Electronic Supplementary Material (ESI) for Energy & Environmental Science.

Supporting Information

The significance of Li-ion batteries in electric vehicle life-cycle energy and emissions and recycling's role in its reduction

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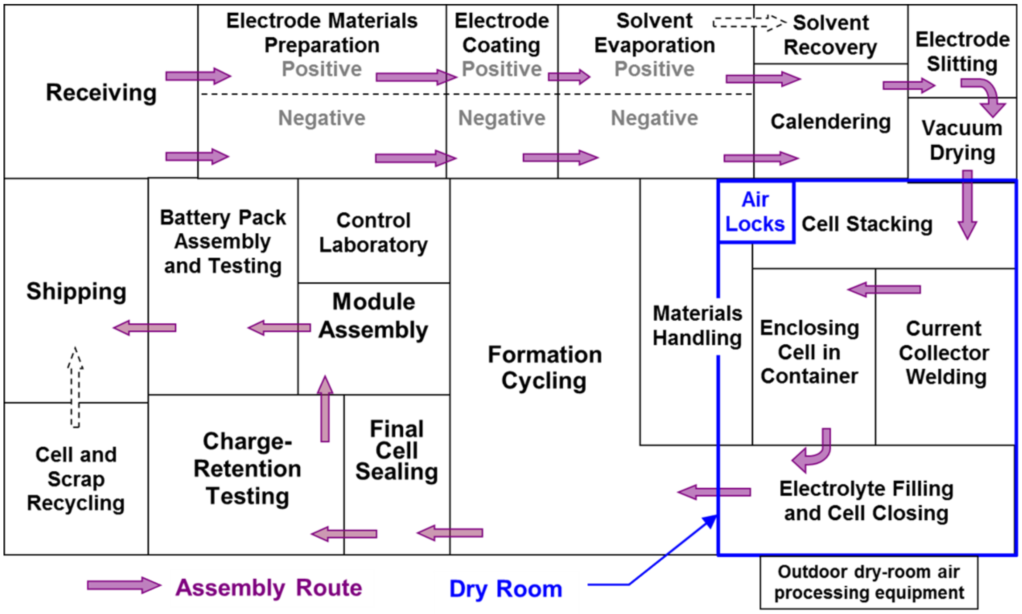

The areas in this diagram for each processing step are approximately proportional to the estimated plant areas in the baseline plant.

Figure S1. Battery assembly plant schematic[1]

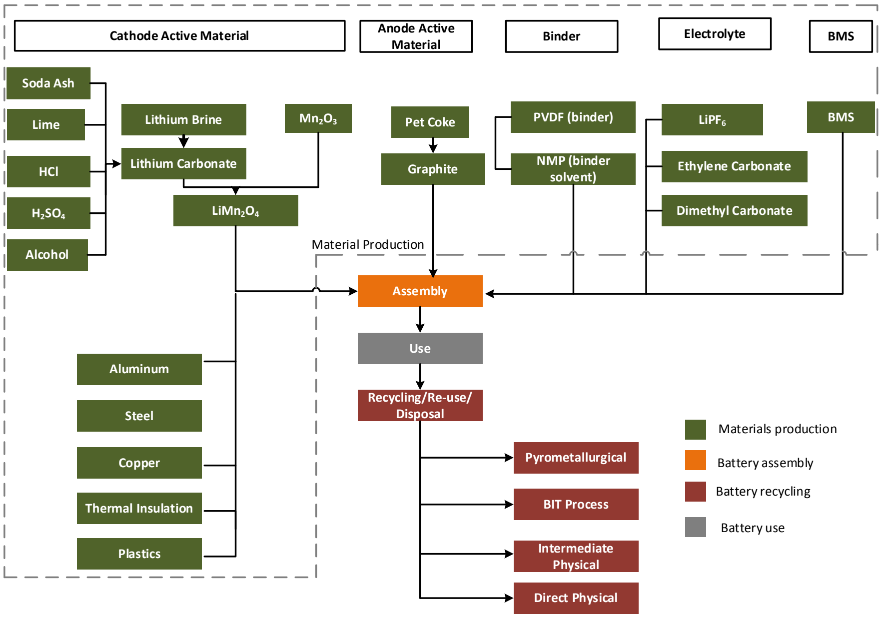

Figure S2. Steps and materials in the production of the lithium-ion battery with the assembly step separated from all material production steps. BMS = battery management system

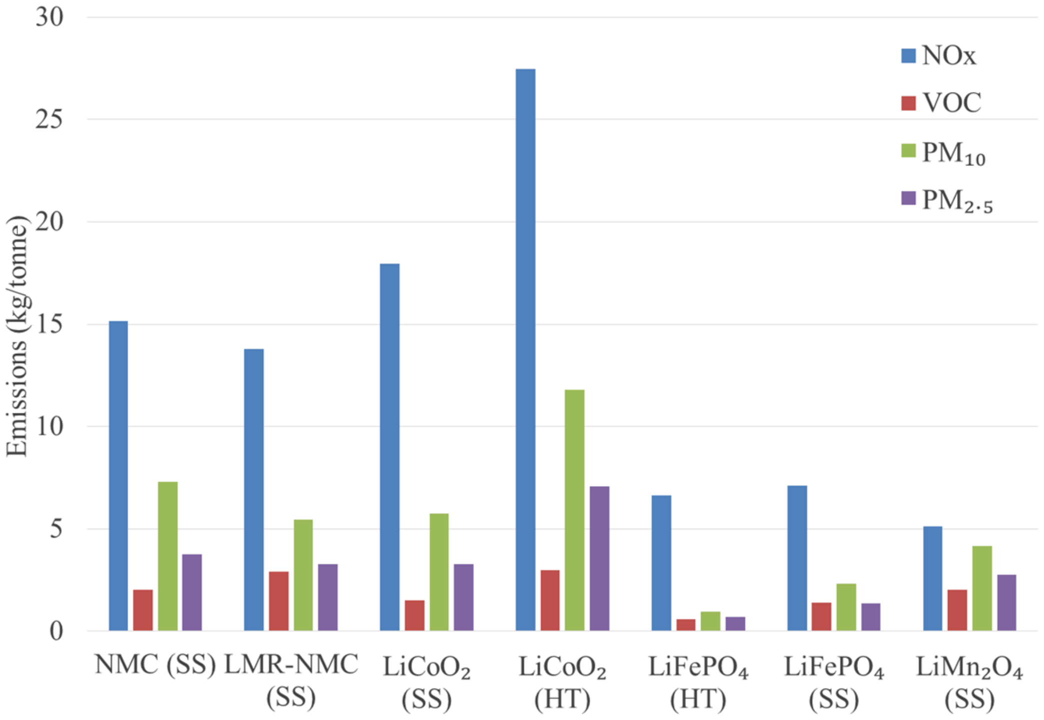

Figure S3. Cradle-to-gate NOx, VOC, PM_{10}, and $PM_{2.5}$ emissions (kg/tonne) for different cathode materials

The following table provides material and purchased energy flows for the preparation of cathode materials by solid-state (SS) or hydrothermal (HT) preparation techniques. Complete material and energy flows for all compounds used in this analysis are provided in Dunn et al. 2014[2] and in the 2014 release of the GREET model (http://es.greet.anl.gov).

Table S1. Material (kg/kg) and purchased energy (MJ/kg) inputs for the production of cathode materials via solid-state (SS) or hydrothermal (HT) preparation.

	NCM SS	LFP HT	LMR-NMC SS	LCO SS	LCO HT	LFP SS	LMO SS
Material Inputs (kg/kg cathode)							
$Ni_{0.4}Co_{0.2}Mn_{0.4}(OH)_2$	0.95		0.85				
Lithium Hydoxide	0.25	0.27			0.25		
Oxygen	0.08		0.37				
Phosphoric Acid		0.37					
Iron Sulfate		0.57					
Lithium Carbonate			0.52	0.38		0.23	0.20
Cobalt Oxide				0.82			
Hydrochloric acid					0.12		
Sodium Chlorate					0.45		
Sodium Hydroxide					1.9		
Cobalt Chloride					1.3		
Iron Oxide						0.49	
Diammonium Phosphate						0.84	
Manganese Oxide							0.87
Purchased Energy Inputs (MJ/kg cathode)							
Natural Gas					34		15
Electricity	2.2	36	3.2	1.2		2.9	0.15

Table S2. Cathode material properties[3]

Chemical Formula	Abbreviation	Specific Energy (Wh/kg vs Li-metal)	Capacity (mAh/g)	Advantages	Drawbacks
$LiMn_2O_4$	LMO	405	100	• Low cost • High power density	• Lower energy density • Accelerated capacity fade
$LiCoO_2$	LCO	610	150	• High energy density	• High cost • Moderate stability
$LiFePO_4$	LFP	515	150	• High power density • Very stable	• Lower energy density
$LiNi_{0.4}Co_{0.2}Mn_{0.4}O_2$	NMC	675	150	• Performs well for all metrics	• Moderate cost • Moderate stability
$0.5Li_2MnO_3 \cdot 0.5LiNi_{0.44}Co_{0.25}Mn_{0.31}O_2$	LMR-NMC	940	250	• High energy density • Low cost	• Not commercial • Degrades quickly

The following tables report battery parameters as determined with Argonne's BatPaC model[3] and incorporated into GREET.

Table S3. BEV Battery Properties

	LMO	LCO	NMC	LFP	LMR-NMC
Power (kW)	149				
Energy (kWh)	28				
Energy Requirement (Wh/km)	136				
Cells in Battery	96	96	96	100	100

Table S4. PHEV Battery Properties

	PHEV		
	LMO	NMC	LFP
Power (kW)	60		
Energy (kWh)	9		
Energy Requirement (Wh/km)	136		
Cells in Battery	96	96	100

Table S5. PHEV Battery Composition

	PHEV		
Material (wt%)	NMC	LMO	LFP
Active Material	15	27	17
Wrought Aluminum	26	22	27
Copper	25	15	19
Graphite/Carbon	9.7	12	11
Electrolyte: Ethylene Carbonate	4.7	4.8	6.3
Electrolyte: Dimethyl Carbonate	4.7	4.8	6.3
Electrolyte: $LiPF_6$	1.6	1.7	2.2
Electronic Parts	2.2	2.8	2.2
Steel	2.0	2.0	2.1
Binder	1.3	2.1	1.4
Polypropylene	3.7	2.2	2.9
Polyethylene	0.75	0.38	0.52
Polyethylene Terephthalate	1.6	1.7	1.8
Glycol (coolant)	1.1	1.3	1.2
Thermal Insulation	0.30	0.34	0.42
Total Mass (kg)	108	85	107

Table S6. BEV Battery Composition

	BEV					
Material (wt%)	LFP	NMC	LCO	LMO	LMR-NMC (Gr anode)	LMR-NMC (Gr/Si anode)
Active Material	24	28	29	34	20.	24
Wrought Aluminum	20.	20.	20.	19	22	25
Copper	12	11	11	11	15	20.
Graphite/Carbon	15	18	18	15	20.	5.6
Electrolyte: Ethylene Carbonate	7.8	5.4	5.4	5.4	5.5	5.6
Electrolyte: Dimethyl Carbonate	7.8	5.4	5.4	5.4	5.5	5.6
Electrolyte: $LiPF_6$	2.7	1.9	1.9	1.9	1.9	1.9
Electronic Parts	1.0	1.3	1.4	1.1	1.5	1.7
Steel	1.6	1.4	1.4	1.4	1.4	1.2
Binder	2.1	2.5	2.5	2.5	2.1	2.1
Polypropylene	1.9	1.7	1.6	1.7	2.1	2.8
Polyethylene	0.33	0.30	0.28	0.29	0.40	0.56
Polyethylene Terephthalate	1.4	1.2	1.2	1.2	1.2	1.2
Glycol (coolant)	0.99	1.0	1.1	0.95	1.1	1.3
Thermal Insulation	0.35	0.36	0.37	0.33	0.39	0.41
Total Mass (kg)	230	180	170	210	160	140

Table S7. Contribution (MJ/kg cathode material) to cathode cradle-to-gate energy intensity of cathode inputs. (Data correspond to Figure 1 in the main text.) Values are full fuel cycle (not purchased) energy.

Input	NMC	LMR-NMC	LCO (SS)	LCO (HT)	LFP (HT)	LFP (SS)	LMO (SS)
NiO	62	30					
CoO	31	35	150	150			
MnO	3.7	3.0					
H_2SO_4		0.23					0.02
NH_3		6.9					
NaOH	29	2.4		66			
Lime							0.08
Alcohol							0.0071
Na_2CO_3							3.7
Li Brine							0.68
Ni/Co/Mn precursor	11	9.7					
LiOH	13			13	14		
O_2		1.1					
NMC	4.9						
Li_2CO_3		24	17			11	2.9
LMR-NMC		3.5					
Co_3O_4			0.71				
$LiCoO_2$			2.8	38			
H_2				5.0			0.04
Cl_2				20.			0.14
HCl							0.23
$CoCl_2$				0.70			
NaCl				0.36			0.05
$NaClO_3$				17			
H_3PO_4					1.6		
$FeSO_4$							
$LiFePO_4$					40.	6.5	
Fe_3O_4						0.69	
$(NH_4)_2HPO_4$						16	
Mn_2O_3							12
$LiMn_2O_4$							14
Total	155	116	173	313	56	34	35

Table S8. Contribution of battery components to cradle-to-gate battery energy intensity (MJ/kg battery) (Data correspond to Figure 3 in the main text.) Values are full fuel cycle (not purchased) energy.

	LFP (SS)	LFP (HT)	NMC	LCO (SS)	LCO (HT)	LMO	LMR-NMC: Gr/Si	LMR-NMC: Gr
Cathode material	8.3	14	44	49	91	14	28	23
Graphite	6.5	6.5	7.9	8.0	8.0	6.3	2.4	8.7
Silicon	0	0	0	0	0	0	21	0
Wrought Aluminum	32	32	31	31	31	30	39	35
Copper	4.7	4.7	4.4	4.2	4.2	4.2	7.5	5.6
Battery Management System	4.3	4.3	5.5	5.8	5.8	4.6	7.0	6.2
Binder and binder solvent	0.79	0.79	0.93	0.94	0.97	0.97	0.78	0.79
Plastics	3.0	3.0	2.6	2.5	2.5	2.6	3.7	3.1
Insulation	0.07	0.07	0.07	0.08	0.08	0.07	0.08	0.08
Steel	0.82	0.82	0.75	0.76	0.76	0.75	0.65	0.75
Electrolyte	13	13	9.3	9.3	9.3	9.3	9.6	9.5
Glycol	0.39	0.39	0.41	0.42	0.42	0.38	0.50	0.44
Assembly (nth plant)	3.5	3.5	4.5	4.8	4.8	3.8	5.7	5.1
Assembly (pioneer plant)	610	610	780	830	830	660	990	890

Table S9. Contribution of energy sources to different grid mixes. (Totals may not add due to rounding)

	US Grid	California Grid	Northeast Power Coordinating Council (NPCC) Grid
Residual Oil	0.9%	0.5%	1.1%
Natural Gas	23%	48%	41%
Coal	46%	7.6%	10%
Nuclear Power	20%	17%	31%
Biomass	0.29%	1.3%	1.4%
Other[a]	9.8%	26%	16%

a. Includes hydroelectric, geothermal, wind, solar photovoltaic, and other sources

References

1. P. A. Nelson, K. G. Gallagher, I. Bloom, and D. W. Dees, *Modeling the Performance and Cost of Lithium-Ion Batteries for Electric-Drive Vehicles*, Report number ANL-11/32, Argonne National Laboratory, 2011.
2. J. B. Dunn, C. James, L. Gaines, and K. Gallagher, *Material and Energy Flows in the Production of Cathode and Anode Materials for Lithium Ion Batteries*, Report number ANL/ESD/14/10, Argonne National Laboratory, 2014.
3. Argonne National Laboratory, *BatPaC Model*, 2011.