Anticipatory Life-cycle Assessment of Supercritical Fluid Synthesis of Barium Strontium Titanate Nanoparticles

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This supplementary information document houses the foreground life-cycle inventory used in this study as well as the absolute life-cycle impact assessment values. Any background inventory data (i.e. a unit-process from a life-cycle inventory database such as Ecoinvent[1]) are not included.

1. Foreground inventory

Table S1

Barium isopropoxide, at plant (RER)	Reference Flow Amount: 1kg		Adapted from Ullmann's Encyclopedia of Industrial Chemistry[2]	
Inventory Item	**Amount**	**Units**	**Other**	**Inventory Flow Source**
Barium hydroxide, at plant (RER)	0.69	kg		This study
Electricity, medium voltage, production RER, at grid (RER)	2.0	MJ	Consideration of additional energy consumption during to run auxiliary machines, processes and equipment per the recommendation of "weakly documented chemicals"[1,3]	Ecoinvent[1]
Isopropanol, at plant (RER)	0.471	kg		Ecoinvent
Transport, freight, rail (RER)	0.80	t-km	600 km of freight rail transport	Ecoinvent
Transport, lorry 16-32t, Euro3 (RER)	0.13	t-km	100 km of freight truck transport	Ecoinvent
Water, waste	0.14	kg	Emissions to water	Ecoinvent

Table S2

Barium hydroxide, at plant (RER)	Reference Flow Amount: 1kg		Adapted from Ullmann's Encyclopedia of Industrial Chemistry[4]	
Inventory Item	**Amount**	**Units**	**Other**	**Inventory Flow Source**
Barium oxide, at plant (RER)	0.90	kg		This study
Electricity, medium voltage, production RER, at grid (RER)	2.0	MJ	Consideration of additional energy consumption during to run auxiliary machines, processes and equipment per the recommendation of "weakly documented chemicals"[1,3]	Ecoinvent
Transport, freight, rail (RER)	0.54	t-km	600 km of freight rail transport	Ecoinvent
Transport, lorry 16-32t, Euro3 (RER)	0.090	t-km	100 km of freight truck transport	Ecoinvent
Water, waste	0.95	kg		Ecoinvent
Water, waste	0.84	kg	Emissions to water	Ecoinvent

Table S3

Barium oxide, at plant (RER)	Reference Flow Amount: 1kg		Adapted from Ullmann's Encyclopedia of Industrial Chemistry[4]	
Inventory Item	**Amount**	**Units**	**Other**	**Inventory Flow**

				Source
Barium carbonate, at plant (RER)	0.1.29	kg		This study
Electricity, medium voltage, production RER, at grid (RER)	2.0	MJ	Consideration of additional energy consumption during to run auxiliary machines, processes and equipment per the recommendation of "weakly documented chemicals"[1,3]	Ecoinvent
Hard coal coke, at plant (RER)	0.078	kg		Ecoinvent
Heat, light fuel oil, at industrial furnace 1MW (RER)	1.025	MJ		Ecoinvent
Transport, freight, rail (RER)	0.81	t-km	600 km of freight rail transport	Ecoinvent
Transport, lorry 16-32t, Euro3 (RER)	0.14	t-km	100 km of freight truck transport	Ecoinvent
Carbon monoxide, fossil	0.18	kg	Emissions to air	Ecoinvent

Table S4

Barium carbonate, at plant (RER)	Reference Flow Amount: 1kg		Adapted from Ullmann's Encyclopedia of Industrial Chemistry[4]	
Inventory Item	**Amount**	**Units**	**Other**	**Inventory Flow Source**
Barium sulfide, at plant (RER)	0.86	kg		This study
Electricity, medium voltage, production RER, at grid (RER)	2.0	MJ	Consideration of additional energy consumption during to run auxiliary machines, processes and equipment per the recommendation of "weakly documented chemicals"[1,3]	Ecoinvent
Disposal, inert waste, 5% water, to inert landfill (GLO)	0.40	kg		Ecoinvent
Heat, light fuel oil, at industrial furnace 1MW (RER)	0.0040	MJ		Ecoinvent
Sodium carbonate from ammonium chloride production, at plant (GLO)	0.53	kg		Ecoinvent
Transport, freight, rail (RER)	0.81	t-km	600 km of freight rail transport	Ecoinvent
Transport, lorry 16-32t, Euro3 (RER)	0.14	t-km	100 km of freight truck transport	Ecoinvent

Table S5

Barium sulfide, at plant (RER)	Reference Flow Amount: 1kg		Adapted from Ullmann's Encyclopedia of Industrial Chemistry[4]	
Inventory Item	**Amount**	**Units**	**Other**	**Inventory Flow Source**
Barite, at plant (RER)	1.38	kg		Ecoinvent
Electricity, medium voltage, production RER, at grid (RER)	2.0	MJ	Consideration of additional energy consumption during to run auxiliary machines, processes and equipment per the recommendation of "weakly documented chemicals"[1,3]	Ecoinvent
Hard coal coke, at plant (RER)	0.14	kg		Ecoinvent

Heat, light fuel oil, at industrial furnace 1MW (RER)	0.14	MJ		Ecoinvent
Transport, freight, rail (RER)	0.91	t-km	600 km of freight rail transport	Ecoinvent
Transport, lorry 16-32t, Euro3 (RER)	0.15	t-km	100 km of freight truck transport	Ecoinvent
Carbon dioxide, fossil	0.52	kg	Emissions to air	Ecoinvent

Table S6

Strontium isopropoxide, at plant (RER)	Reference Flow Amount: 1kg		Adapted from Ullmann's Encyclopedia of Industrial Chemistry and based on mass allocation[2]	
Inventory Item	**Amount**	**Units**	**Other**	**Inventory Flow Source**
Ammonia, liquid, at regional storehouse (RER)	0.11	kg		Ecoinvent
Electricity, medium voltage, production RER, at grid (RER)	0.82	MJ	Consideration of additional energy consumption during to run auxiliary machines, processes and equipment per the recommendation of "weakly documented chemicals"[1,3]	Ecoinvent
Isopropanol, at plant (RER)	0.40	kg		Ecoinvent
Strontium chloride, at plant (RER)	0.52	kg		This study
Transport, freight, rail (RER)	0.98	t-km	600 km of freight rail transport	Ecoinvent
Transport, lorry 16-32t, Euro3 (RER)	0.11	t-km	100 km of freight truck transport	Ecoinvent
Ammonium chloride, at plant (GLO)	0.47	kg	Co-product	Ecoinvent

Table S7

Strontium chloride, at plant (RER)	Reference Flow Amount: 1kg		Adapted from Ullmann's Encyclopedia of Industrial Chemistry[5]	
Inventory Item	**Amount**	**Units**	**Other**	**Inventory Flow Source**
Electricity, medium voltage, production RER, at grid (RER)	0.82	MJ	Consideration of additional energy consumption during to run auxiliary machines, processes and equipment per the recommendation of "weakly documented chemicals"[1,3]	Ecoinvent
Heat, natural gas, at industrial furnace > 100kW (RER)	0.33	MJ		Ecoinvent
Hydrochloric acid, from the reaction of hydrogen with chlorine, at plant (RER)	0.23	kg		Ecoinvent
Strontium carbonate, at plant (RER)	0.93	kg		Ecoinvent 3.2*
Transport, freight, rail (RER)	0.55	t-km	600 km of freight rail transport	Ecoinvent
Transport, lorry 16-32t, Euro3 (RER)	0.092	t-km	100 km of freight truck transport	Ecoinvent
Carbon dioxide, fossil	0.28	kg	Emissions to air	Ecoinvent
Carbon monoxide, fossil	0.30	kg	Emissions to air	Ecoinvent
Water, waste	0.11	kg	Emissions to water	Ecoinvent

Table S8

Titanium isopropoxide, at plant (RER)	Reference Flow Amount: 1kg		Adapted from Ullmann's Encyclopedia of Industrial Chemistry and based on mass allocation[2]	
Inventory Item	**Amount**	**Units**	**Other**	**Inventory Flow Source**
Ammonia, liquid, at regional storehouse (RER)	0.12	kg		Ecoinvent
Electricity, medium voltage, production RER, at grid (RER)	0.82	MJ	Consideration of additional energy consumption during to run auxiliary machines, processes and equipment per the recommendation of "weakly documented chemicals"[1,3]	Ecoinvent
Isopropanol, at plant (RER)	0.85	kg		Ecoinvent
Titanium tetrachloride, at plant (RER)	0.67	kg		This study
Transport, freight, rail (RER)	0.98	t-km	600 km of freight rail transport	Ecoinvent
Transport, lorry 16-32t, Euro3 (RER)	0.16	t-km	100 km of freight truck transport	Ecoinvent
Ammonium chloride, at plant (GLO)	0.38	kg	Co-product	Ecoinvent
Hydrochloric acid, from the reaction of hydrogen with chlorine, at plant (RER)	0.23	kg	Co-product	Ecoinvent

Table S9

Titanium tetrachloride, at plant (RER)	Reference Flow Amount: 1kg		Adapted from Ullmann's Encyclopedia of Industrial Chemistry[6]	
Inventory Item	**Amount**	**Units**	**Other**	**Inventory Flow Source**
Carbon black, at plant (GLO)	0.13	kg		Ecoinvent
Chlorine, liquid, production mix, at plant (RER)	0.37	kg		Ecoinvent
Electricity, medium voltage, production RER, at grid (RER)	2.0	MJ	Consideration of additional energy consumption during to run auxiliary machines, processes and equipment per the recommendation of "weakly documented chemicals"[1,3]	Ecoinvent
Heat, natural gas, at industrial furnace > 100kW (RER)	0.47	MJ		Ecoinvent
Ilmenite, 54% titanium dioxide, at plant (AU)	0.42	kg		Ecoinvent
Transport, freight, rail (RER)	0.54	t-km	600 km of freight rail transport	Ecoinvent
Transport, lorry 16-32t, Euro3 (RER)	0.092	t-km	100 km of freight truck transport	Ecoinvent
Carbon monoxide, fossil	0.30	kg	Emissions to air	Ecoinvent

Table S10

Barium acetate, at plant (RER)	Reference Flow Amount: 1kg		Estimated from the reaction of barium carbonate with acetic acid: BaCO3 + 2 CH3COOH --> (CH3COO)2Ba + CO2 + H20	
Inventory Item	**Amount**	**Units**	**Other**	**Inventory Flow**

				Source
Acetic acid, 98% in H2O, at plant (RER)	0.24	kg		Ecoinvent
Barium carbonate, at plant (RER)	0.77	kg		This study
Electricity, medium voltage, production RER, at grid (RER)	1.2	MJ	Consideration of additional energy consumption during to run auxiliary machines, processes and equipment per the recommendation of "weakly documented chemicals"[1,3]	Ecoinvent
Heat, natural gas, at industrial furnace > 100kW (RER)	0.8	MJ	Consideration of additional energy consumption during to run auxiliary machines, processes and equipment per the recommendation of "weakly documented chemicals"[1,3]	Ecoinvent
Ilmenite, 54% titanium dioxide, at plant (AU)	0.42	kg		Ecoinvent
Transport, freight, rail (RER)	0.60	t-km	600 km of freight rail transport	Ecoinvent
Transport, lorry 16-32t, Euro3 (RER)	0.10	t-km	100 km of freight truck transport	Ecoinvent
Carbon dioxide, fossil	0.17	kg	Emissions to air	Ecoinvent
Water, waste	0.071	kg	Emissions to water	Ecoinvent

Table S11

Strontium acetate, at plant (RER)	Reference Flow Amount: 1kg		Estimated from the reaction of strontium carbonate with acetic acid: SrCO3 + 2 CH3COOH --> (CH3COO)2Sr + CO2 + H20	
Inventory Item	**Amount**	**Units**	**Other**	**Inventory Flow Source**
Acetic acid, 98% in H2O, at plant (RER)	0.58	kg		Ecoinvent
Electricity, medium voltage, production RER, at grid (RER)	1.2	MJ	Consideration of additional energy consumption during to run auxiliary machines, processes and equipment per the recommendation of "weakly documented chemicals"[1,3]	Ecoinvent
Heat, natural gas, at industrial furnace > 100kW (RER)	0.8	MJ	Consideration of additional energy consumption during to run auxiliary machines, processes and equipment per the recommendation of "weakly documented chemicals"[1,3]	Ecoinvent
Strontium carbonate, at plant (RER)	0.15	kg		This study
Transport, freight, rail (RER)	0.43	t-km	600 km of freight rail transport	Ecoinvent
Transport, lorry 16-32t, Euro3 (RER)	0.072	t-km	100 km of freight truck transport	Ecoinvent
Carbon dioxide, fossil	0.21	kg	Emissions to air	Ecoinvent
Water, waste	0.088	kg	Emissions to water	Ecoinvent

Table S12

Strontium hydroxide, at plant (RER)	Reference Flow Amount: 1kg		Estimated from the reaction of strontium nitrate and a base such as sodium hydroxide: Sr(NO3)2 + 2NaOH + H2O ==> Sr(OH)2 + 2NaNO3, with consideration of mass allocation.	
Inventory Item	**Amount**	**Units**	**Other**	**Inventory Flow Source**
Electricity, medium voltage, production RER,	0.88	MJ	Consideration of additional energy consumption during to run auxiliary machines,	Ecoinvent

at grid (RER)			processes and equipment per the recommendation of “weakly documented chemicals”[1,3]	
Sodium hydroxide, 50% in H2O, production in mix, at plant (RER)	0.29	kg		Ecoinvent
Strontium nitrate, at plant (RER)	0.77	kg		This study
Transport, freight, rail (RER)	0.42	t-km	600 km of freight rail transport	Ecoinvent
Transport, lorry 16-32t, Euro3 (RER)	0.040	t-km	100 km of freight truck transport	Ecoinvent
Water, ultrapure, at plant (GLO)	0.48	kg		Ecoinvent
Chemicals inorganic, at plant (GLO)	1.26	kg	Co-product	Ecoinvent
Water, waste	0.084	kg	Emissions to water	Ecoinvent

2. Absolute life-cycle impact assessment results

Table S13 Absolute midpoint life-cycle impact results for all supercritical synthesis routes performed in this study.

Scenario Name	Scenario Description	Agri-cultural land	Climate change	Cumulative energy...	Fossil depletion	Freshwater ecotoxicity	Fresh-water eutro...	Human toxicity	Ionising radiation	Marine ecotoxicity	Marine eutrophic-cation	Metal depletion	Natural land transform	Ozone depletion	Particulate matter	Photo-chemical oxidant formation	Terrestrial acidification	Terrestrial ecotoxicity	Urban land occupation	Water depletion
		m2a	kg CO2 eq	MJ-eq	kg oil eq	kg 1,4-DB eq	kg P eq	kg 1,4-DB eq	kg U235 eq	kg 1,4-DB eq	kg N eq	kg Fe eq	m2	kg CFC-11 eq	kg PM10 eq	kg NMVOC	kg SO2 eq	kg 1,4-DB eq	m2a	m3
BST (default)	Default	1.61E+00	5.84E+02	9.82E+03	2.11E+02	1.90E-03	8.25E-02	5.46E+00	1.61E+01	8.71E-02	2.95E-02	5.63E+00	7.52E-02	3.04E-05	3.03E-01	1.25E+00	8.66E-01	1.45E-02	8.12E-01	2.31E+02
BST(0.1M)	0.1 Molar Precursors	3.08E-01	9.77E+01	1.69E+03	3.60E+01	3.73E-04	1.46E-02	1.07E+00	3.70E+00	1.64E-02	5.64E-03	1.02E+00	1.28E-02	5.23E-06	5.38E-02	2.28E-01	1.55E-01	2.57E-03	1.52E-01	4.91E+01
BST(1.0M)	1.0 Molar Precursors	8.65E-02	1.51E+01	3.05E+02	6.24E+00	1.13E-04	3.08E-03	3.22E-01	1.60E+00	4.33E-03	1.59E-03	2.34E-01	2.17E-03	9.35E-07	1.14E-02	5.48E-02	3.37E-02	5.42E-04	3.91E-02	1.81E+01
BST(R)	Default + Recycling	7.00E-01	1.18E+02	2.68E+03	5.51E+01	2.16E-03	2.70E-02	2.98E+00	1.14E+01	5.51E-02	1.21E-02	1.20E+00	2.60E-02	1.21E-05	9.57E-02	3.11E-01	2.80E-01	6.65E-03	4.55E-01	1.39E+02
BST(M)	Methanol Solvent	4.38E-01	5.06E+02	8.25E+03	1.75E+02	1.67E-03	2.70E-02	3.60E+00	1.63E+01	4.10E-02	2.25E-02	2.96E+00	1.18E-01	4.79E-05	1.90E-01	5.85E-01	5.51E-01	1.53E-02	6.50E-01	1.81E+02
BST(M.R)	Methanol + Recycling	5.29E-01	1.04E+02	2.39E+03	4.89E+01	2.12E-03	1.89E-02	2.70E+00	1.14E+01	4.84E-02	1.10E-02	8.14E-01	3.15E-02	1.42E-05	7.87E-02	2.12E-01	2.32E-01	6.72E-03	4.30E-01	1.32E+02
BST(I)	Default + Isopropanol	2.46E+00	6.69E+02	1.20E+04	2.54E+02	3.76E-03	4.71E-02	8.61E+00	2.72E+01	1.27E-01	3.66E-02	8.72E+00	8.76E-02	3.63E-05	4.36E-01	1.53E+00	1.39E+00	1.66E-02	9.58E-01	3.38E+02
BST(I.R)	Isopropanol + Recycling	8.22E-01	1.28E+02	2.94E+03	6.04E+01	2.43E-03	2.18E-02	3.43E+00	1.30E+01	6.08E-02	1.31E-02	1.65E+00	2.71E-02	1.25E-05	1.14E-01	3.49E-01	3.53E-01	6.92E-03	4.75E-01	1.54E+02
BST(BA)	Barium Acetate Precursor	6.39E-02	6.72E+00	1.63E+02	3.19E+00	9.68E-05	2.03E-03	2.54E-01	1.44E+00	3.18E-03	7.90E-04	1.42E-01	1.53E-03	6.71E-07	6.80E-03	2.87E-02	2.02E-02	3.77E-04	3.04E-02	1.55E+01
BSY(BH)	Barium Hydroxide Precursor	5.29E-02	5.87E+00	1.39E+02	2.71E+00	9.13E-05	1.70E-03	2.46E-01	1.18E+00	2.97E-03	7.18E-04	1.13E-01	1.13E-03	5.42E-07	6.10E-03	3.02E-02	1.82E-02	3.33E-04	2.71E-02	1.28E+01
BST(Ti)	Titanium Dioxide Precursor	7.90E-02	7.23E+00	1.51E+02	2.88E+00	1.08E-04	2.27E-03	2.51E-01	1.55E+00	3.89E-03	2.69E-03	1.74E-01	1.55E-03	6.68E-07	1.09E-02	2.85E-02	3.02E-02	4.23E-04	3.18E-02	1.70E+01
BST(R.1.0M)	Recycling + 1.0 Molar	7.20E-02	7.66E+00	1.91E+02	3.77E+00	1.18E-04	2.20E-03	2.82E-01	1.52E+00	3.82E-03	1.32E-03	1.63E-01	1.38E-03	6.43E-07	8.13E-03	3.99E-02	2.44E-02	4.18E-04	3.34E-02	1.67E+01
BST(R.1.0M)*	x = 0.0	7.63E-02	8.06E+00	1.96E+02	3.83E+00	1.21E-04	2.38E-03	2.85E-01	1.71E+00	4.01E-03	1.60E-03	1.67E-01	1.44E-03	6.61E-07	8.54E-03	4.06E-02	2.57E-02	4.47E-04	3.53E-02	1.85E+01
BST(R.1.0M)*	x = 0.2	7.31E-02	7.75E+00	1.90E+02	3.73E+00	1.18E-04	2.25E-03	2.81E-01	1.60E+00	3.87E-03	1.43E-03	1.62E-01	1.40E-03	6.47E-07	8.22E-03	3.97E-02	2.47E-02	4.28E-04	3.40E-02	1.74E+01
BST(R.1.0M)*	x = 0.4	6.99E-02	7.44E+00	1.84E+02	3.62E+00	1.15E-04	2.11E-03	2.77E-01	1.50E+00	3.73E-03	1.25E-03	1.57E-01	1.36E-03	6.33E-07	7.90E-03	3.88E-02	2.37E-02	4.08E-04	3.26E-02	1.63E+01
BST(R.1.0M)*	x = 0.6	6.64E-02	7.09E+00	1.77E+02	3.50E+00	1.13E-04	1.96E-03	2.73E-01	1.37E+00	3.57E-03	1.05E-03	1.52E-01	1.31E-03	6.18E-07	7.54E-03	3.79E-02	2.26E-02	3.86E-04	3.11E-02	1.51E+01
BST(R.1.0M)*	x = 0.8	6.22E-02	6.70E+00	1.69E+02	3.37E+00	1.09E-04	1.79E-03	2.69E-01	1.24E+00	3.39E-03	8.29E-04	1.46E-01	1.25E-03	6.00E-07	7.12E-03	3.67E-02	2.13E-02	3.60E-04	2.93E-02	1.37E+01
BST(R.1.0M)*	x = 1.0	5.79E-02	6.27E+00	1.61E+02	3.22E+00	1.05E-04	1.61E-03	2.63E-01	1.09E+00	3.20E-03	5.86E-04	1.40E-01	1.19E-03	5.81E-07	6.68E-03	3.55E-02	1.99E-02	3.33E-04	2.74E-02	1.21E+01

* Sensitivity analysis where x is the amount of moles of strontium used in the BST using the supercritical synthesis route that includes a 1.0 M precursor concentration and recycling of ethanol as a solvent

Table S14 Percent contribution of critical life-cycle stages to the total impacts of the 0.015 M (*default)* supercritical synthesis scenario

	Precursors	Solvent	Reaction	Drying/Dewater	Other
Agricultural land	3.77%	91.48%	0.41%	0.00%	4.34%
Climate change	0.95%	94.64%	3.27%	0.02%	1.12%
Cumulative energy demand	1.48%	93.91%	3.41%	0.02%	1.18%
Fossil depletion	1.35%	94.27%	3.39%	0.03%	0.96%
Freshwater ecotoxicity	4.38%	91.16%	1.45%	0.01%	3.00%
Freshwater eutrophication	2.12%	94.65%	0.35%	0.00%	2.88%
Human toxicity	4.32%	92.55%	0.83%	0.00%	2.30%
Ionising radiation	8.27%	77.96%	1.20%	0.01%	12.56%
Marine ecotoxicity	3.38%	93.76%	0.27%	0.00%	2.59%
Marine eutrophication	7.03%	87.57%	1.77%	0.02%	3.61%
Metal depletion	2.52%	92.63%	0.33%	0.00%	4.52%
Natural land transform	1.22%	90.47%	5.61%	0.05%	2.65%
Ozone depletion	1.40%	87.38%	8.76%	0.07%	2.39%
Particulate matter	2.13%	91.63%	1.48%	0.01%	4.75%
Photochemical oxidantant formation	2.78%	92.13%	1.46%	0.01%	3.62%
Terrestrial acidification	2.25%	92.32%	1.58%	0.01%	3.84%
Terrestrial ecotoxicity	2.13%	93.60%	2.11%	0.02%	2.14%
Urban land occupation	3.01%	79.48%	0.91%	0.00%	16.60%
Water depletion	6.18%	83.21%	0.91%	0.00%	9.70%
Average	3.19%	90.25%	2.08%	0.01%	4.46%

Table S15 Percent contribution of critical life-cycle stages to the total impacts of the 1.0 M + recycling supercritical synthesis scenario

	Precursors	Solvent	Reaction	Drying/Dewater	Other
Agricultural land	84.36%	12.80%	0.15%	0.07%	2.62%
Climate change	73.35%	18.09%	3.96%	1.88%	2.72%
Cumulative energy demand	76.74%	17.29%	2.79%	1.33%	1.85%
Fossil depletion	75.70%	18.18%	3.02%	1.43%	1.67%
Freshwater ecotoxicity	70.99%	27.59%	0.37%	0.28%	0.77%
Freshwater eutrophication	80.00%	16.35%	0.21%	0.10%	3.34%
Human toxicity	83.75%	14.50%	0.26%	0.12%	1.37%
Ionising radiation	87.41%	8.11%	0.20%	0.10%	4.18%
Marine ecotoxicity	77.35%	20.79%	0.10%	0.05%	1.71%
Marine eutrophication	78.00%	17.54%	1.86%	0.05%	2.55%
Metal depletion	87.24%	7.70%	0.18%	0.09%	4.79%
Natural land transform	66.74%	21.63%	4.86%	2.31%	4.46%
Ozone depletion	66.37%	20.41%	6.59%	3.14%	3.49%
Particulate matter	79.47%	13.77%	0.87%	0.42%	5.47%
Photochemical oxidant formation	86.98%	8.48%	0.72%	0.34%	3.48%

Terrestrial acidification	80.55%	13.93%	0.89%	0.42%	4.21%
Terrestrial ecotoxicity	73.98%	21.54%	1.16%	0.55%	2.77%
Urban land occupation	73.37%	13.69%	0.35%	0.17%	12.42%
Water depletion	85.98%	9.59%	0.20%	0.10%	4.13%
Average	78.33%	15.89%	1.51%	0.68%	3.58%

3. Comparison to Conventional Synthesis Routes

Solid-state synthesis was compared to supercritical fluid synthesis in order to make an eternal comparison of the life-cycle impacts to a more conventional method of particle production. This synthesis route was not completed in the lab nor was industrial-scale data available for most of the inventory, and thus the LCA was dependent on secondary data to create the life-cycle inventory and model. This model was not meant to represent the current technology, but instead, embody an approach to make reasonable comparisons to the supercritical lab-scale inventory.

Solid state (SS) synthesis refers to the direct mechanical processes (e.g. physical impact) of reducing the size of a material. SS synthesis was modelled using high energy ball milling in a planetary ball mill. The inventory (Table S16) was partially taken from previously reported operating parameters for milling of sub-micron copper oxide particles[7] as well as for that typical of mechanical production of barium titanate nanoparticles[8–11]. Barium carbonate, strontium carbonate and titanium dioxide were pre-milled as a dry powder and then calcined at 900°C. A second wet milling procedure took place in ethanol in a 70:30 mixture of solids to wetting agent. Nanomaterials were dewatered, dried and calcined up to 1200°C. All heating was modelled in a low temperature continuous furnace with an efficiency of 25% per hour.

Table S16

Barium strontium titanate nanoparticles, solid state synthesis, at plant (RER)	Reference Flow Amount: 1kg		Adapted from ball milling in procedures typical of producing other metal oxide micron and sub-micron particles at industrial scale[7] and for mechanical production of barium titanate nanoparticles[8–11]	
Inventory Item	**Amount**	**Units**	**Other**	**Inventory Flow Source**
Annealing†	1.08	MJ		Ecoinvent
Barium carbonate	0.42	kg		This study
Calcining†	0.807	MJ		Ecoinvent
Dewatering/Drying†	1.2	MJ		This study
Milling (Wet)	1.0	# items	See Table S17	This study
Pre-milling (Dry)	1.0	# items	See Table S18	This Study
Strontium carbonate	0.32	kg		This study
Titanium dioxide	0.34	kg		Ecoinvent
Transport, freight, rail – RER	21.09	t*km		Ecoinvent
Transport, lorry, 16-32, EURO3 – RER	3.51	t*km		Ecoinvent

†Heat from natural gas

Table S17

Milling (Wet)	Reference Flow Amount: 1 item		Adapted from ball milling in procedures typical of producing other metal oxide micron and sub-micron particles at industrial scale[7].	
Inventory Item	**Amount**	**Units**	**Other**	**Inventory Flow Source**
Electricity, production mix RER – RER	2.69	MJ		Ecoinvent
Ethanol from ethylene, at plant – GLO	0.25	kg		Ecoinvent
Water, ultrapure, at plant – GLO	0.22	kg		Ecoinvent

Table S18

Pre-milling (Dry)	Reference Flow Amount: 1 item		Adapted from ball milling in procedures typical of producing other metal oxide micron and sub-micron particles at industrial scale[7].	
Inventory Item	**Amount**	**Units**	**Other**	**Inventory Flow Source**
Electricity, production mix RER – RER	2.69	MJ		Ecoinvent

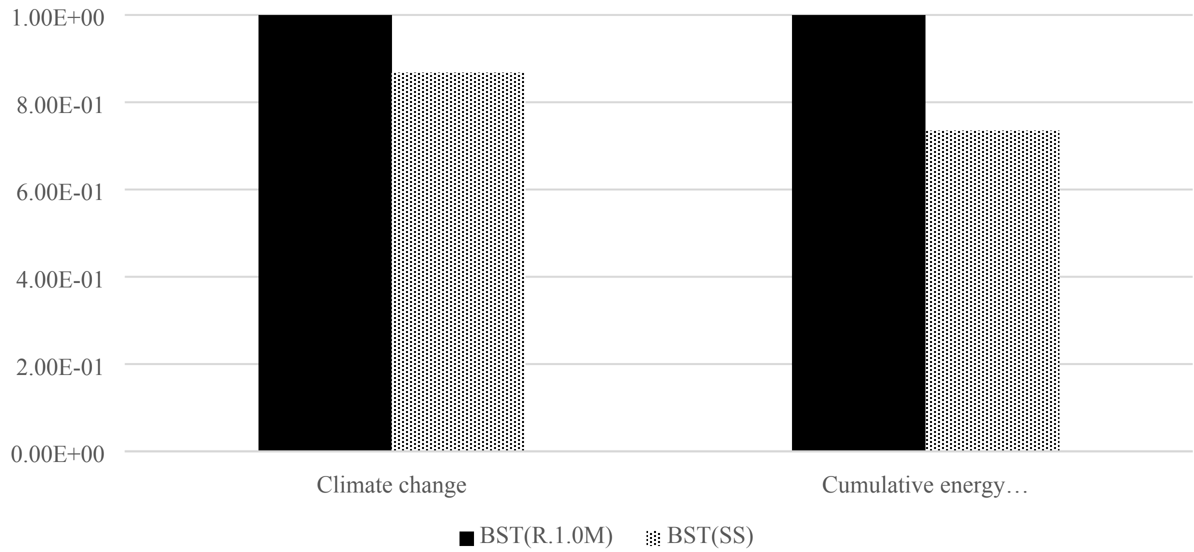

Figure S1 Comparison of the best case supercritical synthesis route (1.0 molar precursor concentration plus recycling of the ethanol solvent) with an estimated solid state manufacturing process. Absolute values of climate change were 7.66 and 6.95 kg CO_2-eq. and for cumulative energy demand were 191.15 and 140.98 MJ-eq. for the supercritical and solid-state pathways, respectively. SS: solid-state. R: recycling.

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