

POWER THE FUTURE:

Battery Materials



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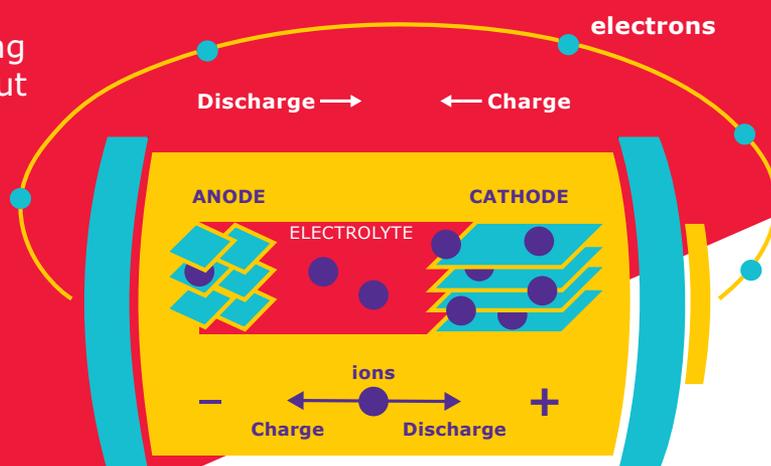
Sigma-Aldrich®
Lab & Production Materials

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

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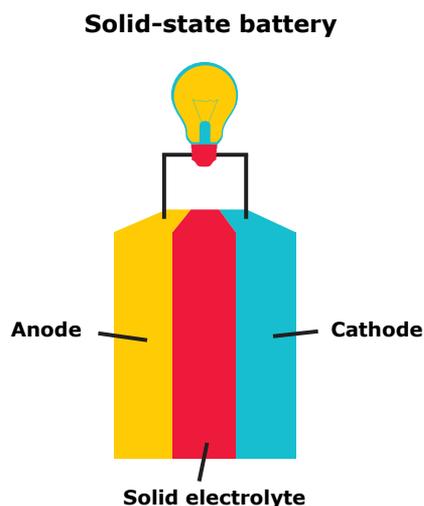
Battery Materials for Development, Device Prototyping, and Manufacturing

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

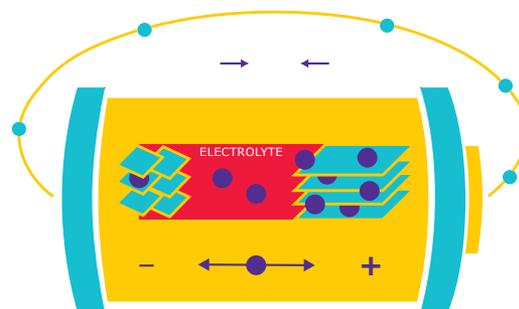
Name	Composition	Cat. No.
Al-doped Lithium Lanthanum ZirconateOxide (LLZO) powder, battery grade	$\text{Li}_{6.24}\text{La}_3\text{Zr}_2\text{Al}_{0.24}\text{O}_{11.98}$	915874
Carbon-coated lithium titanate (LTO) powder, battery grade		916196
LATP-coated Lithium Manganese Nickel Oxide (LMNO), powder, battery grade	$\text{LiMn}_{1.5}\text{Ni}_{0.5}\text{O}_4 + \text{Li}_{1.4}\text{Al}_{0.4}\text{Ti}$	915173
Lithium aluminum titanium phosphate (LATP) powder, battery grade	$\text{Li}_{1.4}\text{Al}_{0.4}\text{Ti}_{1.6}(\text{PO}_4)_3$	915394
Lithium lanthanum titanate (LLTO) powder, battery grade	LiLaTiO_4	916099
Lithium manganese nickel oxide, spinel, powder, battery grade	$\text{Li}_2\text{Mn}_3\text{NiO}_8$	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 (LPSCI) powder, battery grade	$\text{Li}_6\text{PS}_5\text{Cl}$	916137
Lithium tin phosphorus sulfide (LSPS), battery grade	$\text{Li}_{10}\text{SnP}_2\text{S}_{12}$	915114
Lithium titanate, spinel LTO powder, battery grade	$\text{Li}_4\text{Ti}_5\text{O}_{12}$	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.
H₂O < 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 ₂ O	C ₁₁ H ₂₀ F ₆ N ₂ O ₄ S ₂	900873
1-Ethyl-1-methylpyrrolidinium bis(trifluoromethylsulfonyl)imide	≥99%, <500 ppm H ₂ O	C ₉ H ₁₆ F ₆ N ₂ O ₄ S ₂	900813
Diethyl carbonate	≥99%, greener alternative composition	C ₂ H ₅ O ₂ CO	517135
Fluoroethylene carbonate	≥99%, acid <200 ppm, anhydrous	C ₃ H ₃ FO ₃	901686
Lithium tetrafluoroborate	≥98%, acid <200 ppm, anhydrous	LiBF ₄	901695

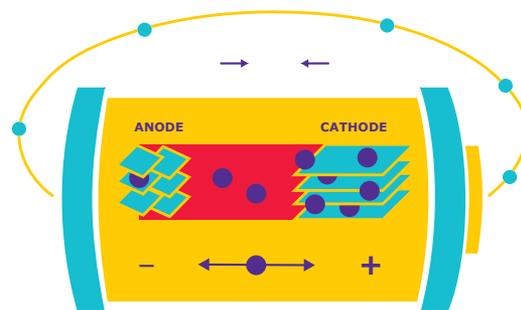
Solvents and Additives for Electrolytes

Name	Specifications	Composition	Cat. No.
Acetonitrile	electronic grade, 99.999% trace metals basis	CH ₃ CN	733466
Adiponitrile	>99%, acid <200 ppm, H ₂ O <100 ppm	NC(CH ₂) ₄ CN	900020
Allyl methyl sulfone	96%	C ₄ H ₈ O ₂ S	718203
<i>tert</i> -Amylbenzene	≥99%, acid <200 ppm, H ₂ O <100 ppm	C ₁₁ H ₁₆	900001
Bis(trifluoromethane)sulfonimide lithium salt		CF ₃ SO ₂ NLiSO ₂ CF ₃	449504
1-Butyl-3-methylimidazolium thiocyanate	for energy applications, ≥95%	C ₉ H ₁₅ N ₃ S	724408
1,4-Di- <i>tert</i> -butyl-2,5-bis (2-methoxyethoxy)benzene	99.5%, anhydrous	C ₂₀ H ₃₄ O ₄	900797
Diethyl carbonate	anhydrous, ≥99%	(C ₂ H ₅ O) ₂ CO	517135
	≥99%, acid <10 ppm, H ₂ O <10 ppm	(C ₂ H ₅ O) ₂ CO	900018
Diethyl sulfite	98%	(C ₂ H ₅ O) ₂ SO	774278
Dimethyl carbonate	≥99.9%, acid <10 ppm, H ₂ O <10 ppm	(CH ₃ O) ₂ CO	809942
1,2-Dimethyl-3-propylimidazolium bis(trifluoromethylsulfonyl)imide	for energy applications	C ₁₀ H ₁₅ F ₆ N ₃ O ₄ S ₂	724416
2,2-Dimethyl-3,6,9,12-tetraoxa-2-silatridecane	≥98%, anhydrous	C ₁₀ H ₂₄ O ₄ Si	900871
Ethyl methyl carbonate	99%	C ₄ H ₈ O ₃	754935
	99.9%, acid <10 ppm, H ₂ O <10 ppm	C ₄ H ₈ O ₃	809934
Ethyl methyl sulfone	for energy applications, 97%	C ₃ H ₈ SO ₂	709980
Ethylene carbonate	≥99%, acid <10 ppm, H ₂ O <10 ppm	C ₃ H ₄ O ₃	809950
Ethylene sulfite	≥99.0%	C ₂ H ₄ O ₃ S	774251
1-Ethyl-3-methylimidazolium tetrachloroaluminate	for energy applications	C ₆ H ₁₁ AlCl ₄ N ₂	724424
Fluoroethylene carbonate	99%	C ₃ H ₃ FO ₃	757349
3-(Methylsulfonyl)-1-propyne	95%	C ₄ H ₆ O ₂ S	718319
Methyl-trioctylammonium bis(trifluoromethylsulfonyl)imide	for energy applications	C ₂₇ H ₅₄ F ₆ N ₂ O ₄ S ₂	724432
Phenylcyclohexane	≥99%, acid < 200 ppm, H ₂ O < 100 ppm	C ₆ H ₅ C ₆ H ₁₁	810002
1,3-Propanesultone	≥99%, acid <200 ppm, H ₂ O <100 ppm	C ₃ H ₆ O ₃ S	809985
Propylene carbonate	≥99%, acid <10 ppm, H ₂ O <10 ppm	C ₄ H ₆ O ₃	809969
1,3-Propylene sulfite	99%	C ₃ H ₆ O ₃ S	774243
1,2-Propyleneglycol sulfite	≥98%	C ₃ H ₆ O ₃ S	774456
2-Propynyl methanesulfonate	≥99.5%, acid <200 ppm, H ₂ O <100 ppm	C ₄ H ₆ O ₃ S	809993
2,2,4,4-Tetramethyl-3,8,11,14,17-pentaoxa-2,4-disilaoctadecane	99%	C ₁₅ H ₃₆ O ₅ Si ₂	900763
Vinylene carbonate	contains 80 ppm BHT as stabilizer, 99%	C ₃ H ₂ O ₃	757144
	99.5%, acid <200 ppm, H ₂ O <100 ppm	C ₃ H ₂ O 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 ₃ O ₄ /graphene nanocomposite	Fe ₃ O ₄	10 mg/mL, dispersion in acetone	5-25 nm	803715
Graphene oxide, organic solvent dispersible	C _x H _y O _z	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 ₂ Mn ₃ NiO ₈	powder, >99%	particle size <0.5 μm (BET)	725110
Lithium manganese oxide, LMO	LiMn ₂ O ₄	powder, >99%	particle size <0.5 μm (BET)	725129
Lithium manganese(III,IV) oxide, LMO	LiMn ₂ O ₄	-	particle size <5 μm	482277
Lithium molybdate	Li ₂ MoO 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

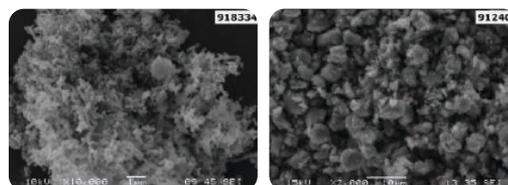
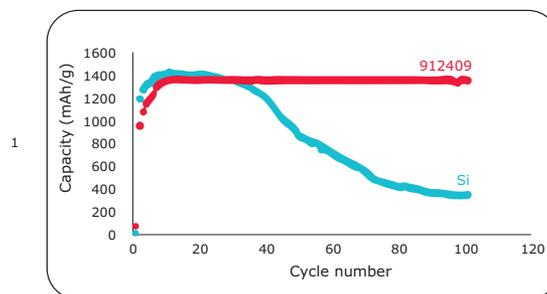
Silicon Anode Materials

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}



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

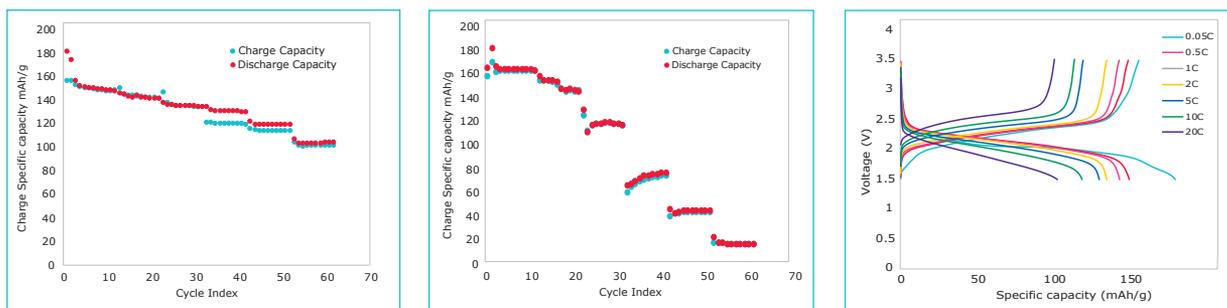
References:

- 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

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.

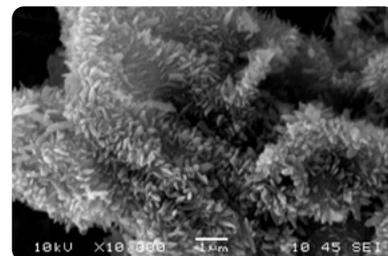


Figure 2: SEM image showing PMDA polymer coated on reduced graphene oxide.

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)

MoS₂

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 SiO ₂ /Si	901479
	Single crystalline monolayer flakes on sapphire	901615
Molybdenum disulfide	particle size: ≤500 nm	900724

WS₂

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

MoSe₂

Name	Description	Cat. No.
Molybdenum selenide	single crystalline monolayer flakes on SiO ₂ /Si	901483
	single crystalline monolayer flakes on sapphire	901478

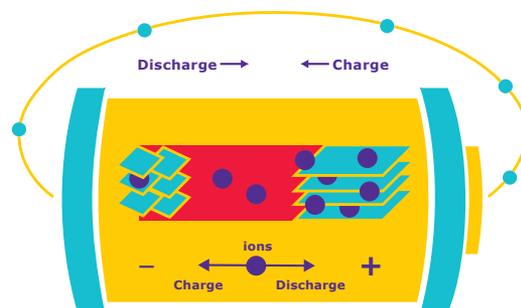
MXene Precursor-MAX Phases

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

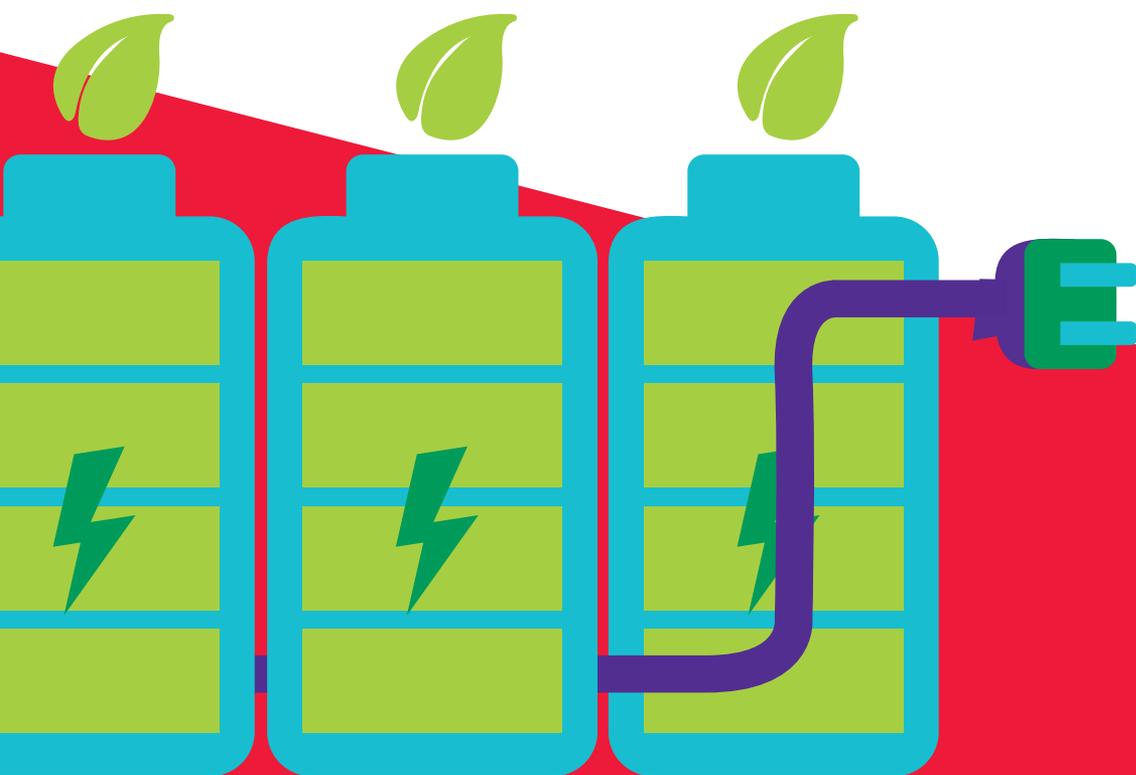
For Device Prototyping

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

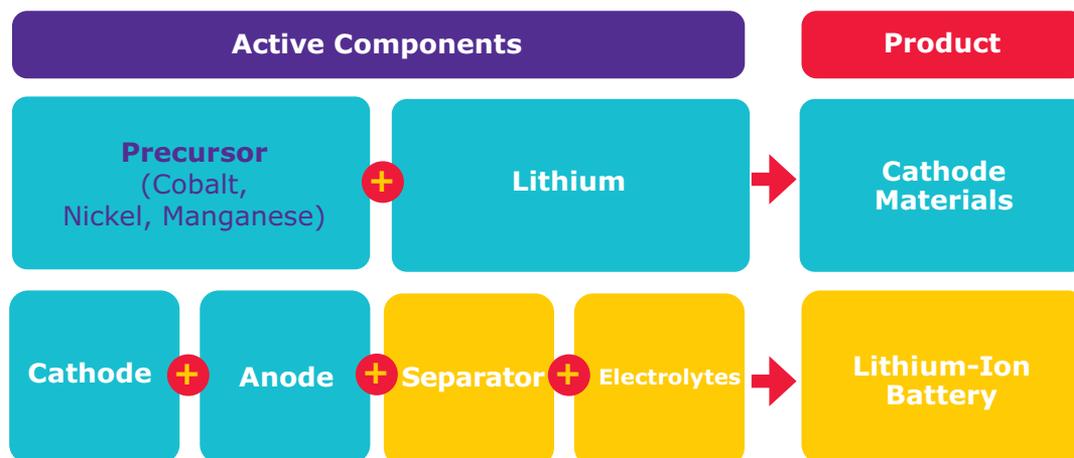
Name	Purity	Cat. No.
1-Butyl-2,3-dimethylimidazolium bis(trifluoromethylsulfonyl)imide	≥99%	900804
1-Butyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide	≥99%	900802
1-Butyl-3-methylimidazolium chloride	≥99%	900856
1-Butyl-1-methylpiperidinium bis(trifluoromethylsulfonyl)imide	≥99%	900807
1-Butyl-1-methylpyrrolidinium bis(trifluoromethylsulfonyl)imide	≥99%	900873
Diethyl carbonate, H ₂ O	≥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 · 9H ₂ O	crystals and lumps	99.997% trace metals basis	229415
Ammonium dihydrogenphosphate	NH ₄ H ₂ PO ₄	crystalline	99.999% trace metals basis	204005
Ammonium hydroxide solution	NH ₄ OH	NH ₃ 28% in H ₂ O	99.99% trace metals basis	338818
Ammonium phosphate dibasic	(NH ₄) ₂ HPO ₄	crystalline	≥99.99% trace metals basis	379980
Cobalt(II) acetate tetrahydrate	(CH ₃ COO) ₂ Co · 4H ₂ O	solid	>99%	1.0253
Cobalt(II) nitrate hexahydrate	Co(NO ₃) ₂ · 6H ₂ O	crystals and lumps	99.999% trace metals basis	203106
Cobalt(II) sulfate heptahydrate	CoSO ₄ · 7H ₂ O	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 ₆ H ₅ FeO ₇	powder	technical grade	F6129
Lithium acetate	LiOOCCH ₃	powder	99.9% trace metals basis	920320
Lithium carbonate	Li ₂ CO ₃	powder	99.997% trace metals basis	203629
Lithium chloride, anhydrous	LiCl	crystals	99.95% trace metals basis	916013
Lithium hydroxide monohydrate	LiOH · H ₂ O	powder or granules	98.0%	402974
Lithium hydroxide monohydrate	LiOH · H ₂ O	crystalline	99.95% trace metals basis	254274
Lithium hydroxide, anhydrous	LiOH	powder	99.9% trace metals basis	920312
Lithium sulfate, anhydrous	Li ₂ SO ₄	crystals	99.5% trace metals basis	920339
Lithium-7Li2 carbonate	7Li ₂ CO ₃		99% (CP)	601470
Manganese(II) chloride	MnCl ₂	powder and chunks	≥99% trace metals basis	244589
Manganese(II) sulfate monohydrate	MnSO ₄ · H ₂ O	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 · 6H ₂ O	powder and chunks	99.999% trace metals basis	203874
Nickel(II) sulfate hexahydrate	NiSO ₄ · 6H ₂ O	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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