Human Health Impacts from Nanoparticles in Life-Cycle Assessment: Case Study on 3rd-Generation Organic Photovoltaics

Michael Tsang, Guido Sonnemann*, Dario Bassani
Outline

• Background
  • Organic Photovoltaics
  • Nanomaterials
  • Previous LCA Studies on OPVs

• Methods

• Results

• Conclusion
Background: Organic Photovoltaics

Organic polymer

Fullerenes

Encapsulation Layers (50 um): PET and Various Resins
Substrate (50 um): PET
Transparent (Front) Anode (160 nm): Fluorine-Doped Tin Oxide
Hole Transport Layer (100 nm): Molybdenum Oxide
Active Layer (150 nm): PCBM:P3HT
Optical Spacer (30 nm): Titanium Dioxide
Electron Transport Layer (<1 nm): Lithium Fluoride
Opaque (Back) Cathode (150 nm): Aluminum
Encapsulation Layers (50 um): PET and Various Resins
Background: Nanomaterials

• Engineered Nanomaterials
  
  • ‘...1 nm < one dimension < 100 nm...’ (European Commission)

• Unique properties
Background: Prior Cradle-to-Gate Results

![Cumulative Energy Demand (MJ/Wp) Graph]

- OPV-Glass (Garcia-Valverde et al. 2010)
- OPV-Glass (Roes et al. 2009)
- OPV (Espinosa et al. 2011)
- OPV (Espinosa et al. 2012)
- OPV (Espinosa et al. 2013)
- OPV (Anctil et al. 2013)
- OPV (Roes et al. 2009)
- OPV (Emmott et al. 2012)
- OPV (Tsang et al. 2015)
- OPV (Espinosa et al 2012)
- OPV (Espinosa et al. 2013)
- Multicrystalline Silicon

Reference: Prior Cradle-to-Gate Results
Greater resource efficiencies

Some demonstration of lower environmental and human health impacts.

What about impacts from nano?
# Background: Prior Studies Summaries

<table>
<thead>
<tr>
<th>Individual Case Studies</th>
<th>Year</th>
<th>Energy and Material Flows During ENM Production</th>
<th>ENM Emissions</th>
<th>ENM Human- or Eco-tox Impacts</th>
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<tr>
<td>Roes et al.(^{29})</td>
<td>2009</td>
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<tr>
<td>Sondergaard et al.(^{147})</td>
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<td>Sandwell et al.(^{156})</td>
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\(^{156}\) Sandwell et al., 2016.  
\(^{157}\) Hengevoss et al., 2016.
Background: LCA and Nanomaterials

- Human health toxicity across the life-cycle
- Human health toxicity of nanomaterials across the life-cycle
Methods

- Focused on: Occupational Indoor Air Emissions
- Most obvious, direct interaction with raw nanoparticles

**Production (ENM)**
- Large volumes
- Direct Interaction: Handling, Dumping, Packaging
- Inconsistent PPE usage
- Inhalation and Dermal Exposure

**Manufacture (OPV Panel)**
- Potentially Large Volumes, More discreet handling
- Direct Interaction: Handling, Dumping
- Inconsistent PPE usage
- Inhalation and Dermal Exposure

**OPV Use Phase**
- No Direct Interaction: Embedded in matrix
- Release: Leaching unknown but unlikely during use

**End-of-Life Options**
- No Direct Interaction: Embedded in matrix
- Release: Conversion to PCBM to CO₂ during incineration, TiO₂ unknown
- Release: Long term leaching possible but unknown in landfill

Exposure Potential: 4 Nearly Certain 3 Likely 2 Possible 1 Unlikely
Methods

• Nanoparticles of Titanium Dioxide (TiO$_2$)
  • *Model* TiO$_2$ material, 21 nm primary particle size

• Excluded: Fullerenes
  • Lack of specific data needed for models (e.g. toxicological data)
Methods (Tsang et al. 2017)

\[ FF \cdot XF \cdot EF = IF \cdot EF = CF \]
Methods - Emissions

• Considered for a high emissions, worst-case scenario

• Pouring large amount of nano-powder into vessel periodically through an 8-hour work period.

• Work is performed in a hall with low ventilation rate. No personal protection equipment.

• The process is assumed to be of high energy (i.e. pouring nano-powder from a height assumed to be 0.3 m - 1 m).
Methods – Fate & Transport *(Tsang et al. 2017)*

- Two zone, near-field (NF) and far-field (FF) fate and transport model

- Sources of removal
  - Air exchange (\(Q\))
  - Interzonal air flow (\(\beta\))
  - Homoaggregation (\(k_1\))
  - Gravitational settling (\(k_2\))
Methods – Exposure Model (*Tsang et al. 2017*)

- Nano-Inhalation *Exposure* Model

  - Inhalation rate only partial influence in exposure
  - Deposition based on particle size
  - Clearance and retention of particles are driven by physiologic and immune responses
  - Retained-intake fraction likely to be lower with personal-protection equipment
Results

- Preliminary Cradle-to-Gate Results:
  - No significant increase in carcinogenic or non-carcinogenic human health impacts from the release of nano-TiO$_2$ to the indoor occupational compartment.
  - Roughly 62% of these emissions came from handling nano-TiO$_2$ during OPV-manufacturing and the other half during nano-TiO$_2$ production.

<table>
<thead>
<tr>
<th>Percent Contribution by Life-Cycle stage</th>
<th>No ENM-specific Characterization Factor</th>
<th>With ENM-specific Characterization Factor</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Human Tox (non-carcinogenic)</td>
<td>Human Tox (carcinogenic)</td>
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<tr>
<td>Annealing</td>
<td>32.08%</td>
<td>29.55%</td>
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<tr>
<td>Hole Transport Layer</td>
<td>24.66%</td>
<td>2.46%</td>
</tr>
<tr>
<td>PCBM</td>
<td>14.47%</td>
<td>18.02%</td>
</tr>
<tr>
<td>Lamination</td>
<td>12.31%</td>
<td>14.56%</td>
</tr>
<tr>
<td>FTO Substrate</td>
<td>9.61%</td>
<td>10.44%</td>
</tr>
<tr>
<td>P3HT</td>
<td>0.80%</td>
<td>17.82%</td>
</tr>
<tr>
<td>Printing</td>
<td>3.16%</td>
<td>3.14%</td>
</tr>
<tr>
<td>Electron Transport Layer</td>
<td>1.59%</td>
<td>1.38%</td>
</tr>
<tr>
<td>Aluminum Electrode</td>
<td>0.63%</td>
<td>1.96%</td>
</tr>
<tr>
<td>Nano-TiO$_2$ Spacer</td>
<td>0.05%</td>
<td>0.04%</td>
</tr>
<tr>
<td>Other</td>
<td>0.64%</td>
<td>0.63%</td>
</tr>
<tr>
<td>Total Impacts (CTU)</td>
<td>9.35E-09</td>
<td>3.55E-09</td>
</tr>
<tr>
<td>Total contribution from nano-TiO$_2$</td>
<td>N/A</td>
<td>N/A</td>
</tr>
<tr>
<td></td>
<td></td>
<td>0.41%</td>
</tr>
</tbody>
</table>

avniR 2017 – Human Health Impacts of Nanoparticles in LCA
Results

• Results are only specific to the release of nano-TiO$_2$ in the workplace

• Does not include potential releases in the environment during the use and/or end-of-life of the OPV panels

• Does not include the potential releases of other nanomaterials such as PCBM (fullerenes)
Conclusions

• Overall indication of potential human health impacts from nanomaterial releases across the life-cycle of OPVs is low

• If goal is to reduce human health impacts, efforts may be best utilized elsewhere in the life-cycle

• Challenges remain:
  • Appropriate nanomaterials' emissions data
  • Characterization factors for nanomaterials
Thank You

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• Dario Bassani
  
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• Emissions estimated as a function of the dustiness of the TiO2 and the handling energy of the work-related activity

\[ E = \left( \frac{A}{t} \right) \cdot [(DI) \cdot (H)] \]

• E: Emissions (mg/min)
• A: Amount of nano-TiO2 handled in work-cycle (kg)
• t: Time length of work-cycle (min)
• DI: Dustiness index of nano-TiO\(_2\) (unitless)
• H: Force applied to the ENM (unitless)
ENM Concentrations: 1-Work Day

**Dynamic**
Average concentration during emission event: 24.9 mg/m$^3$

**Steady-State**
Average concentration: 3.52 mg/m$^3$
Extra Slides – *(Retained)* Intake Fraction

- *(Conventional)* Intake Fraction for indoor exposure (e.g. USEtox):

\[
iF = \frac{IR}{V \cdot m \cdot k_{ex}} \cdot N
\]

- *(Retained)-intake Fraction (RiF, unitless)* in the lung (target organ):
  
  \[
  RiF = \frac{\text{Exposure}}{E} \cdot (\text{Population Exposed})
  \]

- 1-Year and *Lifetime* exposures (i.e. RiF) values calculated
  
  Lung burden measured at the area under curve after the total exposure time (i.e. after 1-year of work)

- Population of 8 workers (Walser et al. 2015)
• ENM distribution in the lung shifts:
  • Inhalation at low airborne nano concentrations: phagocytosis (light blue)
  • Inhalation at higher airborne nano concentrations: translocation of nano to pulmonary and interstitial spaces (grey and yellow)
Extra Slides – Retained Intake Fraction

- Inverse relationship between emitted amount and retained-intake fraction
- Intake fraction not changing in existing steady-state models
Extra Slides – Methods – Dose Response (*Tsang et al. 2017*)

Cancerous Effect Factor: Lung Tumors

Non-Cancerous Effect Factor: Inflammation

\[ EF = \frac{0.5}{ED_{50,\text{int}}} \]

Percent Cancer Cases vs. Surface area of TiO\textsubscript{2} / g-lung

Percent Inflammation vs. \(\mu g\) TiO\textsubscript{2} / g-lung
Extra Slides – Effect Factor

• Effect Factor:

  • Non-Carcinogenic: sub-chronic animal study (Bermudez et al. 2004)
  
  • Carcinogenic: chronic animal studies (Lee et al. 1985, Muhle et al. 1991, Heinrich et al. 1995)

\[
EF = \frac{0.5}{ED_{50,h,int}}
\]

\[
ED_{50,h,int} = \frac{ED_{50,a,int}}{UF_a \cdot UF_t}
\]

0.5 Fraction of the population that will be impacted
EF: Effect Factor
\(ED_{50,h,int}\): Effective dose at which 50% of the humans have response from internal exposure
\(ED_{50,a,int}\): Effective dose at which 50% of the animals have response from internal exposure
\(UF_a\): Uncertainty factor based on animal to human extrapolation
\(UF_t\): Uncertainty factor based on study time (e.g. acute to chronic)