) are 1.24 E02 kg CO_2 eq, 2.81 E-05 CTUh and 1.54 E03 MJ in climate change, human toxicity and resource use (fossil) respectively, but values of gold per kg are 1.79 E04 kg CO_2 eq, 2.83 E-03 CTUh and 2.54 E05 MJ separately, which indicates the huge difference of this two metals in the same original database. Generally, from the figure 5.1, this thesis's selected perovskite PV module with the silver cathode has the lowest environmental impacts in material inventory, which shows the environmentally-friendly application of silver cathode.

5.1.2. Energy consumption environmental impact analysis

To make the comparison more concentrated on the material side and homogeneous, in this thesis, three different PV modules choose the same energy consumption inventory. The specific energy consumption calculated in MJ during the manufacturing process of the studied PSC is shown in table 4.3, which clearly indicates seven steps of producing a 20-year lifetime perovskite solar module when generating one kWh electricity as the functional unit, they are separately substrate patterning, blocking layer deposition, electron-transport layer deposition, perovskite layer deposition, hole-transport layer deposition cathode deposition and encapsulation. All operations are conducted by using electric equipment and all energy is calculated in MJ, which is consistent with Gong's energy inventory [46]. Combining the energy inventory with the life cycle impacts in Idemat 2023 database, the LCA of energy consumption during the manufacturing seven steps are illustrated in figure 5.2.

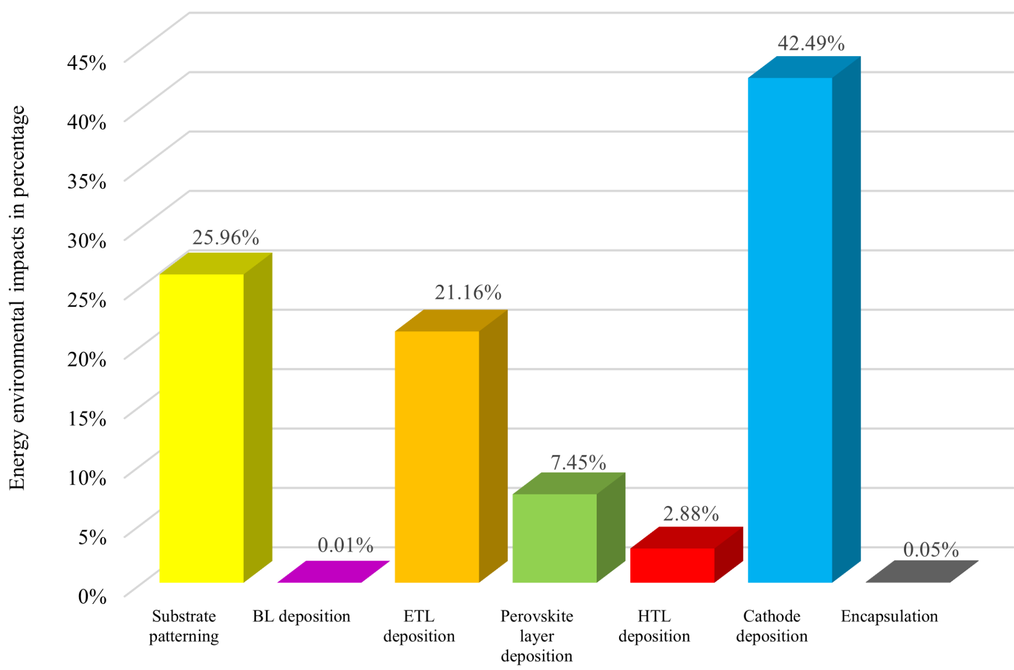

Figure 5.2: Energy consumption related environmental impacts (%) relative to the literature reference

According to the figure, the highest energy consumption happens at the cathode deposition phase which contributes 42.29%, this can be explained by the vacuum-based process during cathode deposition. For instance, some cathode materials, especially metal electrodes like gold or silver, are deposited using vacuum-based processes such as thermal evaporation or sputtering [69]. The thermal evaporation requires an evaporator as equipment, it works by heating the material to be deposited to its evaporation temperature in a vacuum, allowing it to condense on the substrate. Creating and maintaining a vacuum requires energy, and the deposition process itself can be energy-intensive. Besides, the high processing temperature also requires energy to heat the substrate or deposition sources, which may lead to the second-highest 25.96% energy consumption of substrate patterning. As discussed previously in subsection 4.3.3, all the energy consumption is evaluated in terms of electricity or heat. Compared to other deposition processes, the spray pyrolysis applied in the blocking layer deposition shows a considerably low value in energy consumption, which can be explained by the low operating temperature, simple equipment without complex vacuum systems and rapid film formation [70]. According to the evaluation by Espinosa *et al* [71], the encapsulation values are close to zero, since the encapsulation process doesn't require too much electrical equipment to consume electricity.

Compared to material inventory, the energy consumption during the seven manufacturing processes takes up 27% and 38% out of the total impacts in climate change and resource use (fossil) categories, but 0.0048% in human toxicity category. Idemat 2023 database determines the human toxicity value of electricity produced (EU) is relatively low since they are mainly generated from renewable energy or low-emission sources like wind, solar and hydrogen, which does not exert too much influence on human health. Hence, compared to climate change or resource use (fossil), the energy contribution to human toxicity in the manufacturing of perovskite solar cells can be negligible.

5.1.3. Life cycle environmental impact analysis

In this study, for the manufacturing process of perovskite solar modules, life cycle environmental analysis combines the material environmental impact analysis and energy environmental impact analysis together.

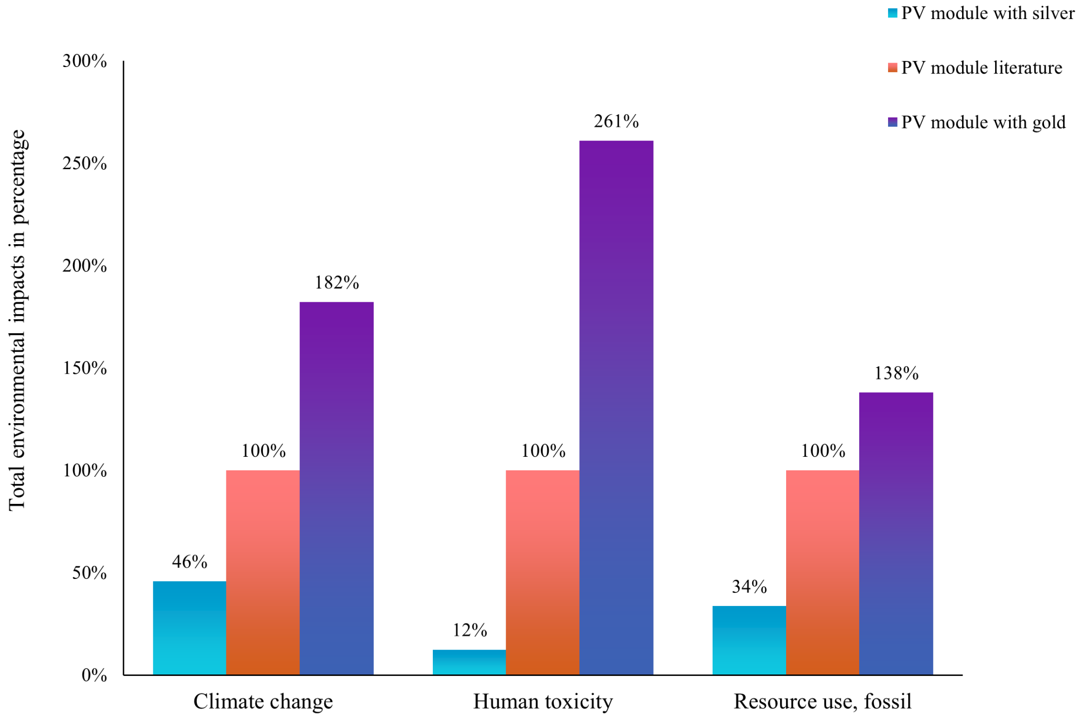

Figure 5.3: Total environmental impacts (%) of three perovskite modules relative to the literature reference

As illustrated in figure 5.3, the total amount of life cycle environmental impact for manufacturing a perovskite module is shown in percentage. The results are calculated in the functional unit, which is per kWh electricity generated by each module, and measured in three categories. For better comparison, the results are shown in percentage in this figure. Similar to material environmental impact analysis, the literature's results are set to be 100% in climate change, human toxicity and resource use (fossil). Compared to figure 5.1, the total life cycle impacts are higher than the material inventory in climate change and resource use (fossil), which can be explained by the energy consumption taking up a part of total impacts, just as discussed in section 5.1.2. For human toxicity, the values share the same 12% percentage as material analysis. This is due to the small amount of energy inventory in human toxicity, for instance, energy consumption takes up 1.30×10^{-3} kg CO_2 equivalent in climate change, 5.50×10^{-15} CTUh in human health, 2.54×10^{-2} MJ in resource use (fossil), which means the scale of the energy part is less than 1000 times the material part, so figure 5.3 shows the same percentage in human toxicity. Even though the percentage of the PV module with gold cathode has a slightly lower percentage in climate change and resource use (fossil), the total environmental impact of three modules shows a similar trend as material inventory. Generally, compared to the original literature's LCA results in 2015, the selected perovskite PV module (with silver cathode) in this report succeeds in reducing the environmental impact of LCA study, which reaches the goal of sustainable energy and decarbonization.

Since the thesis is based on the assumptions made previously, it's essential to discuss the results with respect to these assumptions. For example, the thesis chooses the same module efficiency as the literature's for simplification and better comparison. Due to the rapid development of technologies, there exist commercialized perovskite solar cells with higher efficiency up to 16% [72]. If applying this efficiency to the thesis model, to generate the same 1 kWh electricity of one perovskite module, the coefficient of unit conversion from literature will be smaller, which would lead to lower environmental impacts. Besides, the thesis choose 1391 kWh $\mathrm{year}^{-1}\mathrm{m}^{-2}$ as the average EU irradiation, if the solar modules are implemented in the southern Europe area with higher solar energy resource, the coefficient of unit conversion will be lower to generate 1 kWh electricity, which finally gives rise to lower LCA results in this study.

5.2. Comparison between modules gold and silver cathode

After discussing the LCA results of three different perovskite solar modules, there is a large difference in life cycle impacts between the gold cathode and silver cathode, it's necessary to take a deeper dive into the reasons behind. The figure below lists the top five components that contribute to the largest environmental impacts of each PV module and the rest are calculated in the 'Others' element. One big improvement on the updated $\mathrm{TiO_2}$ perovskite solar module is to choose silver as a cathode instead of gold. Gold is a commonly used metal in $\mathrm{TiO_2}$ perovskite solar cell manufacturing, more specifically made as the cathode of PV modules. Applying gold as the cathode of one PV module has some advantages, for instance, excellent conductivity makes gold transfer generated charge carriers efficient, and gold may provide better interface contact with certain perovskite materials [73]. However, the usage of gold is not practical and commercial, since the price of gold is very expensive. Meanwhile, the environmental impacts of gold are relatively unsustainable, which will be discussed in this section later. Even though most of the perovskite solar cells are still not in the commercial stage, this study prefers the manufacturing process of PSC to be more feasible, so both from the economic and environmental perspective, gold is not the best option. Among all the metals, silver has the highest electrical conductivity, which can facilitate excellent charge transfer [74]. Compared to gold, silver is less expensive lowering the production costs. Both gold and silver may diffuse into perovskite under thermal stress, which may degrade the device's performance over time. Therefore, the selection of silver to replace gold as the metal cathode in the manufacturing process of the studied perovskite solar module is determined.

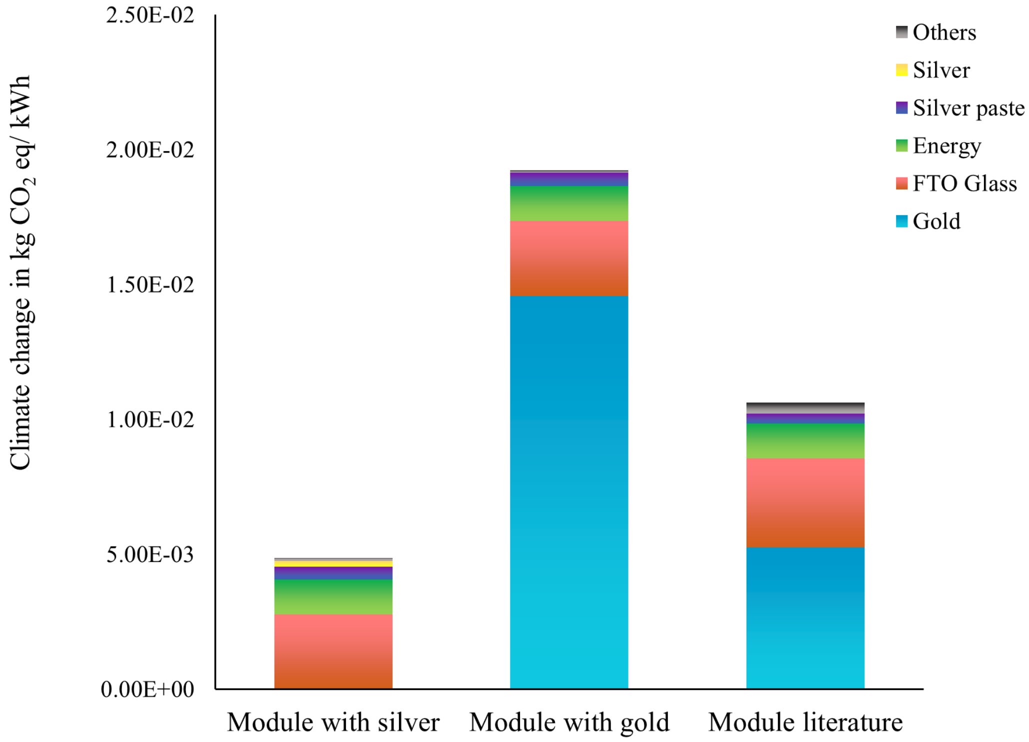

Figure 5.4: Climate change (kg CO_2 eq) impacts of three perovskite modules

Figure 5.4 indicates the climate change of updated perovskite PV modules with silver or gold cathode. From the vertical coordinate's absolute value, the difference between metal silver and metal gold is considerably huge. The climate change single indicator of gold material reaches a value close to 1.46 E-02 kg CO_2 equivalent, which is higher than the sum of all other contributions in TiO_2 module with silver cathode. This can be explained by the intensive mining processes and refinement processes of gold extraction. Meanwhile, the scarcity and geographic dispersion of gold also represent more extensive mining operations, leading to more carbon dioxide emissions, and contributing to climate change significantly. Therefore, from CO_2 emission's perspective, gold exerts more negative environmental impacts than silver. Besides, FTO glass production and energy consumption are the second and third highest elements in climate change analysis, which reaches the value of 2.78 E-03 CO_2 eq and 1.30 E-03 CO_2 eq separately. The production of FTO glass requires high processing temperatures and the synthesis and deposition methods of FTO glass, such as chemical vapor deposition, spray pyrolysis, or sputtering, can be energy-intensive [75].

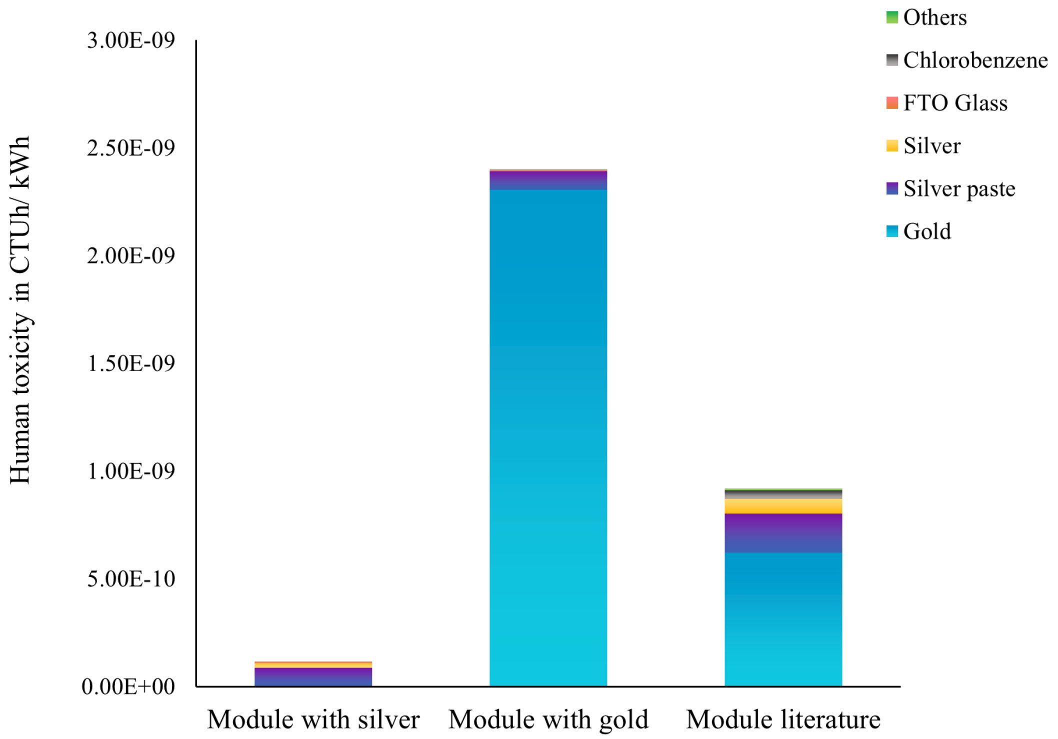

Figure 5.5: Human toxicity (CTUh) impacts of three perovskite modules

As illustrated in figure 5.5, the difference between perovskite modules with silver and gold cathode in human toxicity is relatively bigger displayed, for instance, in the perovskite module with gold cathode, the human toxicity of gold is 2.31×10^{-9} CTUh, which is more than ten times the sum of the rest. The reason why gold's human toxicity is heavy should be explained. Gold (primary) is relatively inert and does not pose significant human toxicity risks under normal conditions. However, the mining and extraction processes for gold often involve hazardous chemicals such as mercury and cyanide, which are highly toxic [73]. Improper handling or disposal of these substances during gold mining can result in contamination of water sources and soil, posing serious health risks to nearby human populations [76]. In this figure, energy consumption does not take up too much human toxicity, this may be because the electricity and heat generated in the basic forms are not inherently toxic to humans, so for human toxicity, the Idemat 2023 and Ecoinvent databases did not take electricity or heat into account.

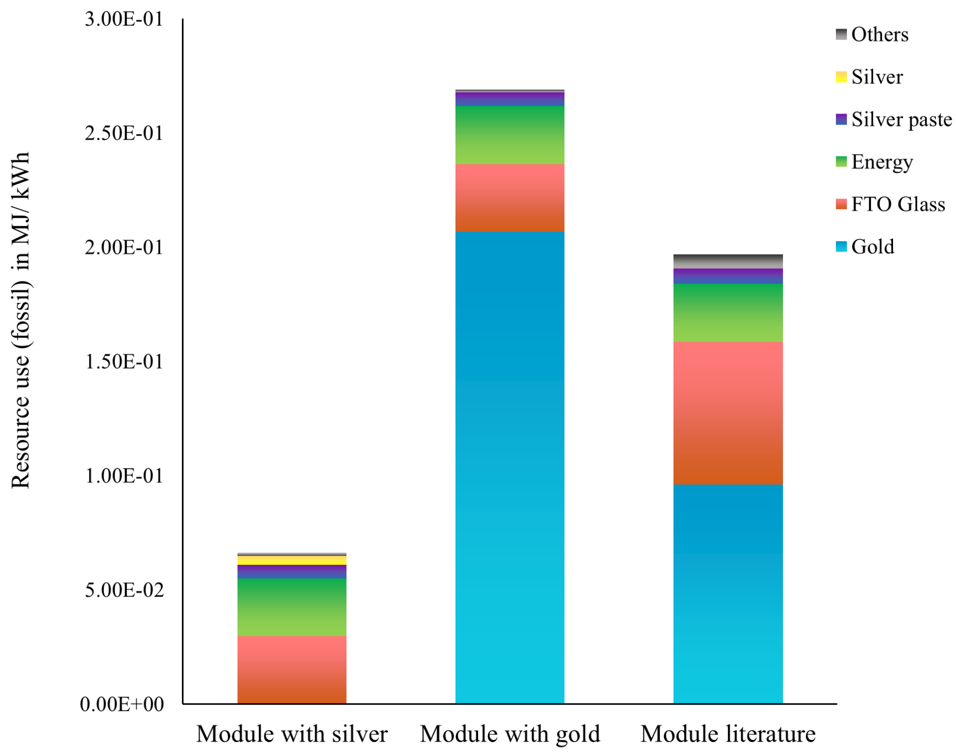

Figure 5.6: Resource use, fossil (MJ) impacts of three perovskite modules

Similar to climate change, gold, FTO glass and energy take up the highest three values in resource use (fossil). The absolute value of gold is 0.207 MJ, which is more than thirty times that of silver's 3.93 E-03 MJ. Comparable with the climate change category, gold is less abundant and more dispersed than silver in the Earth's crust, making the mining and refining processes for gold more energy-intensive. This energy is often supplied by burning fossil fuels, which leads to higher consumption of these resources for gold production.

From the three figures above, all indications are that the perovskite PV module with silver cathode has much lower life cycle environmental impacts than with gold cathode. From the environmental perspective, applying silver cathode is more sustainable and eco-friendly in every impact category studied. The results of climate change and resource use (fossil) show similar characteristics in the performance of LCIA results, which demonstrates gold contributes the most to each impact category, and FTO glass and energy consumed during the manufacturing process occupy the second and third contributions.

After figuring out that silver cathode has lower environmental impacts during the manufacturing process of perovskite solar modules, it comes up with a question: Do the same type of module with gold cathode and silver cathode have different efficiency? Do they have a huge difference? In solar cells, the role of metal electrodes (like silver or gold) is to form the electrical contact that allows the flow of electrons from the semiconductor to the external circuit, providing a low resistance path for the collected charge carriers [77]. Some recent studies show that some high-efficiency tandem perovskite solar cells have taken silver contacts into account [78]. Nevertheless, the choice of metal typically does not directly influence the efficiency of the solar cell in converting sunlight to electricity, which is more dependent on the semiconductor materials used (such as silicon, perovskite, etc.) and the design of the cell. For instance, the properties of semiconductor materials, such as light absorption, charge carrier mobility and bandgap, primarily determine the conversion ability efficiency of the solar module [79]. Therefore, in this study, assuming the perovskite module with silver cathode has the same efficiency as the one with gold cathode is reasonable. Besides, it's interesting to explore more alternative cathode materials like copper in the manufacturing process of solar modules in the future.

5.3. Contribution analysis

This section introduces the difference between the updated perovskite PV module (with silver and gold cathode) and literature [46]'s PV module. To clarify the structure of the perovskite PV modules and make the comparison more persuasive, the selected perovskite module refers to the same layer structure of the literature except for the cathode. However, as discussed previously in chapter 4, differences in databases and changes in the material inventory lead to differences in the updated PV module and literature module. For instance, among all the material inventory, cathode deposition plays the highest share in differences, specifically in the usage of gold or silver. Besides, the set-up of gold cathode and silver cathode aims to analyze the influence of gold and silver in LCA. The comparison is also conducted in the studied three categories, which are climate change, human toxicity and resource use (fossil) respectively. In this section, all the calculations of results are considered in percentage, in order to describe how significant the portion of each component takes in the production process of PSC. Same rules as previously, the results pick out the top five or six elements from the life cycle inventory, and the rest are added up as the element 'Others' in the figures below.

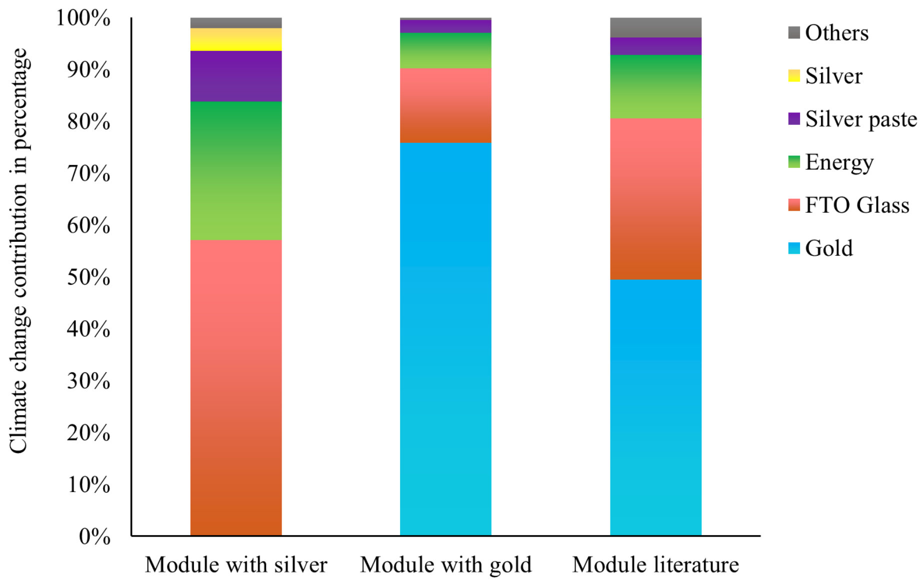

Figure 5.7: Contribution of climate change (%) of three perovskite modules

From figure 5.7, it is clear that FTO glass consumes the most CO_2 emissions in the updated perovskite module with silver cathode, and gold consumes the most CO_2 emissions in the both literature's module and updated perovskite module with gold cathode. In the module with silver, FTO glass takes up more than 50% of the total amount, and energy consumption is 26.7%. From the raw material perspective, FTO glass is made from high-purity tin(II) oxide (SnO) doped with fluorine, these raw materials are relatively scarce and the processes to refine them to the necessary purity are resource-intensive, which leads to the CO_2 emissions caused by relevant machines or factories during the refining process. In the modules with gold cathode, gold, FTO glass and energy consumption occupy the top three components in climate change successively. Note that silver and silver paste do not conduct too much environmental impact in climate change, which makes the studied PV module with silver cathode more advantageous.

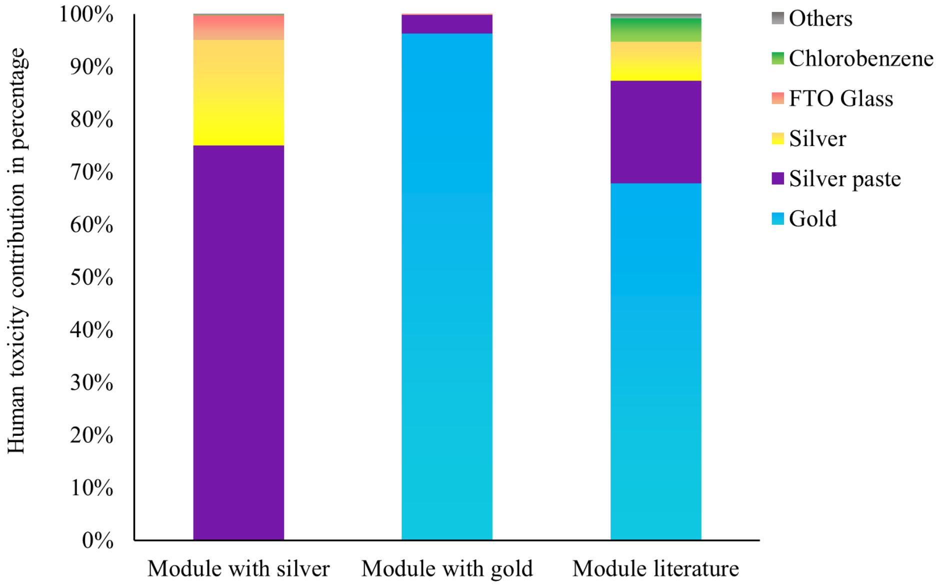

Figure 5.8: Contribution of human toxicity (%) of three perovskite modules

As shown in figure 5.8, the characteristics of human toxicity show quite different layouts in the perovskite module with silver cathode. Chemicals used in the production and processing of silver cathode and silver paste contribute significantly to human toxicity, for instance, silver mining and refinement often involve hazardous substances, and silver paste manufacturing may utilize potentially harmful organic compounds and solvents such as terpineol, ethylene glycol, etc [80]. These negative effects on human toxicity are considered in the original Ideamat 2023 and Ecoinvent V3.8 databases, and turn out in the percentage in figure 5.8. When it comes to the PV modules with gold cathode, gold still takes up the most significant portion of human toxicity, which is especially obvious in the selected perovskite module with gold cathode. Another aspect of the result is material C_6H_5Cl named chlorobenzene since it is the third highest percentage of 7.43 % during the manufacturing process of the module. As a solvent in the fabrication of perovskite solar modules, C_6H_5Cl's contribution to human toxicity is mainly embodied in the inhalation, ingestion, or skin contact with chlorobenzene, which can cause irritation and central nervous system effects such as dizziness or unconsciousness [81]. In addition, chronic exposure may result in liver, kidney, or lung damage. Even though the absolute value of human toxicity is considerably low compared to climate change or resource use, the human toxicity analysis significantly influences human health during the process of manufacturing. For example, in this study, the human toxicity evaluation includes assessing the toxicity of fluorine emissions compounds from FTO glass production.

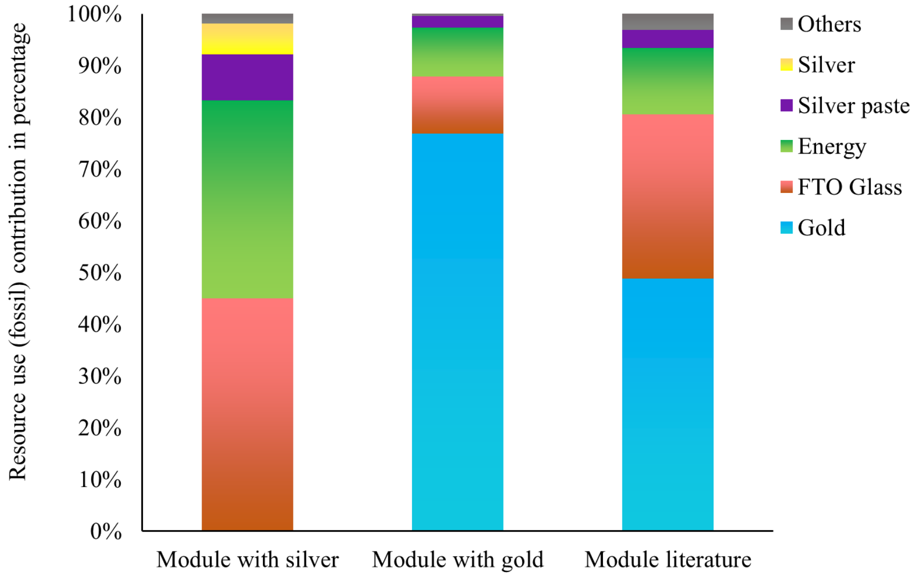

Figure 5.9: Contribution of resource use, fossil (%) of three perovskite modules

Similar to climate change, the life cycle impact on resource use (fossil) indicates that gold still occupies the main percentage of resource use, and the second and third highest contributions are FTO glass and energy consumption. From the percentage perspective, material gold in the total resource (fossil) use shows 76.83% and 48.81% in the selected module and literature module respectively. From the absolute value perspective, material gold shares 0.207 MJ and 0.096 MJ to generate 1 kWh of electricity in the selected module and literature module respectively. In the PV module with the silver cathode, the FTO glass substrate production costs 44.94% of the total energy resource use, as explained previously in section 5.2, high-temperature processing, synthesis and raw material extraction may cause the largest contribution in resource use (fossil). In addition, silver as the cathode material doesn't consume too much resource use in the selected PV module, which shares the percentage of 5.93%. Compared to gold, material silver in the databases all show quite low value in the resource use (fossil) aspect, this may explain the reason for the low contribution of silver.

Compared to climate change, environmental impacts in resource use (fossil) in both absolute values and contribution analysis show similar characteristics, as illustrated in fig 5.4, fig 5.6, fig 5.7 and fig 5.9. When diving into the reason why they look similar, the burning of fossil fuels to produce energy is a significant source of CO_2 emissions. When fossil fuels are consumed, they release CO_2 a greenhouse gas that contributes to climate change. Besides, a significant amount of energy production is still dependent on fossil fuel sources. Therefore, trends in energy consumption (MJ) from fossil sources would correlate with trends in CO2 emissions. For instance, in this LCA study of perovskite solar cells, if the manufacturing process is energy-intensive and primarily relies on fossil fuel based energy, both the CO2 emissions and fossil resource use would be high during the manufacturing stage, exhibiting a similar trend in the figures.

5.4. Comparisons with PERC PV modules in climate change

Once the LCIA results of manufacturing a perovskite solar module are calculated, it's necessary to compare this study's results with other types of PV modules, for instance, crystalline silicon (c-Si) glass-backsheet (G-BS) and glass-glass (GG) modules, to see how perovskite and c-Si solar cells perform in LCA. The reason why selecting these two crystalline silicon instead of multi-crystalline silicon is that it shares with a polysilicon market share of 65% in 2019 and an expected market share of 80% by 2030 [82]. Due to the availability of existing data, the comparison only focuses on the climate change category, as shown in figure 5.10 below. This section compares the perovskite solar module (with silver cathode) with G-BS and G-G modules which are separately manufactured in Europe and China. The data of c-Si modules is based on Mueller et al.'s research [83], and the functional unit keeps the same as this thesis's model which is CO_2 emissions in one kWh of electricity generated by each PV module over the lifetime. Both this thesis and the paper conduct a cradle-to-gate LCA assessment on the manufacturing process of a module. For these different PV modules, the different assumptions and parameters are listed in the table below.

Parameter	Unit	Perovskite module	G-BS module	G-G module
Lifetime (LT)	year	20.00	25.44	29.89
Performance ratio (PR)	%	80%*	85%**	85%***
Solar irradiation r	kWh/ $(\mathrm{m}^2\mathrm{yr})$	1391	1391	1391
Efficiency η	%	9.10%	19.79%	19.40%

* No DR is applied to this value, as Perovskite DR is still very unknown.
** DR 2.67% in the first year and 0.64% in the following year will be applied to this value.
*** DR 2.55% in the first year and 0.45% in the following year will be applied to this value.

Table 5.1: Overview of parameters and assumptions of different PV modules

According to table 5.1, the parameters or assumptions of three different PV modules are different except the solar irradiation. All the assumptions of perovskite solar module analyzed in this thesis are introduced in section 4.2.2 previously, and the parameters of c-Si solar modules are extracted from Mueller et al's research [83]. In Mueller et al.'s paper, the assumptions of module efficiency, lifetime and performance ratio of G-BS and G-G modules are based on the IEA LCA PV guidelines [51]. For the performance ratio (PR), the perovskite solar module keeps the same 80% as the previous assumption, and this value does not consider the degradation rate (DR) due to the unavailability of supporting data. The PR of G-BS and G-G modules including the DR is set to be 85% derived from the paper [83]. It's worth noting that the main purpose of this section is to generally evaluate how good the LCA performance of this thesis is compared with other types of solar cells, and different types of solar cells also vary in many other properties, so the comparison keeps the parameters as the original paper [83] without controlling variables.

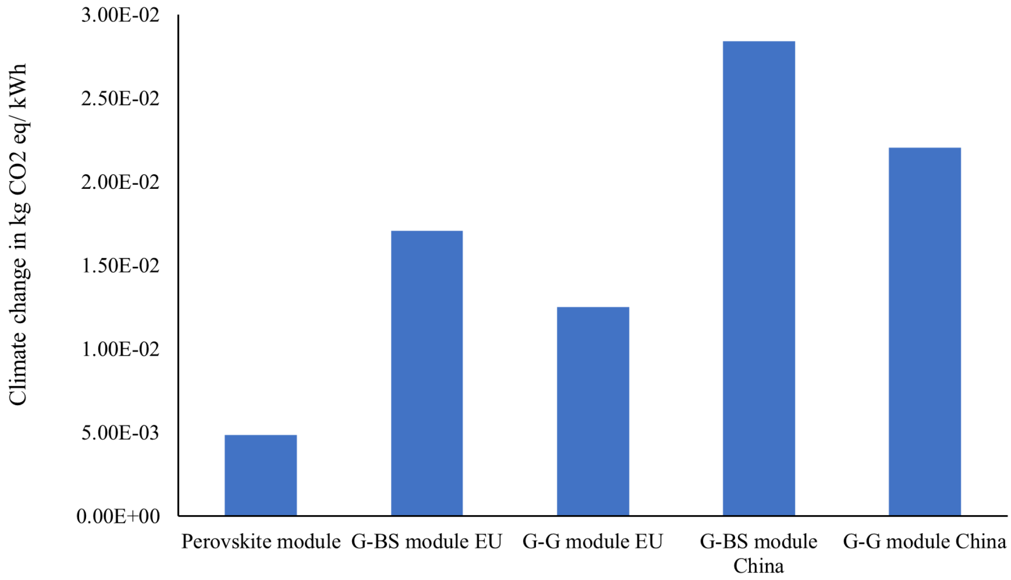

Figure 5.10: Comparisons with G-BS and G-G modules in climate change (kg CO_2 eq)

As illustrated in figure 5.10, the perovskite solar module has the lowest life cycle impacts in climate change to generate one kWh electricity, the value comes to 4.87×10^{-3} kg CO_2 equivalent. This result indicates that perovskite solar cells are less energy-intensive than typical c-Si cells, which demonstrates the commercialized perovskite module is more environmentally friendly from an LCA's perspective. The G-BS module has the highest CO_2 emissions among the three kinds of solar modules, this can be interpreted by the fact that the production of high-purity silicon material, crystalline silicon wafers involves substantial material waste and higher energy consumption. The reason why perovskite solar module has lower CO_2 emissions can be explained by the different raw materials and manufacturing methods from c-Si modules. For instance, the manufacturing of perovskite solar cells involves solution-based processes, typically conducted at lower temperatures compared to silicon cell manufacturing. Perovskite solar cells can be fabricated using methods like spin-coating or inkjet printing, which is more energy-efficient compared to the batch processes used for c-Si cells. Besides, from the raw material aspect, the manufacturing process of perovskite solar cells requires different materials from that of c-Si, for example, PSC doesn't need the high-purity silicon as raw material as c-Si modules, which explains less energy consumption and lower CO_2 emissions in climate change. Therefore, from figure 5.10's comparison, the perovskite solar module analyzed in this thesis has lower environmental impacts than the other two c-Si modules with the same functional unit, which aligns with the sustainable goal of reduction in CO_2 emissions. Certainly, this section only gives an initial LCA results comparison, further research on LCA in PSC and other types of solar cells should be made in the future.

5.5. Research implications

As perovskite solar cells continue to develop and scale up to commercialization, conducting LCA on their manufacturing process becomes crucial to evaluate the environmental impact. Embracing principles of the circular economy is fundamental, which means placing emphasis on the reuse, refurbishment, and recycling of materials, especially given the potential toxicity of some PSC components. Investing in R&D is paramount, not only to discover up-to-date non-toxic and more abundant material alternatives but also to innovate the manufacturing technologies that are less energy-intensive and environmentally negative, for example, roll-to-roll processing or inkjet printing could offer scalable and energy-efficient deposition techniques to replace lab-scale methods like spin-coating [84]. Moreover, optimizing module design can lead to material and energy conservation, while advanced sensors and automation can monitor and streamline manufacturing processes for minimal waste and energy use.

Simultaneously, LCA models should stay current, integrating real-time data and reflecting the latest material and technologies. Standardizing LCA practices will ensure global consistency, while transparency in publishing results promotes trust and industry-wide progress. Engaging diverse stakeholders, investing in continuous LCA training, and drawing insights from other industries will further enrich the assessment, ensuring that PSC developments remain aligned with environmental sustainability.

6 Conclusion

Perovskite solar cells have marked a promising shift in the development of PV technology recently. Applying the LCA method to the production of perovskite PV modules aims to assess the environmental impacts that happen during the whole production process. This thesis focuses on understanding the manufacturing of perovskite PV modules, conducting a cradle-to-gate life cycle assessment of chosen perovskite solar modules either with silver and gold cathode, also making the comparison with the LCA results from the literature and single-crystalline silicon modules.

The thesis begins with the selection of PSCs with mesoporous TiO_2 scaffold. Second, the thesis clearly defines the research goal, functional unit, assumptions and system boundaries of LCA, to define the range of the whole study. For instance, the research goal is to evaluate the environmental impacts on the manufacturing of perovskite solar cells, and the functional unit is set to be per kWh of electricity generated by one module over lifetime. After determining to combine Idemat 2023 and Ecoinvent V3.8 together as the original databases, this work creates the updated life cycle inventory, especially in the material aspects during the manufacturing process. Due to the limitation of existing LCI data, some of the materials cannot be derived from the databases directly, so the thesis makes some reasonable alternatives or improvements to calculate these unavailable materials. For the energy inventory of manufacturing PSCs, the thesis chooses the same energy inventory data for PV modules because of similar manufacturing technologies and the constrained availability of data. Following the selection of three life cycle impact categories (climate change, human toxicity and resource use, fossil), the LCIA results indicate the difference between perovskite modules with silver and gold cathode, showing that silver's lower environmental impacts than gold during the production of solar cells. The total results show that compared to the literature PV module's 100% percentage, the module with silver cathode takes up 46%, 12% and 34% in climate change, human toxicity and resource use (fossil) respectively. This can be explained by intensive mining processes and refinement processes of gold extraction. The thesis also analyzes the top five elements that contribute to the LCIA results and discusses the explanations of the characteristics shown in the figures. When analyzing modules with the gold cathode (selected module and literature module), the metal gold occupies the highest contributions in three categories, and FTO glass and energy consume the second and third contributions in climate change and resource use (fossil). Besides, the thesis makes comparisons with the LCA results of two single-crystalline silicon solar modules produced in EU and China, turning out perovskite solar modules have better LCA performance during manufacturing. Finally the thesis describes the research implications and provides potential advice for the future.

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