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Environmental impact assessment of hole conductor layer free and flexible organo lead iodide perovskite solar cell

Boşluk iletim tabakasız ve esnek organo kurşun iyodür perovskit güneş hücresinin çevresel etki değerlendirmesi

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Environmental Impact Assessment of Hole Conductor Layer Free and Flexible Organo Lead Iodide Perovskite Solar Cell

Highlights

- *In this work, a life cycle assessment of an Hole transport layer free and flexible (HFF) Perovskite solar cell is performed.*
- *Environmental impact values for each layer were determined in six ILCD (International Reference Life Cycle Data System) impact categories.*

Graphical Abstract

Figure 1 demonstrates the contribution of each PSC layer to every impact category. In five of the six environmental impact categories (except eutrophication), the Al metal electrode layer represents up to 70 percent of the total impact value.

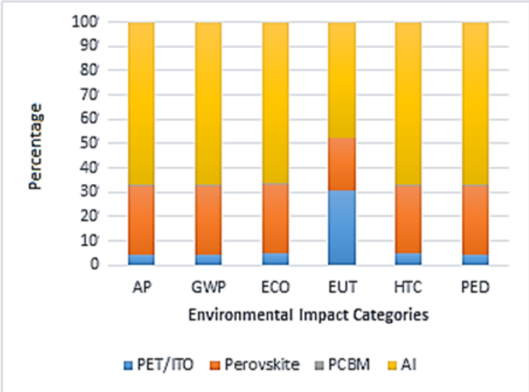

Figure. Share of total environmental impacts of each HFF PSC layers

Aim

The aim of this work is to determine the potential environmental impacts of a representative Hole transport layer free and flexible (HFF) Perovskite solar cell device that has 10% power conversion efficiency.

Design & Methodology

Six midpoint environmental impact categories in ILCD impact assessment model were used for impact assessment. All results were calculated with characterization factors provided by Gabi 8.1 software.

Originality

In this work, the life cycle assessment of an HTL-free flexible (HFF) PSC is performed for the first time in the literature.

Findings

In this work, it was found that the contributions of environmental impact values of PSC layers are largely in line with the amount of electricity required for fabrication (~ 90).

Conclusion

The results show that the majority of environmental impacts come from Al metal electrode deposition in all environmental impact categories. The high electricity consumptive vacuum-based fabrication process of the metal electrode is responsible for this high impact values.

Declaration of Ethical Standards

The author(s) of this article declare that the materials and methods used in this study do not require ethical committee permission and/or legal-special permission.

Boşluk İletim Tabakasız ve Esnek Organo Kurşun İyodür Perovskit Güneş Hücresinin Çevresel Etki Değerlendirmesi

Araştırma Makalesi / Research Article

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ÖZ

Perovskit güneş pilleri (PSC) esneklik ve düşük maliyetli rulodan ruloya üretim gibi avantajlarla birlikte son zamanlarda güç dönüşüm verimliliğinde de önemli bir ilerleme kat etmiştir. PSC'lerin ticarileştirilmesinden önce çevresel performansının yaşam döngüsü değerlendirme (LCA) yöntemi ile araştırılması önemlidir. Bu çalışmada, literatür verilerinden istifade edilerek, esnek Polietilen tereftalat (PET) alt tabaka ve boşluk iletim katmanı (HTL) eliminasyonunu içeren çözelti bazlı organo-kurşun iyodür perovskit güneş hücresinin beşikten kapıya yaşam döngüsü analizi (LCA) gerçekleştirilmiştir. 1 m2 hücre alanı üretiminden kaynaklanan çevresel etkiler altı Uluslararası Referans Yaşam Döngüsü Veri Sistemi (ILCD) kategorisinde belirlenmiştir. Analizin sonucunda, en fazla etki değerinin yüksek elektrik enerjisi tüketimine sahip vakum biriktirme işlemi gereksinimine sahip olan alüminyum metal elektrot tabakasının imalatından kaynaklandığı bulunmuştur. Ticari fotovoltaik teknolojilerle karşılaştırma yapabilmek için en yaygın kullanılan çevresel göstergelerden birisi olan küresel ısınma potansiyeli (GWP), birim kWh elektrik üretimi için hesaplanmıştır. Buna göre, bu çalışmada incelenen HTL'siz esnek (HFF) PSC'nin ticari PV'lerle rekabetçi GWP değerine ulaşmak için 15-20 yıl cihaz ömrüne ihtiyacı olduğu bulunmuştur.

Anahtar Kelimeler : Perovskit güneş hücreleri, yaşam döngüsü değerlendirmesi, fotavoltaik teknolojiler, sürdürülebilir enerji, çevresel etki analizi.

Environmental Impact Assessment of Hole Conductor Layer Free and Flexible Organo Lead Iodide Perovskite Solar Cell

ABSTRACT

Perovskite solar cells (PSCs) have shown a significant increment in power conversion efficiency recently with advantages such as flexibility and low-cost roll-to-roll production. Prior to the commercialization of PSCs, it is significant to investigate its environmental performance with life cycle assessment method. In this work, cradle to gate LCA of solution-based organo-lead iodide perovskite solar cell performed according to the one reported literature method that comprises flexible Polyethylene terephthalate (PET) substrate and hole transport layer (HTL) elimination. Environmental impacts from the generation of 1 m^2 of cell area production are determined in six International Reference Life Cycle Data System (ILCD) categories. It is found that the major impact comes from the fabrication of the aluminum metal electrode layer due to the high electrical energy required in the vacuum deposition process. The life cycle global warming potential (GWP) that the most widely used environmental indicator has been calculated for per kWh electricity production to make a comparison with commercial photovoltaic technologies. It is found that the HTL-free flexible (HFF) PSC needs 15-20 years of device lifetime to reach competitive GWP value with commercial PVs.

Keywords : Perovskite solar cells, life cycle assessment, photovoltaic technologies, sustainable energy, environmental impact assessment.

1. INTRODUCTION

Global energy demand has been increasing by the rising world population and advances in technology. It enhances the interest in renewable energy sources to meet this need and ensure environmental and economic sustainability. One of the most important renewable energy sources is solar energy with its large capacity and abundance. Photovoltaic (PV) technologies are systems that convert photon energy emitted from the sun into usable electrical energy. PV technologies are categorized as first-generation crystalline silicon technology, second-generation thin-film technology, and third or next-generation technologies such as organic, dye sensitize, and perovskite.

PSC technology stands out among third-generation solar cells due to its high efficiency and cheap production. Despite fast power conversion efficiency development recently, there are some problems in cell architecture that prevent the commercialization of PSC technology. One of these obstructions is Spiro-OMeTAD which is widely used as Hole Transport Layer (HTL) creates negative effects on PSC cell stability [1]. The other is high electricity

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consumptive vacuum-based fabrication techniques used in perovskite active layer production [2]. Therefore, HTL-free solution based PSC architectures have been studied recently [3]. Besides, replacing the rigid glass substrate with flexible materials led to the production of cheaper and portable PSC devices [4]. Although these eliminations cause some loss of efficiency in device, it has many advantages in terms of ensuring cell stability and cost.

Before the commercialization of PSCs, it is important to quantify its environmental performance with LCA tool. In this work, the life cycle assessment of an HTL-free flexible (HFF) PSC is performed for the first time in the literature. First, the environmental impact values (per m^2) for each layer were determined in six ILCD (International Reference Life Cycle Data System) impact categories. Secondly, GWP (global warming potential) impact value converted to 1kWh electricity production to compare this value with those of commercial PVs.

2. MATERIAL and METHOD

LCA is a method that has its ISO standard that is used to assign the environmental impacts of products [5]. It comprises four stages, which are goal and scope definition, inventory analysis, impact assessment, and interpretation.

The goal of this work is to determine the potential environmental impacts of a representative HFF PSC device that has 10% power conversion efficiency [6]. The which is deposited on a glass substrate and serves as a front electrode, an electron transport layer (ETL) has electron mobility that allows electron flow across the layer, a perovskite active layer has the ability to absorb a wide range of photons, a hole transport layer for hole transfer (HTL), and the metal back electrode. In this work, the representative device consists of PET (Polyethylene terephthalate) / ITO (Indium doped Tin Oxide) substrate, $CH_3NH_3PbI_3$ active layer, PCBM (Phenyl-C61-butyric acid methyl ester) ETL, and Al metal electrode. As can be seen from the structure of the architecture, the PET flexible substrate is used instead of the glass and the architecture does not contain an HTL. structure of a typical PSC is composed of five main layers [7]. They are a transparent conducting oxide (TCO)

The system boundary for this LCA is cradle to gate (from raw materials supply to the finished solar cell). Important parameter specifications and assumptions are shown in Table 1.

Table 1. Specifications and assumptions of flexible PSC device

Active Area (A) (m^2)	75 %
Performance Ratio (PR)	80 %
Cell to Module Efficiency Loss	20 %
Annual Solar Insolation (I) [10]	1700 (kWh/m^2-yr)
Device Lifetime (LT) (year)	5 years
Flexible PSC Efficiency (η)	10 %

The inventory table has been created by using literature data and ecoinvent v3.4 (Table 2 and Table 3). In the reference work, it was reported that the highest efficiency value was obtained when the perovskite active layer thickness is 340 nm. Since no data were mentioned for other layers, thickness values were assumed by the benefit of the literature data. One step spin coating fabrication is assumed for PCBM deposition while two sequential step spin coating is selected for perovskite active layer with an annealing process at 100 ^{0}C and 1h. ITO production and deposition values are provided by the benefit of the work of Espinosa et.al [8]. The vacuum deposition fabrication technique with 50% efficiency is assumed for the production of the Al metal electrode.

Table 2. Inventory table of PET/ ITO substrate, ETL and Metal Electrode. I stand for material input, P for process energy requirement, O for output, and E for emission.

Materials and processes		Input	Unit
PET/ITO Substrate Assumption: 50 µm layer thickness [14] Density: 1.38 g/cm3 [15] ITO Production [8]			
I	Polyethylene terephthalate compound (PET)	6.90E-02	kg
I	Indium, liquid, at plant	4.78E-05	kg
I	oxygen, liquid, at plant	9.10E-03	kg
I	tin, at regional storage	4.78E-06	kg
Energy Input			
P	US: electricity, production mix US (ITO and Oxygen plasma)	10.7	MJ
Electron Transport Layer Assumption: 60 nm layer thickness [16] Density: 1.5 g/cm3 [17]			
PCBM Production		**1.80E-03**	**kg**
I	Cumene (Assumed instead of 1,2,4-Trimethylbenzene)	1.02	kg
I	Graphite production (Assumed instead of C_{60} Fullerene)	5.93E-03	kg
I	Diazomethane Production	2.34E-03	kg
I	Chlorobenzene	9.00E-02	kg
Energy Input [13 1]			
P	Spin Coating	0.9	MJ
Metal Electrode Assumption: 100 nm layer thickness			
I	Aluminum	5.40E-04	kg
Energy Input (50 % efficiency assumed) [13 1]			
P	Evaporation	34.6	MJ
P	Vacuum	132	MJ

Table 3. Inventory table of Perovskite Active Layer. I stand for material input, P for process energy requirement, O for output, and E for emission.

Materials and processes		Input	Unit
Perovskite Active Layer Assumption: 340 nm layer thickness [6] Density: 1.368 g/ml [11]			
$CH_3NH_3PbI_3$ Production		**9.30E-03**	**kg**
PbI_2 Production		**6.90E-03**	**kg**
I	lead, at regional storage	3.11E-03	kg
I	nitric acid, 50% in H2O, at plant	1.89E-03	kg
E	Hydrogen	2.43E-05	kg
I	Iodine	4.56E-03	kg
I	potassium hydroxide, at regional storage	2.02E-03	kg
O	Water	3.28E-04	kg
O	RER: potassium nitrate	3.04E-03	kg
I	N, N-dimethylformamide, at plant Density: 0.95g/ml [12]	9.65E-03	kg
CH_3NH_3I Production		**2.39E-03**	**kg**
I	hydrazine, at plant	1.21E-04	kg
I	Iodine	1.91E-03	kg
O	Nitrogen	9.71E-05	kg
I	methylamine, at plant	4.70E-04	kg
W	CH_3NH_3I	2.19E-04	kg
W	PbI_2	6.56E-04	kg
E	Nitrogen	9.71E-05	kg
Energy Input [13 1]			
P	Spin Coating	1.8	MJ
P	Annealing (100^{0}C, 1h)	45.43	MJ

3. RESULTS AND DISCUSSION

Six midpoint environmental impact categories in ILCD impact assessment model were used for impact assessment (Table 4). All results were calculated with characterization factors provided by Gabi 8.1 software. Table 4 shows the environmental impact values of each layer of the HFF PSC required to manufacture 1 m^2 of the solar cell.

In previously published studies examined the environmental effects of PSCs [2,8], it was found that the contributions of environmental impact values of PSC layers are largely in line with the amount of electricity required for fabrication (~ 90). Hence, environmental impact values for each layer calculated in this study can be predicted to be proportional to the electricity consumption values stated in the inventory table. Table 5 shows the manufacturing electricity consumption and percentages of each PSC layers.

Table 4. Environmental Impacts of manufacturing 1 m^2 HFF PSC

Impact Category	PET/ITO	Perovskite	PCBM	Al	Total
Acidification (AP) [Mole of H+ eq.]	0.019	0.121	0.002	0.29	0.433
Global Warming Potential (GWP) [kg CO_2 eq.]	2.441	14.639	0.4	34.96	52.44
Ecotoxicity (ECO) [Comparative Toxic Units ecotoxicity (CTUe)]	12.35	70.28	2.29	166.07	250.99
Eutrophication (EUT) [kg N eq.]	0.019	0.013	0.0002	0.029	0.061
Human toxicity (HTC) [Comparative Toxic Unit for human (CTUh)]	1.39 E-07	8.17 E-07	2.12 E-08	1.95 E-06	2.93 E-06
Primary energy demand (PED) [MJ]	37.353	245.49	10.029	582.9	875.77

Table 5. Manufacturing electricity consumptions and percentages of each PSC layers

PSC Layer	Manufacturing Electricity Consumption (MJ)	Percentage (%)
PET / ITO Substrate	10.7	4.75
PCBM ETL	0.9	0.4
Perovskite	47.23	20.95
Metal Electrode	166.6	73.9

Figure 1 demonstrates the contribution of each PSC layer to every impact category. In five of the six environmental impact categories (except eutrophication), the Al metal electrode layer represents up to 70 percent of the total impact value. The main reason for this is the vacuum-based manufacturing with high electricity consumption used in the fabrication of the Al metal electrode layer. Except for eutrophication (PET/ITO substrate caused a significant change), the distribution of impact values in each impact category is proportional to the amount of electricity consumed for the manufacturing. The PET/ITO layer has a 30% percent contribution in the eutrophication impact category while in other categories this contribution is about 5%. Indium used as in the ITO front electrode on PET is responsible for this increase in the Eutrophication category.

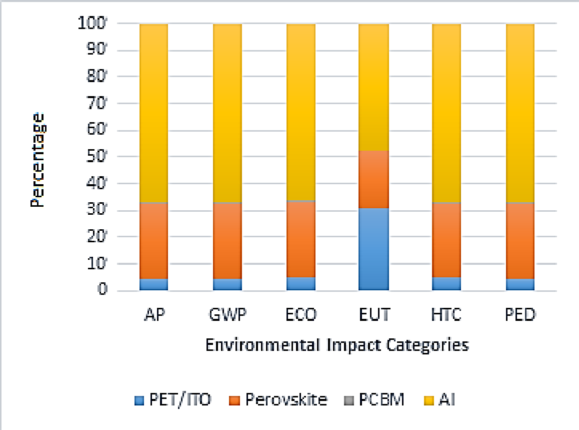

Figure 1. Share of total environmental impacts of each HFF PSC layers

GWP of the photovoltaics is generally determined as the ratio of life cycle greenhouse gas emissions (g CO_2-eq) to lifetime power generation (kWh). Therefore, a correlation is applied to convert the GWP impacts from 1 m^2 cell area ($Impact_{m^2}$) to 1kWh ($Impact_{kWh}$) by using the equation 1 [1].

$$Impact_{kWh} = \frac{Impact_{m^2}}{I\ x\ \eta\ x\ A\ x\ PR\ x\ LT} \qquad (1)$$

As a result of the calculation, the GWP value of HFF PSC is determined as 128.5 g CO_2-eq / kWh. It is reported that the mean global warming potential values of commercial PVs vary between 24 to 37 g CO_2-eq per kWh [9]. As can be seen in Figure 2, HFF PSC has 3.5-5 times higher GWP value than commercial PVs. If the lifetime of HFF PSC was within the range of 15-20 years rather than 5 years as we assumed in this study, then the GWP value would reach a competitive value (~ 30-40 g CO_2-eq / kWh) with commercial PVs.

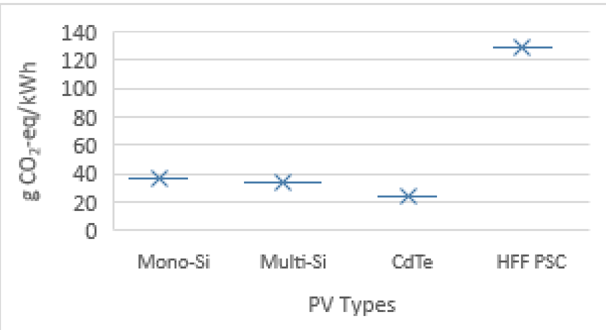

Figure 2. Comparison of HFF PSC with commercial PV technologies in terms of GWP results

4. CONCLUSION

The cradle-to-gate life cycle assessment of manufacturing hole transport layer free flexible perovskite solar cell shows that the majority of environmental impacts come from Al metal electrode deposition in all environmental impact categories. The high electricity consumptive vacuum-based fabrication process of the metal electrode is responsible for this high impact values.

As envisaged, most of the environmental impact values for each layer were proportional to the electricity consumption values stated in the inventory table. The only exception in this regard was seen in the eutrophication category. Indium used as in the ITO front electrode on PET caused to rise the impact share of PET/ITO layer up to 30 % from around 5% in the eutrophication category.

In the light of the results obtained in this study, one of the suggestions that can be made for future studies is to choose lower electricity consumptive materials and deposition methods alternatives for the back electrode instead of the metal electrode, which causes high electricity consumption. Another one is that instead of using indium based front electrodes that are already in the rare earth element category, fluorine-doped front electrodes can be investigated on flexible layers to reduce the environmental impact in eutrophication category. Finally, in order to bring the global warming potential value to a level that can compete with commercial photovoltaic technologies, it is necessary to increase the lifetime of the cell as well as reducing the manufacturing electricity consumption.

ACKNOWLEDGEMENT

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DECLARATION OF ETHICAL STANDARDS

The author(s) of this article declare that the materials and methods used in this study do not require ethical committee permission and/or legal-special permission.

AUTHORS' CONTRIBUTIONS

Hüseyin SARIALTIN: Performed the experiments and analyse the results. Wrote the manuscript.

CONFLICT OF INTEREST

There is no conflict of interest in this study.

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