

Lithium-ion Battery Chemicals

As the world moves increasingly toward electricity-based fuel, one important aspect is storage of that energy. Solar cells can only generate power during daylight hours and electric cars need to bring the electricity with them. The need for high performance batteries is higher than ever.

Lithium-ion batteries satisfy these needs and AEE can supply Lithium X-Y-Z Oxide cathode materials in coin cells as well as our typical targets, powders, and shapeless pieces.

When evaluating battery materials, the factors of importance are **Energy Density**: the amount of energy stored per unit weight or sometimes per volume. **Specific Power**: the speed you can deliver that energy. **Lifespan**: how many charge-discharge cycles can the battery sustain before chemical changes render it too weak to function. We should also consider **Safety** since lithium tends to cause fires without proper circuit controls, **Cost**, and **Durability** against high and low temperatures and idle time, and Recharge Rate.

Lithium-Ion batteries are rechargeable, have high energy densities, low memory-effect, and low passive charge loss.

They are heavily utilized in portable electronics such as flashlights, phones and laptops, power tools, electric vehicles including cars and aircraft and backup power sources.

The needs of the application will influence which material should be used. There are tradeoffs to be considered between Total Capacity, Power, and Longevity



A Li-ion battery from a [Nokia 3310 mobile phone](#)

Specific energy	100–265 W·h/kg ^{[1][2]} (0.36–0.875 MJ/kg)
Energy density	250–693 W·h/L ^{[3][4]} (0.90–2.43 MJ/L)
Specific power	~250 – ~340 W/kg ^[1]
Charge/discharge efficiency	80–90% ^[5]
Energy/consumer-price	6.4 Wh/US\$ ^[6] US\$156/kWh
Self-discharge rate	0.35% to 2.5% per month depending on state of charge ^[7]
Cycle durability	400–1,200 cycles ^[8]
Nominal cell voltage	3.6 / 3.7 / 3.8 / 3.85 V , LiFePO4 3.2 V

	Structure	Potential [V] (Versus Li/Li ⁺)	Physical Density [g/cc]	Specific Capacity [Ah / kg] (theoretical / practical)	Specific Energy [Wh / kg]	Maximum Discharge Rate [C-rate]	Lifespan [cycles]	Cost	Safety & Durability
LiNiO₂	Layered	4.2	4.71	220/160	640	1	200	Medium	Medium
LiCoO₂	Layered	3.9	5.10	272/145	520	1	700	Medium	Medium
LiMn₂O₄	Spinel	4.1	4.31	148/105	410	1-10	500	Medium	Medium
LiFePO₄	Olivine	3.45	3.60	170/155	540	1-25	2000	Medium	Highest
Li (Ni_{1/3}Mn_{1/3}Co_{1/3}) O₂	Layered	3.8	4.7	272/200	760	1-2	1000	Medium	Medium
Li (Ni_{0.8}Co_{0.15}Al_{0.05}) O₂	Layered	3.8	4.7	300/200	680	1	700	Low	Medium
Li₄Ti₅O₁₂	Spinel	1.55	3.73	175/145	230	10	5000	Low	Highest
Notes: C-Rate is the allowable fraction of capacity discharged per hour. Carbon is the typical anode to the above cathode materials. Li ₄ Ti ₅ O ₁₂ may be used as an anode or cathode.									

References

Wikipedia: https://en.wikipedia.org/wiki/Lithium-ion_battery
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Julien, Christian M., et.al. (2014) Comparative Issues of Cathode Materials for Li-Ion Batteries
Chen, Hungru (2012) Simulations for new battery materials.

Item	Formula	Applications
Cathodes		
Lithium Cobalt Oxide	LiCoO ₂	Power Tools, Electric Vehicles, Few Medical Tools
Lithium Nickel(II) Phosphate	LiNiPO ₄	Rechargeable lithium batteries for electric vehicles, power tools, RC cars
Lithium Cobalt Phosphate	LiCoPO ₄	Energy storage systems, hybrid electric vehicles or electric vehicles
Lithium Manganese Phosphate	LiMnPO ₄	Pouch Cell, Rechargeable lithium batteries
Lithium Iron Phosphate	LiFePO ₄	Automobiles (Electric and hybrid vehicles) and renewable energy generation
Lithium Manganese Nickel Oxide	LiMnNiO (Mn1.5Ni0.5)	Electric vehicles (EVs) and plug-in hybrid electric vehicles (HEVs)
Lithium Manganese Oxide	LiMn ₂ O ₄	Precursors to NMC batteries, Electric vehicles (Nissan Leaf had LMO-NMC in their older models. Nissan expected to switch to pure NMC cathode in second gen models)
Lithium Nickel Cobalt Aluminum Oxide	LiNiCoAlO ₂ (Al0.03Co0.09Ni0.88)	Electric vehicles, Grid storage (Energy density is increased from 150-200Wh/kg range to >280 Wh/kg Tesla is currently using NCA cell chemistry)
Lithium Nickel Cobalt Aluminum Oxide	LiNiCoAlO ₂ (Al0.01Co0.14Ni0.85)	
Lithium Nickel Cobalt Aluminum Oxide	LiNiCoAlO ₂ (Al0.05Co0.15Ni0.8)	
Lithium Nickel Manganese Cobalt Oxide NMC	LiNiMnCoO ₂	Power Banks, Flashlights, Electric Vehicles, Cordless Power Tools, Laptop Battery Packs (Recently battery manufacturers are moving toward higher nickel content in cathodes due to the high cost and toxic nature of cobalt Because of its increased energy density it is used more frequently in long range EVs)
Lithium Nickel Manganese Cobalt Oxide NMC	LiNi0.5Mn0.3Co0.2O ₂	
Lithium Nickel Manganese Cobalt Oxide NMC	LiNi0.6Mn0.2Co0.2O ₂	
Lithium Nickel Manganese Cobalt Oxide NMC	LiNi0.8Mn0.1Co0.1O ₂	
Lithium Nickel Manganese Cobalt Oxide NMC	LiNi0.4Mn0.4Co0.2O ₂	
Lithium Nickel Manganese Cobalt Oxide NMC	LiNi0.4Mn0.2Co0.4O ₂	
Lithium Nickel Oxide	LiNiO ₂	Rechargeable lithium batteries for electric vehicles

Anodes		
Lithium	Li	Anode in Lithium-ion batteries and coin cells
Lithium Titanate (Lithium Titanium Oxide)	Li ₄ Ti ₅ O ₁₂	Batteries for Samsung's Bluetooth S-Pens, Seiko's wristwatches, Electric vehicles, energy storage systems
Lithium Titanate (Lithium Titanium Oxide)	Li ₂ TiO ₃	
Lithium Tungsten Oxide	Li ₂ WO ₄	Used for preparation of ceramics with ultra-low sintering temp. Catalyst for oxidative coupling reactions
Electrolytes		
Lithium Nitride	Li ₃ N	Originally proposed for use as an electrolyte in all solid- state Li ion batteries given its exceptional ionic conductivity at RT. Used in the fabrication of lithium-ion batteries as cathode additive
Lithium Phosphorus Sulfide	Li ₃ PS ₄	Solid state electrolyte material for all solid-state lithium-ion batteries.
Lithium Phosphorus Sulfide	Li ₇ P ₃ S ₁₁	
Lithium Silicate	Li ₂ SiO ₃	Fuel cell Li-Ion batteries
Lithium Phosphorus Oxynitride	LiPON	Thin film LiPON - All solid-state batteries Layers of LiPON are deposited over the cathode material at ambient temperatures by RF magnetron sputtering, forms the solid electrolyte used for ion conduction between anode and cathode in a lithium-ion battery cell.
Lithium Phosphate	Li ₃ PO ₄	Solid state electrolyte material for all solid-state lithium-ion batteries.
Germanium Sulfide	GeS ₂	Commonly used as a precursor material for sulfide based solid state electrolyte materials used in advanced lithium batteries (all-solid-state batteries, lithium-sulfur batteries, etc.) In addition, GeS ₂ is also used in electronic materials, catalysts, and optical materials.

Lithium Sulfide	Li ₂ S	All solid-state batteries Lithium sulfide is an important precursor material for synthesizing sulfide solid state electrolyte materials, such as LPS, LGPS, Argyrodite type Li ₆ PS ₅ Cl.
Lithium Germanium Phosphorus Sulfide	Li ₁₀ GeP ₂ S ₁₂	Have high ionic conductivity exceeding liquid electrolytes are not stable with Li metal exhibiting the lowest coulombic efficiency when using high voltage cathode
Lithium Germanium Phosphorus Sulfide Chloride	Li ₁₀ GeP ₂ S ₁₂ Cl	Used as a solid-state electrolyte material for advanced lithium batteries (all-solid-state batteries, lithium-sulfur batteries, etc)
Lithium Phosphorus Sulfide Bromide	Li ₆ PS ₅ Br	Solid state electrolyte material for all solid-state lithium-ion batteries. Cathode electrolyte (catholyte).
Lithium Phosphorus Sulfide Chloride	Li ₆ PS ₅ Cl	
Lithium Aluminum Germanium Phosphate	LiAlGeP ₃ O ₁₂	NASICON-type electrolyte, Lithium-sulfur battery system Superior to LATP because of the better electrochemical stability
Lithium Lanthanum Titanium Oxide	LiLaTiO ₃	Commercial solid electrolyte in thin film batteries
Lithium Aluminum Titanium Phosphate	Li _{1.3} Al _{0.3} Ti _{1.7} (PO ₄) ₃	Lithium-Air, Lithium-sulfur, Lithium-bromine battery systems
Lithium Lanthanum Zirconium Oxide	Li ₇ La ₃ Zr ₂ O ₁₂	Patented by QuantumScape as catholytes, electrolytes and/or anolytes for all solid-state lithium rechargeable batteries.
Aluminum doped Lithium Lanthanum Zirconium Oxide	Li _{6.75} Al _{0.25} La ₃ Zr ₂ O ₁₂	
Gallium doped Lithium Lanthanum Zirconium Oxide	Li _{6.4} Ga _{0.2} La ₃ Zr ₂ O ₁₂	Researched as solid electrolyte materials for lithium ion and lithium metal batteries
Niobium doped Lithium Lanthanum Zirconium Oxide	Li _{6.5} La ₃ Zr _{1.5} Nb _{0.5} O ₁₂	
Tantalum doped Lithium Lanthanum Zirconium Oxide	Li _{6.4} La ₃ Zr _{1.4} Ta _{0.6} O ₁₂	
Tungsten doped Lithium Lanthanum Zirconium Oxide	Li _{6.3} La ₃ Zr _{1.65} W _{0.35} O ₁₂	
Sodium Thioantimonate	Na ₃ SbS ₄	Solid-state sodium ion batteries
Sodium Phosphorus Sulfide	Na ₃ PS ₄	