Electronic Supplementary Material (ESI) for Energy Advances.

Supplementary Information

Life Cycle Assessment of Low-Dimensional Materials for Perovskite Photovoltaic Cells

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- The environmental impacts attributed to 1g of each LD material analyzed in this study across ten TRACI impact categories are presented in Table S.1.

- The environmental impacts of the incorporation of the various LD materials in different layers of PSC have been calculated, and a comparative analysis of the environmental impacts for each LD material within every layer has been presented in Table S.2- S.4.
- LD materials that show lower environmental impacts in each layer have been chosen for Alt-1 *ld*-PSC configuration (highlighted in green in Table S.2-S.4), while those with higher impacts among the analyzed LD materials have been selected for the Alt-2 *ld*-PSC (highlighted in red in Table S2-S4).

- The environmental impacts of PSCs for 1 m^2 are provided in Table S.5.

- The Energy Payback Time (EPBT) calculations were performed using Eq. S1 follows an approach similar to Celik et al[1].

- The improved photovoltaic parameters after the incorporation of LD materials into various layers of the PSC structure are provided in Table S.6.

- Table S.7 provides the environmental impacts comparison of organic HTL i.e., spiro-OMeTAD, and inorganic HTL i.e., CuSCN for 1m^2 of PSC.

- Table S.8 provides an environmental impact comparison between two Alt-1 configurations, one with spiro-OMeTAD as HTL and the other employing CuSCN as HTL. In both of these Alt-1 configurations, the HTL integrates rGO, the ETL includes graphene, and the absorber layer with BP-nano. Our results show that the environmental performance of the spiro-OMeTAD-based Alt-1 and CuSCN-based Alt-1 are similar.

Table S.1. Environmental impacts attributed to materials and energy utilized in the synthesis of 1g of various LD materials across all TRACI impact categories.

TRACI impact categories	rGO		Graphene		GQDs		BP-nano		MoS_2	
	Materials	Energy	Materials	Energy	Materials	Energy	Materials	Energy	Materials	Energy
Acidification (kg SO_2-eq)	3.28E-04	3.06E-06	1.91E-05	7.08E-04	4.05E-02	1.97E-01	2.18E-01	4.81E-02	1.47E-02	1.15E-05
Ecotoxicity (CTUe)	4.08E+00	8.71E-03	6.58E-02	2.01E+00	5.70E+01	8.22E+02	3.83E+02	2.00E+02	8.98E+01	4.80E-02
Eutrophication (kg N-eq)	1.98E-04	6.39E-06	1.13E-05	1.48E-03	8.21E-03	6.52E-01	2.02E-01	1.59E-01	1.04E-02	3.81E-05
GWP (kg CO_2-eq)	3.27E-02	1.10E-03	3.53E-03	2.55E-01	2.28E+00	8.65E+01	4.58E+01	2.11E+01	2.06E+00	5.05E-03
Particulate Air (kg $PM_{2.5}$- eq)	9.22E-05	2.69E-06	6.45E-06	6.23E-04	5.51E-03	2.94E-01	1.01E-01	7.17E-02	2.67E-03	1.72E-05
Human toxicity, cancer (CTUh)	3.40E-09	7.80E-11	3.52E-10	1.80E-08	2.60E-07	7.52E-06	3.34E-06	1.83E-06	1.36E-07	4.40E-10
Human toxicity, non-canc. (CTUh)	2.94E-08	2.64E-10	1.36E-09	6.10E-08	1.00E-06	2.45E-05	1.15E-05	5.97E-06	6.32E-07	1.43E-09
Ozone Depletion Air (kg CFC 11-eq)	9.26E-09	6.66E-11	4.12E-10	1.54E-08	2.21E-07	4.97E-06	3.24E-06	1.21E-06	3.24E-07	2.90E-10
Resources, Fossil fuels (MJ surplus energy)	3.72E-02	1.07E-03	3.72E-03	2.48E-01	3.19E+00	8.06E+01	5.12E+01	1.97E+01	3.95E+00	4.71E-03
Smog Air (kg O_3-eq)	2.47E-03	3.08E-05	2.53E-04	7.11E-03	1.50E-01	2.81E+00	2.99E+00	6.87E-01	1.14E-01	1.64E-04

Table S.2 Environmental impacts of graphene, BPQDs, and GQDs integrated into ETL per m^2 of *ld*-PSC. The LD material highlighted in green indicates lower environmental impact, while the LD material highlighted in red shows higher environmental impacts for ETL integration.

TRACI impact categories	**Graphene**	**BPQDs**	**GQDs**
Acidification (kg SO_2-eq)	9.66E-05	8.45E-04	1.24E-03
Ecotoxicity (CTUe)	1.73E-01	1.83E+00	4.59E+00
Eutrophication (kg N-eq)	9.76E-05	1.12E-03	3.45E-03
GWP (kg CO_2-eq)	2.07E-02	2.09E-01	4.63E-01
Particulate Air (kg $PM_{2.5}$- eq)	2.48E-05	5.24E-04	1.56E-03
Human toxicity, cancer (CTUh)	1.59E-09	1.62E-08	4.06E-08
Human toxicity, non-canc. (CTUh)	4.98E-09	5.46E-08	1.33E-07
Ozone Depletion Air (kg CFC 11-eq)	6.99E-10	1.35E-08	2.71E-08
Resources, Fossil fuels (MJ surplus energy)	4.95E-02	2.39E-01	4.37E-01
Smog air (kg O_3-eq)	1.19E-03	1.16E-02	1.55E-02
CED (MJ)	6.00E-01	4.66E+00	9.99E+00

Table S.3 Environmental impacts of GQDs, BP-nano, and rGO integrated into absorber layer per m^2 of *ld*-PSC. The LD material highlighted in green indicates a lower environmental impact, while the LD material highlighted in red shows higher environmental impacts for absorber layer integration.

TRACI impact categories	**GQDs**	**BP-nano**	**rGO**
Acidification (kg SO_2-eq)	1.22E-02	1.60E-03	2.43E-01
Ecotoxicity (CTUe)	4.25E+01	2.34E+00	2.27E+02
Eutrophication (kg N-eq)	3.17E-02	1.39E-03	1.22E-01
GWP (kg CO_2-eq)	4.27E+00	2.46E-01	1.93E+01
Particulate Air (kg $PM_{2.5}$- eq)	1.42E-02	5.21E-04	1.96E-02
Human toxicity, cancer (CTUh)	3.72E-07	1.81E-08	1.24E-06
Human toxicity, non-canc. (CTUh)	1.22E-06	6.15E-08	4.35E-06
Ozone Depletion Air (kg CFC 11-eq)	2.62E-07	2.53E-08	3.71E-06
Resources, Fossil fuels (MJ surplus energy)	4.22E+00	3.96E-01	5.68E+01
Smog air (kg O_3-eq)	1.45E-01	1.33E-02	9.96E-01
CED (MJ)	9.27E+01	5.86E+00	5.55E+02

Table S.4 Environmental impacts of rGO, MoS_2, and BP-nano integrated into HTL per m^2 of *ld*-PSC. The LD material highlighted in green indicates a lower environmental impact, while the LD material highlighted in red shows higher environmental impacts for HTL integration.

TRACI impact categories	**rGO**	**MoS_2**	**BP-nano**
Acidification (kg SO_2-eq)	1.34E-04	9.40E-03	1.61E-02
Ecotoxicity (CTUe)	5.92E-01	4.06E+01	3.54E+01
Eutrophication (kg N-eq)	4.24E-04	7.11E-03	2.18E-02
GWP (kg CO_2-eq)	5.46E-02	1.80E+00	4.04E+00
Particulate Air (kg $PM_{2.5}$- eq)	1.78E-04	1.66E-03	1.04E-02
Human toxicity, cancer (CTUh)	4.74E-09	9.87E-08	3.12E-07
Human toxicity, non-canc. (CTUh)	1.53E-08	4.72E-07	1.06E-06
Ozone Depletion Air (kg CFC 11-eq)	3.80E-09	1.44E-07	2.68E-07
Resources, Fossil fuels (MJ surplus energy)	5.84E-02	5.27E+00	4.35E+00
Smog air (kg O3-eq)	1.91E-03	9.97E-02	2.22E-01
CED (MJ)	1.22E+00	4.95E+01	8.86E+01

Table S.5 Environmental impacts of PSCs for 1m² of module across all TRACI impact categories.

TRACI impact categories	**PSC**	**Alt-1**	**Alt-2**
Acidification (kg SO_2-eq)	3.45E-01	3.47E-01	6.06E-01
Ecotoxicity (CTUe)	5.83E+03	5.83E+03	6.09E+03
Eutrophication (kg N-eq)	2.46E-01	2.48E-01	3.93E-01
GWP (kg CO_2-eq)	3.64E+01	3.67E+01	6.02E+01
Particulate Air (kg $PM_{2.5}$- eq)	8.14E-02	8.19E-02	1.13E-01
Human toxicity, cancer (CTUh)	7.63E-06	7.65E-06	9.22E-06
Human toxicity, non-canc. (CTUh)	6.18E-05	6.19E-05	6.73E-05
Ozone Depletion Air (kg CFC 11-eq)	3.73E-06	3.76E-06	7.74E-06
Resources, Fossil fuels (MJ surplus energy)	4.94E+01	4.98E+01	1.11E+02
Smog air (kg O3-eq)	3.97E+00	3.99E+00	5.21E+00
CED (MJ)	6.72E+02	6.80E+02	1.33E+03

Table S.6 Photovoltaic parameters of PSC structure after incorporation of various LD materials into ETL, the absorber layer, and HTL.

PSC layer	LD material integration	Jsc (mA/cm²)	V_{oc} (V)	FF (%)	η (%)	Reference
ETL	Graphene	23.21	1.08	69.0	17.4	[2]
	GQDs	22.97	1.13	75.4	19.7	[3]
	BPQDs	24.4	1.13	76.1	21.0	[4]
Absorber layer	BP-nano	22.95	1.06	80.0	19.7	[5]
	rGO	17.67	0.93	70.0	11.6	[6]
	GQDs	22.91	1.05	76.3	18.4	[7]
HTL	BP-nano	20.22	1.06	76.1	16.4	[8]
	MoS_2	21.70	1.12	72.0	17.5	[9]
	rGO	23.05	1.11	71.0	18.2	[10]

Conversion of $\text{Impacts}_{\text{kWh}}$ to $\text{Impacts}_{\text{m2}}$

$$Impacts_{kWh} = \frac{Impacts_{m^2}}{I * PCE * PR * Lt} \quad Eq. S1$$

where $\text{impacts}_{\text{m2}}$ represents the environmental impacts of 1m2 of module area manufacturing; $\text{impacts}_{\text{kWh}}$ is the impacts per kWh electricity generation from PV module; I denote the solar insolation constant (1700 kWh/m²/year); PR is the performance ratio of the module (75%); Lt is the lifetime of the PV modules (years).

Energy Payback Time (EPBT)

$$EPBT = \frac{CED \times \varepsilon}{I \times \eta \times PR \times CF} \quad Eq. S2$$

where CED represents the cumulative energy demand (MJ/m^2), ε is the electrical to primary energy conversion factor (35%), PR is the performance ratio (75%), η is the PCE (%) of PV technology, I denote the global irradiation constant (1700 kWh/ m^2/ year), and CF is the conversion factor (3.6MJ/kWh).

Low-cost inorganic HTL (CuSCN)

Table S.7 Environmental impacts comparison of organic HTL i.e., spiro-OMeTAD, and inorganic HTL i.e., CuSCN for $1m^2$ of PSC. Note: The thickness of CuSCN is 40nm and spiro-OMeTAD is 150nm.

TRACI impact categories	**CuSCN**	**spiro-OMeTAD**
Acidification (kg SO_2-eq)	1.58E-04	9.33E-07
Ecotoxicity (CTUe)	2.46E-01	1.74E-03
Eutrophication (kg N-eq)	2.82E-04	5.43E-07
GWP (kg CO_2-eq)	2.73E-02	2.32E-04
Particulate Air (kg $PM_{2.5}$- eq)	1.77E-05	2.15E-07
Human toxicity, cancer (CTUh)	2.08E-09	1.19E-11
Human toxicity, non-canc. (CTUh)	8.33E-09	3.76E-11
Ozone Depletion Air (kg CFC 11-eq)	4.08E-09	2.32E-11
Resources, Fossil fuels (MJ surplus energy)	3.19E-02	8.80E-04
Smog air (kg O3-eq)	1.20E-03	1.24E-05
CED (MJ)	6.01E-01	7.44E-03

Table S.8 Environmental impacts comparison between two Alt-1 *ld*-PSC configurations, one incorporates organic HTL spiro-OMeTAD and the other using inorganic HTL CuSCN for 1kWh electricity production. In two Alt-1configurations, ETL is integrated with graphene and absorber layer with BP-nano. We substituted spiro-OMeTAD with inorganic CuSCN for the HTL and following a previous study[11] that incorporated rGO on CuSCN, we calculated the environmental impacts.

TRACI impact categories	**Alt-1 with spiro-OMeTAD+rGO**	**Alt-1 with CuSCN+rGO**
Acidification (kg SO_2-eq)	4.30E-05	4.31E-05
Ecotoxicity (CTUe)	7.23E-01	7.23E-01
Eutrophication (kg N-eq)	3.07E-05	3.08E-05
GWP (kg CO_2-eq)	4.55E-03	4.56E-03
Particulate Air (kg $PM_{2.5}$- eq)	1.02E-05	1.02E-05
Human toxicity, cancer (CTUh)	9.49E-10	9.50E-10
Human toxicity, non-canc. (CTUh)	7.67E-09	7.67E-09
Ozone Depletion Air (kg CFC 11-eq)	4.66E-10	4.67E-10
Resources, Fossil fuels (MJ surplus energy)	6.18E-03	6.20E-03
Smog air (kg O3-eq)	4.94E-04	4.95E-04
CED (MJ)	8.43E-02	8.44E-02

Environmental impact comparison between regular and inverted PSCs after the incorporation of LD materials

- Table S.9 provides the environmental impact comparison between Alt-1 *ld*-PSC and an inverted *ld*-PSC configuration. The inverted *ld*-PSC includes BPQDs additional coating on the top of PEDOT: PSS. Following previous study[12], we assumed a 15% increase in the PCE value for the inverted *ld*-PSC after the integration of BPQDs.

Table S.9 Environmental impacts comparison between Alt-1 *ld*-PSC configuration and inverted *ld*-PSC with PEDOT: PSS as HTL and PCBM as ETL. In inverted PSC, BPQDs were applied on the PEDOT: PSS to enhance the hole extraction in p-i-n PSC structure.

TRACI impact categories	**Alt-1 PSC**	**Inverted PSC PEDOT: PSS +BPQDs**
Acidification (kg SO_2-eq)	4.30E-05	4.44E-05
Ecotoxicity (CTUe)	7.23E-01	7.26E-01
Eutrophication (kg N-eq)	3.07E-05	3.29E-05
GWP (kg CO_2-eq)	4.55E-03	4.98E-03
Particulate Air (kg $PM_{2.5}$- eq)	1.02E-05	1.05E-05
Human toxicity, cancer (CTUh)	9.49E-10	9.70E-10
Human toxicity, non-canc. (CTUh)	7.67E-09	7.71E-09
Ozone Depletion Air (kg CFC 11-eq)	4.66E-10	5.33E-10
Resources, Fossil fuels (MJ surplus energy)	6.18E-03	7.50E-03
Smog air (kg O3-eq)	4.94E-04	5.12E-04
CED (MJ)	8.43E-02	8.72E-02

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