SUPPLEMENTARY INFORMATION

S1. Estimation of Nanowire Mass

Sol-gel/CBD Methodology

The mass of ZnO NWs produced in a single reaction was determined using existing literature published from the research group. The sol-gel methodology to produce ZnO NWs has been extensively studied by the research team and as such, there exists a deep understanding of the density and dimensions of the produced NWs.

In this protocol, the resulting NWs have an average length and diameter of 2.8µm and 78nm, respectively [1]. Both the length and diameter of the NW is a function of the growth duration, which was specified in the article as 3 hours. From this, we can calculate the mass of one ZnO NW, assuming the NW is a perfect cylinder:

$$V = \pi r^2 h \#(S1)$$

where *V* is the NW volume, *r* is the NW radius, and *h* is the NW length.

$$V = \pi(3.9 \times 10^{-6} cm)^2 (2.8 \, x \, 10^{-4} cm)$$

$$V = 1.34 \, x \, 10^{-14} \, cm^3$$

We can then derive the mass of a single NW using the density of ZnO (5.61g/cm^3):

$$m_{single} = V\rho \#(S2)$$

where m_{single} is the NW mass and ρ is the density of ZnO.

$$m_{single} = (1.34 \, x \, 10^{-14} \, cm^3)(\frac{5.61g}{cm^3})$$

$$m_{single} = 7.51 \, x \, 10^{-14} g$$

The mass of one NW is equal to $7.51 \, x \, 10^{-14} g$, or 7.51 $x \, 10^{-11}$ mg.

Further, the research group found that the density of ZnO NWs is a function of the sol-gel concentration and deposition method. In this article, a 1M sol-gel is prepared and deposited in one layer, as described in the manuscript. As such, the resulting NW array has a density of 30/µm^2 [1]. From this information, the number of NWs produced in a single growth reaction on a silicon wafer substrate with an area of 9cm^2 can be determined.

$$N = \rho_{NW} * A_{substrate} \#(S3)$$

where N is the number of NWs synthesized, ρ_{NW} is the NW density and $A_{substrate}$ is the growth area of the reaction.

$$N = \frac{30NWs}{\mu m^2} * 9 \, x \, 10^8 \, \mu m^2$$

$$N = 2.70 \, x \, 10^{10} \, NWs$$

With the total number of NWs produced in one chemical reaction and the mass of a single NW, the total mass of NWs synthesized can be derived:

$$m_{total} = m_{NW} * N \#(S4)$$

where m_{total} is the total mass of NWs synthesized.

$$m_{total} = 2.70 \, x \, 10^{10} \, NWs * 7.51 \, x \, 10^{-14} g \frac{g}{NW}$$

$$m_{total} = 2.03mg$$

In-Solution Methodology

The mass of ZnO NWs produced in a single synthesis reaction was determined by weighing the filter paper before and after the filtration and drying steps. The difference in mass corresponds to the mass of NWs collected. This measurement was repeated several times under identical synthesis conditions to ensure consistency. The average yield was 1.51 mg of ZnO nanowires per reaction, with a standard deviation of 0.30 mg. This experimental uncertainty was incorporated into the LCA model and propagated through the Monte Carlo analysis to account for its influence on the overall results.

S2. Breakdown of Chemicals Not Available in EcoInvent

Zinc Nitrate Hexahydrate

In this study, zinc nitrate hexahydrate (ZNH) is used as a precursor to the formation of zinc oxide nanowires (ZnO NWs) in-solution. ZNH is not found in the EcoInvent database and therefore, the environmental impacts of this chemical must be estimated and modelled in OpenLCA using the best available information from literature. For the case of ZNH, the best available literature for the synthesis of this chemical at the industrial scale is from patent US3206281A [2]. For this example, we will build the inventory to produce 1 mole of ZNH.

According to patent US3206281A, ZNH is fabricated at the industrial scale in a two-step process. First, zinc oxide is dissolved in nitric acid. The resulting solution is then evaporated until crystallization. The resulting crystal is $Zn(NO_3)_2 \bullet 6H_2O$, with a molecular weight of 297.49 g/mol [2]. The process reaction is shown below in Equation S1 (not shown that additional water is absorbed during crystallization):

$$ZnO + 2HNO_3 \rightarrow Zn(NO_3)_2 + H_2O\#(S5)$$

Based on this stoichiometry, to produce 1 mole of ZNH, the inputs are 1 mole of zinc oxide and 2 moles of nitric acid. Additionally, some extra water is added in the process for hydration during crystallization, which is accounted for in the mass balance below. Converting this to a mass basis using molecular weights, the inputs for 1 mole of ZNH production (297.5g) become:

Input	Amount (g)
Zinc Oxide	81.38
Nitric Acid	126.0
Water	90.11

Hexamethylenetetramine

Hexamethylenetetramine (HMTA) is a highly soluble compound used as a chemical precursor for the fabrication of ZnO NWs in-solution. HMTA is not found in the EcoInvent database and therefore, the environmental impacts of this chemical must be estimated and modelled in OpenLCA using the best available information from literature. In this study, we reference patent US2542315A [3]. For this example, we will build the inventory to produce 1 mole of HMTA.

According to patent US2542315A, HMTA is fabricated at the industrial scale by reacting gaseous ammonia absorbed in aqueous solutions of formaldehyde under controlled temperature. The resulting product is HMTA with a molecular weight of 140.186 g/mol. Given that we are modelling 1 mole of HMTA, the total weight of the product will be 140.186g. The process reaction is shown below in Equation S2 [3]:

$$6CH_2O + 4NH_3 \rightarrow (CH_2)_{6N_4} + 6H_2O + Heat\#(S6)$$

Based on this stoichiometry, to produce 1 mole of HMTA, the inputs are 6 moles of formaldehyde and 4 moles of ammonia. By-products of the reaction include water and heat. Converting this to a mass basis based on molecular weights, the inputs for 1 mole (140.2g) of product become:

Input	Amount (g)
Formaldehyde	180.2
Ammonia	68.14

Zinc Acetate Dihydrate

Zinc acetate dihydrate (ZAD) is a hydrated salt of zinc and acetate. In this paper, ZAD is used as in the preparation of the ZnO sol-gel for the growth via CBD. ZAD is not found in the EcoInvent database and therefore, the environmental impacts of this chemical must be estimated and modelled in OpenLCA using the best available information from literature. For the case of ZAD, the best available literature at the industrial scale is from patent RU2483056C2 [4]. For this example, we will build the inventory to produce 1 mole of ZAD.

According to patent RU2483056C2, ZAD is fabricated at the industrial scale by dissolving powdered zinc oxide in an aqueous acetic acid solution with ratio of reactants - zinc oxide (zinc hydroxide):water: acetic acid equal to 1:(1.6-2.0):(1.8-2.2) by weight. [4]. The resulting product is crystallized $(CH_3COO)_2Zn \cdot 2H_2O$ with a molecular weight of 219.5 g/mol [2]. The balanced process reaction is shown below in Equation S3 (not shown that additional water is absorbed during crystallization):

$$ZnO + 2CH_3COOH \rightarrow Zn(CH_3COO)_2 + H_2O\#(S7)$$

Based on this stoichiometry, to produce 1 mole of ZAD, the inputs are 1 mole of zinc oxide and 2 moles of acetic acid. Converting this to a mass basis based on molecular weights, the inputs for 1 mole (219.5 g) of product become:

Input	Amount (g)
Zinc Oxide	81.38
Acetic Acid	120.1
Water	18.02

Tartaric Acid

Tartaric acid (TA) is not directly used in this study, but is a precursor to a different chemical used in the ZnO NW synthesis process – sodium tartrate dibasic dihydrate. The literature reference for the production of TA at the industrial scale is patent US3923884A [5]. The production of tartaric acid is a two-step synthetic route from maleic anhydride. The two chemical reactions are shown below in Equations S4 and S5. The first reaction begins with maleic anhydride which is hydrogenated to form maleic acid. For this example, we will build the inventory to produce 1 mole of TA (molecular weight = 150.09 g/mol).

$$C_4H_2O_3 + H_2O \rightarrow C_4H_4O_4 \# (S8)$$

In the next reaction, this maleic acid is reacted with hydrogen peroxide to form tartaric acid.

$$C_4H_4O_4 + \ H_2O_2 \rightarrow C_4H_6O_6 \# (S9)$$

Based on this stoichiometry, to produce 1 mole of TA, the inputs are 1 mole of maleic anhydride, 1 mole of water, and 1 moles of hydrogen peroxide. Converting this to a mass basis based on molecular weights, the inputs for 1 mole (150.1 g/mol) of product become:

Input	Amount (g)
Maleic Anhydride	98.06
Water	18.02
Hydrogen Peroxide	34.01

Sodium Tartrate Dibasic Dihydrate

Sodium tartrate dibasic dihydrate (STDD) is used in this study in the production of ZnO NWs in-solution. In literature, it is documented that STDD is produced by dissolving tartaric acid in water and neutralizing it with sodium hydroxide [6]. The balance chemical reaction is shown below in Equation S6. For this example, we will build the inventory to produce 1 mole of STDD (molecular weight = 230.08g/mol).

$$C_4H_6O_6 + 2NaOH \rightarrow Na_2C_4H_4O_6 + 2H_2O \# (S10)$$

Based on this stoichiometry, to produce 1 mole of STDD, the inputs are 1 mole of tartaric acid and 2 moles of sodium hydroxide. Converting this to a mass basis based on molecular weights, the inputs for 1 mole (230.08g) of product become:

Input	Amount (g)
Tartaric Acid	150.12
Sodium Hydroxide	80.00

References

[1] T. Demes, C. Ternon, D. Riassetto, V. Stambouli, and M. Langlet, “Comprehensive study of hydrothermally grown ZnO nanowires,” *J. Mater. Sci.*, vol. 51, no. 23, pp. 10652–10661, Dec. 2016, doi: 10.1007/s10853-016-0287-8.

[2] M. August, “Process for preparing pulverulent hydrates of zinc nitrate,” US3206281A, Sep. 14, 1965 Accessed: Sep. 25, 2025. [Online]. Available: https://patents.google.com/patent/US3206281A/en

[3] A. G. Eickmeyer, “Method for production of hexamethylenetetramine,” US2542315A, Feb. 20, 1951 Accessed: Sep. 26, 2025. [Online]. Available:

https://patents.google.com/patent/US2542315A/en?q=(%22method+for+production+of+Hexamethylenetetramine%22)&oq=%22method+for+production+of+Hexamethylenetetramine%22

[4] Д. В. Тимофеев *et al.*, “Способ получения двухводного ацетата цинка,” RU2483056C2, May 27, 2013 Accessed: Sep. 26, 2025. [Online]. Available: https://patents.google.com/patent/RU2483056C2/en?q=(%22METHOD+OF+PRODUCING+ZINC+ACETATE+DIHYDRATE%22)&oq=%22METHOD+OF+PRODUCING+ZINC+ACETATE+DIHYDRATE%22

[5] E. Yonemitsu, H. Miyamori, M. Takeda, and Y. Sasaki, “Process for producing DL-tartaric acid,” US3923884A, Dec. 02, 1975 Accessed: Oct. 01, 2025. [Online]. Available: https://patents.google.com/patent/US3923884A/en

[6] “Sodium Tartrate Production Cost Reports,” Procurement Resource. Accessed: Oct. 01, 2025. [Online]. Available: https://www.procurementresource.com/production-cost-report-store/sodium-tartrate?