MERCK

POWER THE FUTURE:

Battery Materials

The Life Science business of Merck operates as MilliporeSigma in the U.S. and Canada.

Sigma-Aldrich®

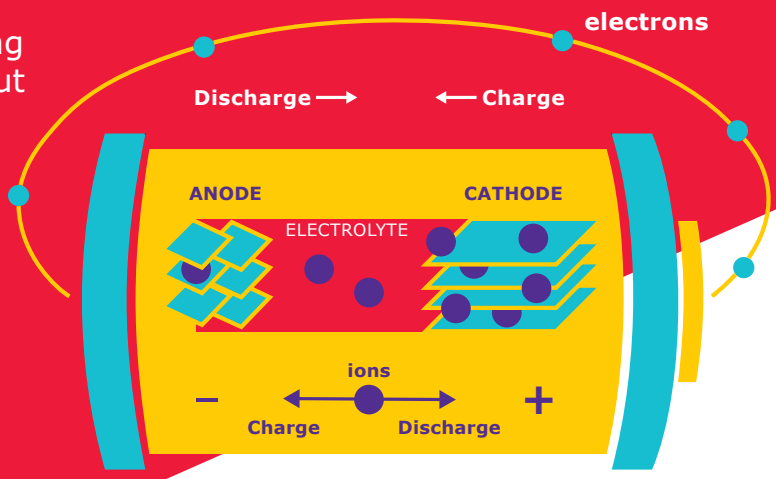
Lab & Production Materials

Battery Materials

Lithium-ion batteries have revolutionized the electronics industry with uses ranging from mobile devices to electric vehicles due to their high energy efficiency, power density, light weight, improved safety and lower material costs.

We offer reliable building blocks for successfully producing high-performance batteries with outstanding durability and dependability throughout your battery development workflow.

In this brochure, we will explore different parts of the battery and key products that are used to develop the next generation of materials.



Battery Materials Workflow

Material Development

- High-Purity Salts
- Oxides & Ceramics
- Metals & Alloys
- Chalcogenides
- Solvents

Device Prototyping

- Battery Materials
- Inorganic & Metallic Nanomaterials
- Carbon Nanomaterials
- Speciality & Smart Polymers

Battery Manufacturing

- High-Purity Salts
- Oxides & Ceramics
- Metals & Alloys
- Speciality & Smart Polymers
- Solvents

Analysis of Battery Materials

- Analytical Chromatography
- Titration Reagents
- Chromatography & Spectroscopy Reagents
- ICP & AAS Standards
- Ion Chromatography Standards

Explore more at **SigmaAldrich.com/lib**

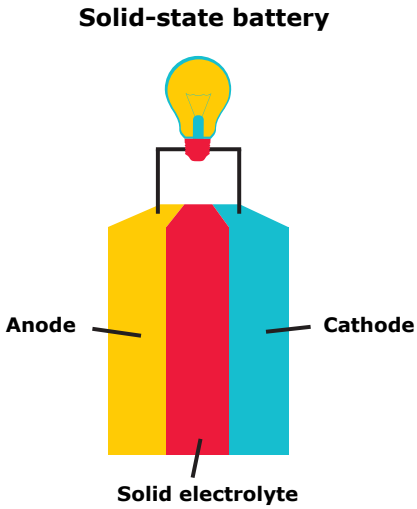
Battery Materials for Development, Device Prototyping, and Manufacturing

Our innovative battery materials are designed to improve the performance of Li-ion batteries, making them more powerful, reliable and affordable.

Solid Electrolytes

For Device Prototyping

Solid-state battery technology uses solid electrodes and a solid electrolyte, instead of the liquid or polymer gel electrolytes found in lithium-ion or lithium polymer batteries.



Solid Electrolytes

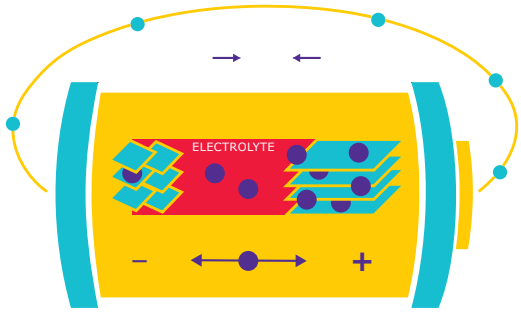
Name	Composition	Cat. No.
Al-doped Lithium Lanthanum ZirconateOxide (LLZO) powder, battery grade	$Li_{6.24}La_3Zr_2Al_{0.24}O_{11.98}$	**915874**
Carbon-coated lithium titanate (LTO) powder, battery grade		**916196**
LATP-coated Lithium Manganese Nickel Oxide (LMNO), powder, battery grade	$LiMn_{1.5}Ni_{0.5}O_4+Li_{1.4}Al_{0.4}Ti$	**915173**
Lithium aluminum titanium phosphate (LATP) powder, battery grade	$Li_{1.4}Al_{0.4}Ti_{1.6}(PO_4)_3$	**915394**
Lithium lanthanum titanate (LLTO) powder, battery grade	$LiLaTiO_4$	**916099**
Lithium manganese nickel oxide, spinel, powder, battery grade	$Li_2Mn_3NiO_8$	**915432**
Lithium manganese oxide spinel (LMO) powder, battery grade	$LiMn_2O_4$	**916439**
Lithium Phosphorus Sulfide (LPS) powder, battery grade	Li_3PS_4	**916374**
Lithium phosphorus sulfur chloride (LPSCl) powder, battery grade	Li_6PS_5Cl	**916137**
Lithium tin phosphorus sulfide (LSPS), battery grade	$Li_{10}SnP_2S_{12}$	**915114**
Lithium titanate, spinel LTO powder, battery grade	$Li_4Ti_5O_{12}$	**915939**

Electrolytes

For Device Prototyping

Electrolytes serve as a catalyst to make a battery conductive, promoting the flow of electrical charge between the cathode and anode.

Our ready-to-use electrolytes are engineered to optimize the performance of advanced lithium-ion cells.



Electrolyte Solutions

Name	Composition	Cat. No.
H_2O < 15 ppm, HF < 50 ppm, APHA < 50		
1.0 M $LiPF_6$ in DEC	in diethyl carbonate	**746770**
1.0 M $LiPF_6$ in DMC	in dimethyl carbonate	**746754**
1.0 M $LiPF_6$ in EC/DEC=50/50 (v/v)	in ethylene carbonate and diethyl carbonate	**746746**
1.0 M $LiPF_6$ in EC/DMC=50/50 (v/v)	in ethylene carbonate and dimethyl carbonate	**746711**
1.0 M $LiPF_6$ in EC/EMC=50/50 (v/v)	in ethylene carbonate and ethyl methyl carbonate	**746738**
1.0 M $LiPF_6$ in EMC	in ethyl methyl carbonate	**746762**
1.0 M $LiPF_6$ in PC	in propylene carbonate	**746789**
2.0 M $LiPF_6$ DEC	in diethyl carbonate	**809543**
2.0 M $LiPF_6$ DMC	in dimethyl carbonate	**809411**
2.0 M $LiPF_6$ EC/DEC=50/50(v/v)	in ethylene carbonate and diethyl carbonate	**809349**
2.0 M $LiPF_6$ EC/EMC=50/50(v/v)	in ethylene carbonate and ethylmethyl carbonate	**809365**
2.0 M $LiPF_6$ EMC	in ethylmethyl carbonate	**809403**
2.0 M $LiPF_6$ in EC/DMC=50/50(v/v)	in ethylene carbonate and dimethyl carbonate	**809357**
2.0 M $LiPF_6$ PC	in propylene carbonate	**809470**

Electrolyte Materials

Name	Specifications	Composition	Cat. No.
1-Butyl-1-methylpyrrolidinium bis(trifluoromethylsulfonyl)imide	>99%, <500 ppm H_2O	$C_{11}H_20F_6N_2O_4S_2$	**900873**
1-Ethyl-1-methylpyrrolidinium bis(trifluoromethylsulfonyl)imide	≥99%, <500 ppm H_2O	$C_9H_{16}F_6N_2O_4S_2$	**900813**
Diethyl carbonate	≥99%, greener alternative composition	$C_2H_5O_2CO$	**517135**
Fluoroethylene carbonate	≥99%, acid <200 ppm, anhydrous	$C_3H_3FO_3$	**901686**
Lithium tetrafluoroborate	≥98%, acid <200 ppm, anhydrous	$LiBF_4$	**901695**

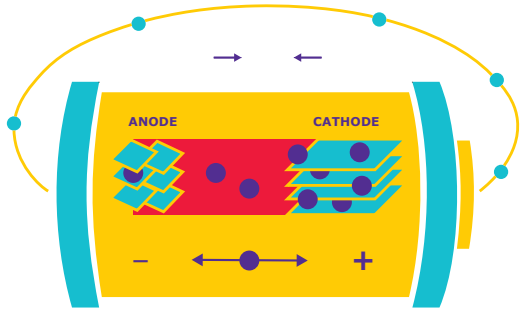
Solvents and Additives for Electrolytes

Name	Specifications	Composition	Cat. No.
Acetonitrile	electronic grade, 99.999% trace metals basis	CH_3CN	**733466**
Adiponitrile	>99%, acid <200 ppm, H_2O <100 ppm	$NC(CH_2)_4CN$	**900020**
Allyl methyl sulfone	96%	$C_4H_8O_2S$	**718203**
tert-Amylbenzene	≥99%, acid <200 ppm, H_2O <100 ppm	$C_{11}H_{16}$	**900001**
Bis(trifluoromethane)sulfonimide lithium salt		$CF_3SO_2NLiSO_2CF_3$	**449504**
1-Butyl-3-methylimidazolium thiocyanate	for energy applications, ≥95%	$C_9H_{15}N_3S$	**724408**
1,4-Di-*tert*-butyl-2,5-bis (2-methoxyethoxy)benzene	99.5%, anhydrous	$C_{20}H_{34}O_4$	**900797**
Diethyl carbonate	anhydrous, ≥99%	$(C_2H_5O)_2CO$	**517135**
	≥99%, acid <10 ppm, H_2O <10 ppm	$(C_2H_5O)_2CO$	**900018**
Diethyl sulfite	98%	$(C_2H_5O)_2SO$	**774278**
Dimethyl carbonate	≥99.9%, acid <10 ppm, H_2O <10 ppm	$(CH_3O)_2CO$	**809942**
1,2-Dimethyl-3-propylimidazolium bis(trifluoromethylsulfonyl)imide	for energy applications	$C_{10}H_{15}F_6N_3O_4S_2$	**724416**
2,2-Dimethyl-3,6,9,12-tetraoxa-2-silatridecane	≥98%, anhydrous	$C_{10}H_{24}O_4Si$	**900871**
Ethyl methyl carbonate	99%	$C_4H_8O_3$	**754935**
	99.9%, acid <10 ppm, H_2O <10 ppm	$C_4H_8O_3$	**809934**
Ethyl methyl sulfone	for energy applications, 97%	$C_3H_8SO_2$	**709980**
Ethylene carbonate	≥99%, acid <10 ppm, H_2O <10 ppm	$C_3H_4O_3$	**809950**
Ethylene sulfite	≥99.0%	$C_2H_4O_3S$	**774251**
1-Ethyl-3-methylimidazolium tetrachloroaluminate	for energy applications	$C_6H_{11}AlCl_4N_2$	**724424**
Fluoroethylene carbonate	99%	$C_3H_3FO_3$	**757349**
3-(Methylsulfonyl)-1-propyne	95%	$C_4H_6O_2S$	**718319**
Methyl-trioctylammonium bis(trifluoromethylsulfonyl)imide	for energy applications	$C_{27}H_{54}F_6N_2O_4S_2$	**724432**
Phenylcyclohexane	≥99%, acid < 200 ppm, H_2O < 100 ppm	$C_6H_5C_6H_{11}$	**810002**
1,3-Propanesultone	≥99%, acid <200 ppm, H_2O <100 ppm	$C_3H_6O_3S$	**809985**
Propylene carbonate	≥99%, acid <10 ppm, H_2O <10 ppm	$C_4H_6O_3$	**809969**
1,3-Propylene sulfite	99%	$C_3H_6O_3S$	**774243**
1,2-Propyleneglycol sulfite	≥98%	$C_3H_6O_3S$	**774456**
2-Propynyl methanesulfonate	≥99.5%, acid <200 ppm, H_2O <100 ppm	$C_4H_6O_3S$	**809993**
2,2,4,4-Tetramethyl-3,8,11,14,17-pentaoxa-2,4-disilaoctadecane	99%	$C_{15}H_{36}O_5Si_2$	**900763**
Vinylene carbonate	contains 80 ppm BHT as stabilizer, 99%	$C_3H_2O_3$	**757144**
	99.5%, acid <200 ppm, H_2O <100 ppm	$C_3H_2O_3$	**809977**

Anodes and Cathodes

For Device Prototyping

Our high-performance anode material provide excellent porosity and conductivity, good durability and light weight at low cost. Our high-purity cathode materials vary according to their electrochemical properties, energy density, thermal stability, and load capacities to achieve unprecedented battery performance.



Cathode Materials

Name	Composition	Purity	Dimensions	Cat. No.
Cobalt monoantimonide	CoSb	99.9% trace metals basis	-80 mesh	**746320**
Fe_3O_4/graphene nanocomposite	Fe_3O_4	10 mg/mL, dispersion in acetone	5-25 nm	**803715**
Graphene oxide, organic solvent dispersible	CxHyOz	solid	-	**921556**
Lithium cobalt(III) oxide	$LiCoO_2$	powder, 99.8% trace metals basis	-	**442704**
Lithium cobalt phosphate, LCP	$LiCoPO_4$	powder, ≥99% (trace metals analysis)	-	**725145**
Lithium iron(III) oxide	$LiFeO_2$	powder, 95%	particle size <1 µm	**442712**
Lithium iron(II) phosphate, LFP	$LiFePO_4$	powder, >97% (XRF)	particle size <5 µm (BET)	**759546**
Lithium manganese dioxide	$LiMnO_2$	powder, >99% trace metals basis	particle size <1 µm	**725137**
Lithium manganese nickel oxide, LMNO	$Li_2Mn_3NiO_8$	powder, >99%	particle size <0.5 µm (BET)	**725110**
Lithium manganese oxide, LMO	$LiMn_2O_4$	powder, >99%	particle size <0.5 µm (BET)	**725129**
Lithium manganese(III,IV) oxide, LMO	$LiMn_2O_4$	-	particle size <5 µm	**482277**
Lithium molybdate	Li_2MoO_4	powder or crystals, 99.9% trace metals basis	-	**400904**
Lithium nickel cobalt aluminium oxide, NCA	$LiNi_{0.8}Co_{0.15}Al_{0.05}O_2$	powder, >98%	particle size <0.5 µm	**760994**
Lithium nickel cobalt oxide, LNCO	$LiNi_{0.8}Co_{0.2}O_2$	powder, >98%	particle size <0.5 µm	**760986**
Lithium nickel dioxide, LNO	$LiNiO_2$	powder, ≥98% trace metals basis	particle size <3 µm (BET)	**757365**
Lithium nickel manganese cobalt oxide, NMC	$LiNi_{0.33}Mn_{0.33}Co_{0.33}O_2$	powder, >98%	particle size <0.5 µm	**761001**

Anode or Cathode Materials

Name	Composition	Purity	Form	Cat. No.
Boron/Nitrogen co-doped graphene	Boron: 2.0-4.0% Carbon: 85-95% Nitrogen: 2.0-4.0%	≥95%	powder	**900535**
Nitrogen/Sulfur co-doped graphene	Carbon: 85-95% Nitrogen: 2.0-4.0% Oxygen: <7.5% Sulfur: 2.0-4.0%	≥95%	powder	**900530**
Nitrogen/Phosphorus co-doped graphene	Carbon: 85-95% Nitrogen: 2.0-4.0% Oxygen: <7.5% Phosphorus: 1.0-3.0%	≥95%	powder	**900531**
Nitrogen-doped graphene	Carbon: >80 wt. % Nitrogen: >4 wt. %	-	powder	**900416**

Separator Material

Name	Molecular Weight (M_w)	λ_{max}	Band Gap	Cat. No.
Poly(9,9-dioctylfluorenyl-2,7-diyl) end capped with dimethylphenyl	50,000-150,000 by GPC	368 nm in THF	2.5 eV	**923222**

Anode Materials

Name	Purity	Description	Form	Cat. No.
Fullerene-C_{60}	99.9%	greener alternative	sublimed	**572500**
Lithium	99%, metals basis	particle size 4 - 10 mesh	granular	**444456**
	99.9% trace metals basis	thickness × W 1.5 × 100 mm	ribbon	**266000**
	99.9% trace metals basis	thickness × W 0.75 × 45 mm	ribbon	**265993**
	99.9% trace metals basis	thickness × W 0.75 × 19 mm	ribbon	**320080**
	99.9% trace metals basis	thickness × W 0.38 × 23 mm	ribbon	**265985**
	≥98%	diam. 3.2 mm	wire	**278327**
Lithium-aluminum alloy	-	-	powder	**426490**
Lithium titanate, LTO	-	−80 mesh	powder	**400939**
Lithium titanate, spinel, LTO nanopowder	>99%	particle size <200 nm (BET)	nanopowder	**702277**
Tin(IV) oxide	-	avg. part. size ≤100 nm	nanopowder	**549657**

R&D Highlight

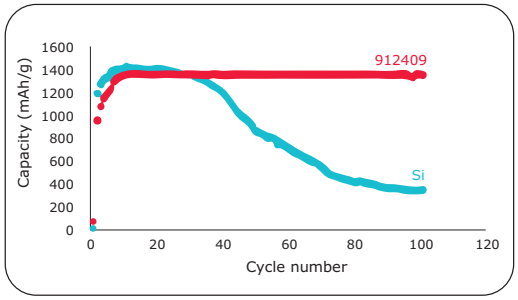
Silicon Anode Materials

High Capacity

With a capacity over 1300 mAh/g, our silicon composite formulation is well suited for use as a counter electrode for new high capacity cathode materials.

Extended Cycle Life

Unlike some silicon-based electrode formulations, our 3D porous conductive polymer prevents capacity loss during the charge/discharge cycles.[1,2]



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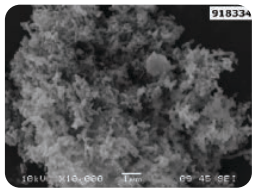
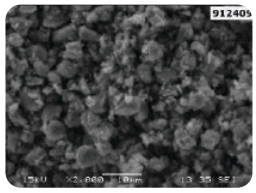




Formula		Cat. No.
High-performance silicon anode material	1 micron (Si)	**910961**
	100 nm (Si)	**910953**

References:

1) Wu, H.; Yu, G. H.; Pan, L. J.; Liu, N.; McDowell, M. T.; Bao, Z. N.; Cui, Y. *Nat. Commun.* **2013,** *4,* 1943. DOI: 10.1038/ncomms2941

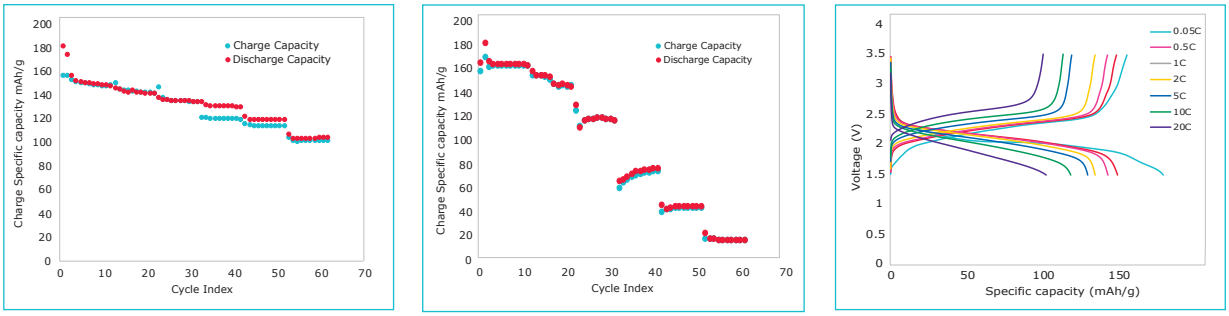
2) Zhao, F.; Bae, J. W.; Zhou, X. Y.; Guo, Y. H.; Yu, G. H. *Adv. Mater.* **2018,** *30,* 1801796. DOI: 10.1002/adma.201801796

R&D Highlight

rGO Battery Electrode Materials

Fast Charge and Discharge Rates

Take advantage of the rate-enhancing capabilities of reduced graphene oxide in your battery research. Our methods transform a thorough mixture of redox polymers into well-dispersed reduced graphene oxide to create high-rate performance electrode materials for lithium-ion batteries.[1]



A) Charge and discharge rate performance of PAQS/rGO composite electrode; B) Charge and discharge rate performance of PAQS electrode; C) Voltage profile of lithium metal half-cell battery with PAQS/rGO composite electrode at 0.5 to 20 C.

Green Batteries

Redox polymers are free of commonly used toxic transition metals, such as cobalt and nickel, used in lithium-ion batteries. This type of battery material also has the potential to be more sustainable.[2,3]

Improved Capacity

Our reduced graphene oxide composites show a fourfold increase in capacity at 10 C compared to PAQS.

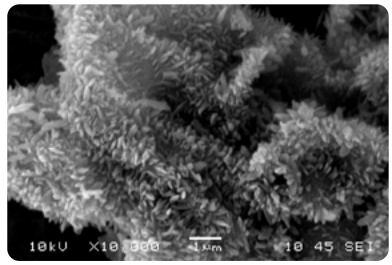


Figure 2: SEM image showing PMDA polymer coated on reduced graphene oxide.

Fast Charge/Discharge Li-Ion Battery Electrode Materials

Cat. No.	Product Description
921351	Reduced graphene oxide enhanced poly (anthraquinonyl sulfide) (PAQS) battery electrode
921378	Reduced graphene oxide enhanced pyromellitic dianhydride (PMDA) battery electrode
921386	Reduced graphene oxide enhanced 1,4,5,8-naphthalenetetracarboxylic dianhydride (NTCDA) battery electrode

References:

[1] Song, Z.; Xu, T.; Gordin, M. L.; Jiang, Y.-B.; Bae, I.-T.; Xiao, Q.; Zhan, H; Liu, J.; Wang, D. *Nano Lett.* **2012,** *12*, 2205. DOI: 10.1021/nl2039666

[2] Song, Z.; Zhan, H.; Zhou, Y. *Angew. Chem. Int. Ed.* **2010,** *49*, 8444. DOI: 10.1002/anie.201002439

[3] Muench, S.; Wild, A.; Friebe, C.; Häupler, B.; Janoschka, T.; Schubert, U. S. *Chem. Rev.* 2016, *116*, 9438. DOI: 10.1021/acs.chemrev.6b00070

2D Materials

For Device Prototyping

Transition Metal Dichalcogenides are 2D semiconductor materials showing unique electrical, mechanical, and optical properties.

TMD-based (MX_2) electrodes have come to light as promising candidates due to their range of operational voltage, long-life, stability, very high surface Li diffusivities, and excellent charge/discharge capabilities.

Transition Metal Dichalcogenides (TMDCs)

MoS_2

Name	Description	Cat. No.
Molybdenum disulfide ink for spin/spray coating	Resistivity: 75-100 kΩ·cm	**901867**
Molybdenum disulfide nanoplatelets	50-1000 nm thickness < 3 layers	**901792**
Molybdenum disulfide quantum dots	-	**914541**
Molybdenum disulfide suspension	50-1000 nm thickness < 3 layers	**901797**
	50-1000 nm thickness < 3 layers	**902012**
Molybdenum sulfide	single crystalline monolayer flakes on SiO2/Si	**901479**
	Single crystalline monolayer flakes on sapphire	**901615**
Molybdenum disulfide	particle size: ≤500 nm	**900724**

WS_2

Name	Description	Cat. No.
Tungsten disulfide nanoplatelets	50-300 nm thickness < 3 layers	**901789**
Tungsten disulfide quantum dots	-	**914290**
Tungsten disulfide suspension	50-300 nm thickness < 3 layers	**901791**
	thickness < 3 layers 50-300 nm	**901775**
Tungsten sulfide	single crystalline monolayer flakes on sapphire	**901474**
	single crystalline monolayer flakes on SiO_2/Si	**901484**
Tungsten(IV) sulfide	90 nm avg. part. size (SEM), 99% trace metals basis	**790583**

$MoSe_2$

Name	Description	Cat. No.
Molybdenum selenide	single crystalline monolayer flakes on SiO_2/Si	**901483**
	single crystalline monolayer flakes on sapphire	**901478**

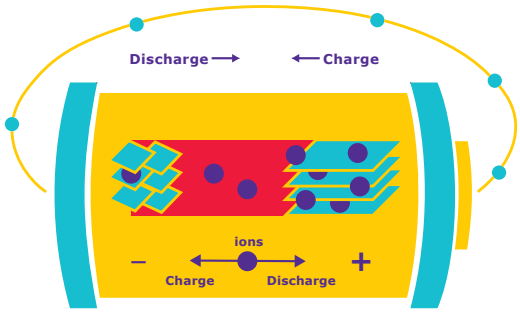
MXene Precursor-MAX Phases

Name	Form	Particle Size (µm)	Purity	Cat. No.
Titanium aluminium carbide 211	powder	≤100	≥80%	**901821**
	powder	≤200	≥80%	**901708**
Titanium aluminium carbide 312	powder	≤40	≥90%	**901775**
	powder	≤100	≥90%	**910767**
	powder	≤200	≥90%	**910740**
Titanium aluminium carbide 211	powder	≤40	≥80%	**910759**

Ionic Liquids

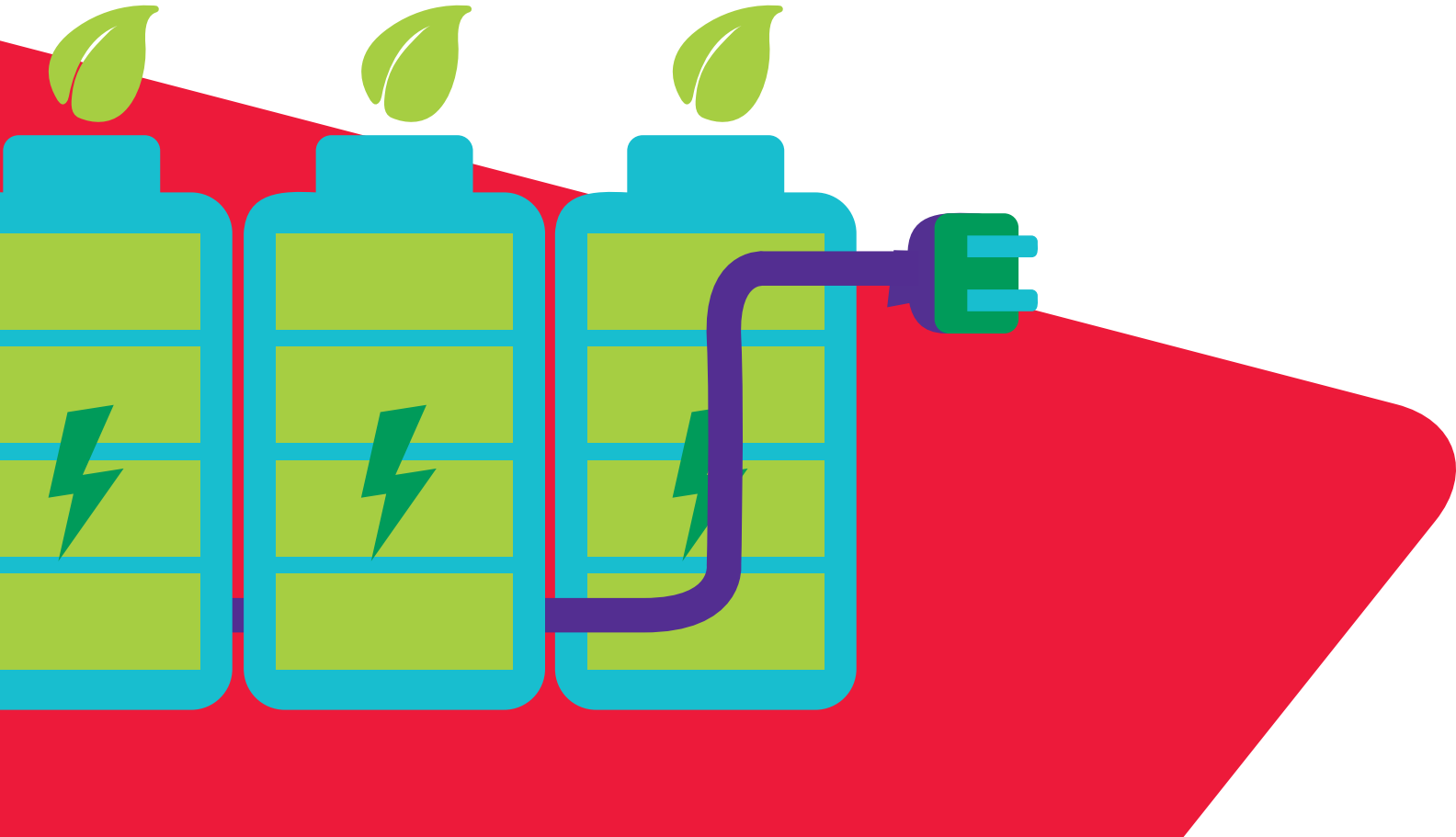
For Device Prototyping

Ionic liquids (ILs) have been dubbed “designer solvents” because their physicochemical properties can be designed to suit application requirements by adjusting cationic and anionic components. Moreover, they are a greener alternative to traditional organic solvents.



Ionic Liquids

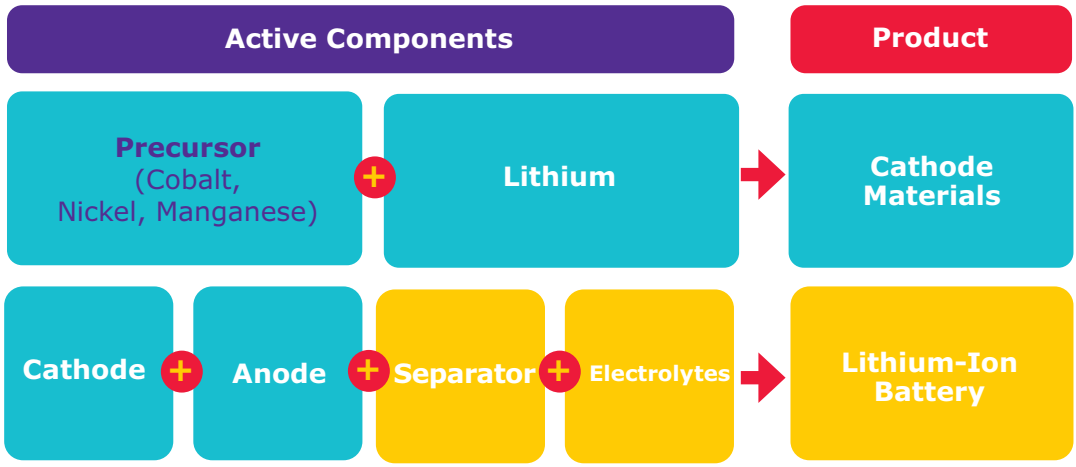
Name	Purity	Cat. No.
1-Butyl-2,3-dimethylimidazolium bis(trifluoromethylsulfonyl)imide	≥99%	**900804**
1-Butyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide	≥99%	**900802**
1-Butyl-3-methylimidazolium chloride	≥99%	**900856**
1-Butyl-1-methylpiperidinium bis(trifluoromethylsulfonyl)imide	≥99%	**900807**
1-Butyl-1-methylpyrrolidinium bis(trifluoromethylsulfonyl)imide	≥99%	**900873**
Diethyl carbonate, H_2O	≥99%	**900018**
1-Ethyl-3-methylimidazolium acetate	≥98%	**900787**
1-Ethyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide	≥99%	**900801**
1-Ethyl-3-methylimidazolium chloride	≥99%	**900771**
1-Ethyl-3-methylimidazolium hexafluorophosphate	≥99%	**900779**
1-Ethyl-3-methylimidazolium tetrafluoroborate	≥99%	**900772**
1-Ethyl-1-methylpyrrolidinium bis(trifluoromethylsulfonyl)imide	≥99%	**900813**
1-Methyl-1-propylpiperidinium bis(trifluoromethylsulfonyl)imide	≥99%	**900806**
Tributylmethylammonium bis(trifluoromethylsulfonyl)imide	≥99%	**900857**



Precursors

For Material Development

We offer a wide variety of precursors to help make your own customizable cathode material to suit your battery development needs.



Name	Composition	Form	Purity	Cat. No.
Aluminum nitrate nonahydrate	$Al(NO_3)_3 \cdot 9H_2O$	crystals and lumps	99.997% trace metals basis	**229415**
Ammonium dihydrogenphosphate	$NH_4H_2PO_4$	crystalline	99.999% trace metals basis	**204005**
Ammonium hydroxide solution	NH_4OH	NH_3 28% in H_2O	99.99% trace metals basis	**338818**
Ammonium phosphate dibasic	$(NH_4)_2HPO_4$	crystalline	≥99.99% trace metals basis	**379980**
Cobalt(II) acetate tetrahydrate	$(CH_3COO)_2Co \cdot 4H_2O$	solid	>99%	**1.0253**
Cobalt(II) nitrate hexahydrate	$Co(NO_3)_2 \cdot 6H_2O$	crystals and lumps	99.999% trace metals basis	**203106**
Cobalt(II) sulfate heptahydrate	$CoSO_4 \cdot 7H_2O$	powder	≥99%	**C6768**
Copper(II) sulfate, anhydrous	$CuSO_4$	powder	≥99.99% trace metals basis	**451657**
Iron(III) chloride	$FeCl_3$	powder or crystals	sublimed grade, ≥99.9% trace metals basis	**701122**
Iron(III) citrate	$C_6H_5FeO_7$	powder	technical grade	**F6129**
Lithium acetate	$LiOOCCH_3$	powder	99.9% trace metals basis	**920320**
Lithium carbonate	Li_2CO_3	powder	99.997% trace metals basis	**203629**
Lithium chloride, anhydrous	LiCl	crystals	99.95% trace metals basis	**916013**
Lithium hydroxide monohydrate	$LiOH \cdot H_2O$	powder or granules	98.0%	**402974**
Lithium hydroxide monohydrate	$LiOH \cdot H_2O$	crystalline	99.95% trace metals basis	**254274**
Lithium hydroxide, anhydrous	LiOH	powder	99.9% trace metals basis	**920312**
Lithium sulfate, anhydrous	Li_2SO_4	crystals	99.5% trace metals basis	**920339**
Lithium-7Li2 carbonate	$7Li_2CO_3$		99% (CP)	**601470**
Manganese(II) chloride	$MnCl_2$	powder and chunks	≥99% trace metals basis	**244589**
Manganese(II) sulfate monohydrate	$MnSO_4 \cdot H_2O$	powder	≥99%	**M7634**
Nickel(II) chloride	$NiCl_2$	powder	98%	**339350**
Nickel(II) chloride, anhydrous	$NiCl_2$	powder	99.99% trace metals basis	**451193**
Nickel(II) nitrate	$Ni(NO_3)_2 \cdot 6H_2O$	powder and chunks	99.999% trace metals basis	**203874**
Nickel(II) sulfate hexahydrate	$NiSO_4 \cdot 6H_2O$	crystals	≥98%	**227676**
Nickel(II) sulfate, anhydrous	$NiSO_4$	powder and chunks	99.99% trace metals basis	**656895**
Sodium Hydroxide, Pellets - CAS 1310-73-2 - Calbiochem	NaOH	pellets (crystalline)	≥95%, titration	**567530**

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