# Advanced Materials for Next Generation Batteries

## Solutions for Battery R&D, Prototyping, Manufacturing, Testing, Recycling

**Dr Adelina Braun**
**Technology Manager/Materials Science**
**EMEA Merck Life Science KGaA**

Battery Tech Expo Sweden, October 2024

# who We are

Who we are

# VIBRANT SCIENCE AND TECHNOLOGY

company with over 350 years of history.

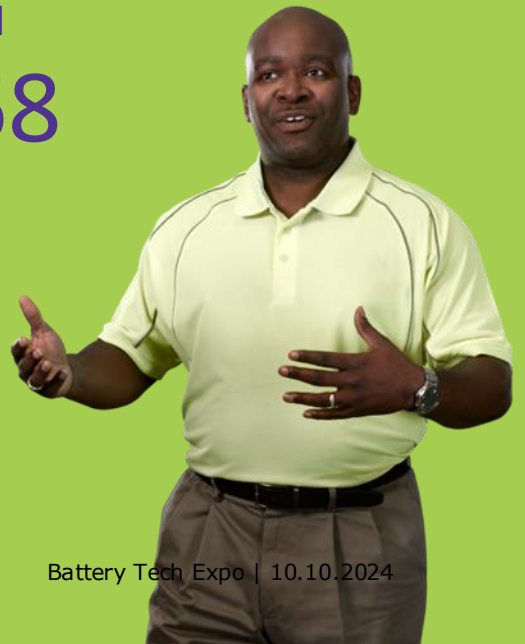
At Merck, science is at the heart of everything we do. It drives the discoveries we make and the technologies we create.

# Key figures

64’000
Employees worldwide

66
Countries

Founded
1668



150
Locations

2.5
R&D (€ billion)

# We are MERCK

A vibrant science and technology company

We are known as **Merck** internationally except for the United States and Canada, where we operate as **EMD Serono** in the biopharmaceutical business, **MilliporeSigma** in the life science business and **EMD Electronics** in the high-tech materials business.

## Healthcare

- Pioneer in cancer treatment
- Advancing care in immunology
- Global market leader in fertility treatments
- Robust R&D pipeline

## Life Science

- Trusted supplier and partner for the scientific community
- From research to large scale production with >300,000 products
- Novel technologies and world-class solutions driving discoveries

## Electronics

- Innovations to change the way we access, store, process and display data
- Enabler of new generations of electronic products for our everyday lives
- Supplier of high-tech materials and solutions to the electronic industry

# Science & Lab Solutions Portfolio

Manufacturing and distributing quality products and services in an ever-changing and competitive world is a challenge that we help our customers tackle.

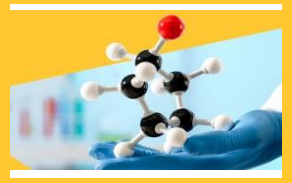
## Chemistry

### Lab Classics

- Solvents
- Inorganics
- High-purity Acids & Bases


### Materials Science

- Inorganic Nanoparticles
- High-purity Metals & Salts
- Electrolytes
- Ceramics
- Battery Grade Materials



### Chemical Synthesis

- Building blocks
- Reagents
- Catalysts

## Analytical

### Mobile Analysis & Sample Preparation

- Mobile Analysis solutions
- Lab-based workflow solutions
- Application-specific kits

### Chromatography & Instr. Analysis

- Chromatography columns
- Solvents & reagents
- Sample Prep, SPE/SPME


### Analytical Reagents

- Titration Reagents
- Karl Fischer and Coulometry

### Reference Materials

- ICP & AAS Standards
- Physical Property Standards
- Ion Chromatography Std

## Lab Separation and Workflow Tools

### Analytical

- Millex® Filters
- Cut discs
- Glassware

## Water Purification

- Milli-Q® Benchtop Systems
- Milli-Q® High-flow Lab Water Systems

## Greener Alternatives

- Re-engineered products
- Greener Alternatives
- 12 principle aligned products

# Materials for Energy Applications

## Batteries

- **Ready-to-use battery grade**
  - Electrode sheets
  - Electrolyte solutions
- **Electrode materials**
- **Electrolyte materials in battery grades with very low water content**

## Fuel Cells

- **Solid Oxide Fuel Cells**
  - Electrode and Electrolyte materials
  - Fuel Cell catalysts
- **Proton exchange membrane fuel cells**
  - Membranes, Materials for hydrogen storage

## Solar Energy

- **Solar energy materials (Perovskites)**
- **Quantum dots**

## Hydrogen Storage

- **Complex Metal Hydrides**
- **Metal Organic Frameworks (MOF)s**
- **Hydrogen Storage Alloys**

**SigmaAldrich.com/Battery**



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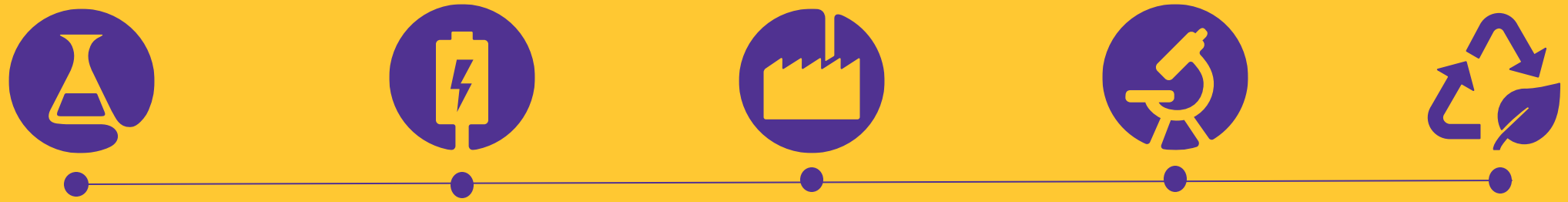
SigmaAldrich.com/battery-manufacturing

# Solutions for Battery R&D and Manufacturing



**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
- Specialty & Smart Polymers
- Solvents

**Quality Control**

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

**Recycling**

- Reagents for Hydrometallurgy
- Bio-renewable Solvents

SigmaAldrich.com/Battery

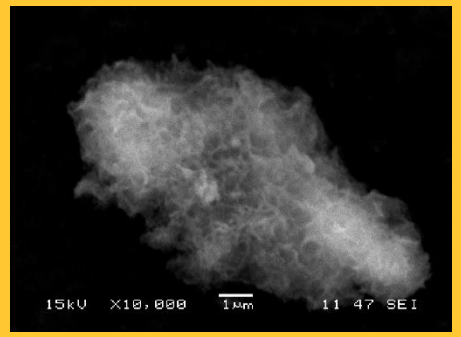
# Battery Material Development

**Material Development**

- Full range of materials for battery development
- Including Monomers, Polymers, and Initiators

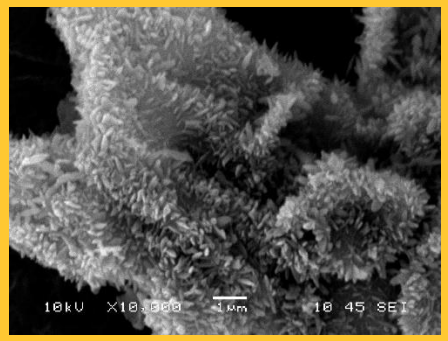
## Fast charging Graphene Polymer Nanocomposites

- 3-6 min charge rate
- No toxic metals




Poly(anthraquinonyl sulfide) (PAQS)/graphene

- Tunable voltage
- Excellent yield

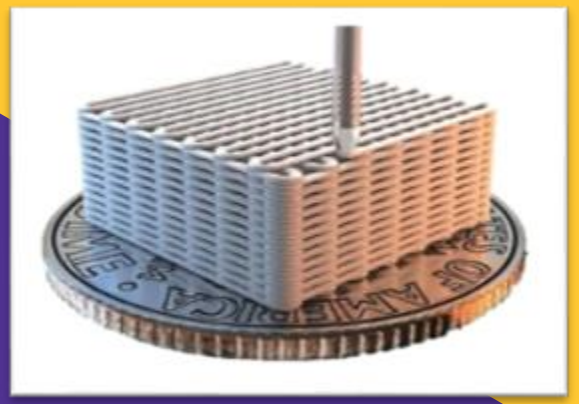



Pyromellitic dianhydride (PMDA)/graphene

# Battery Material Development

## 3D-Printable Inks for Energy Storage Applications

Illustration of 3D-printed materials generated using product number 916579



**Partnering additive manufacturing (3D printing) with functional nanomaterial-based inks for printing electrodes:**

- 3D Printable Yttria-stabilized Zirconium(IV) Oxide Ink(#918571)
- 3D Printable Ultra-High Temperature Boron Carbide Ink (#921912)
- **3D Printable Graphene Oxide Ink (#916579)**

2022 R&D 100 WINNER



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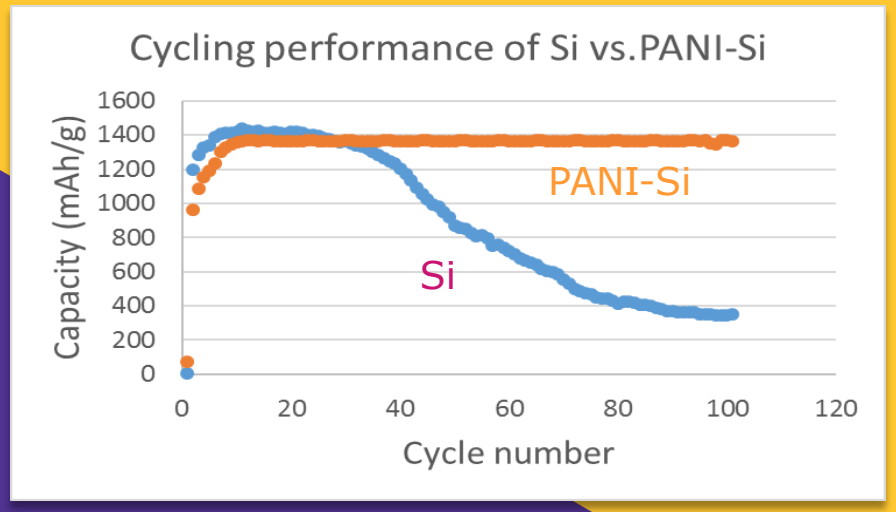
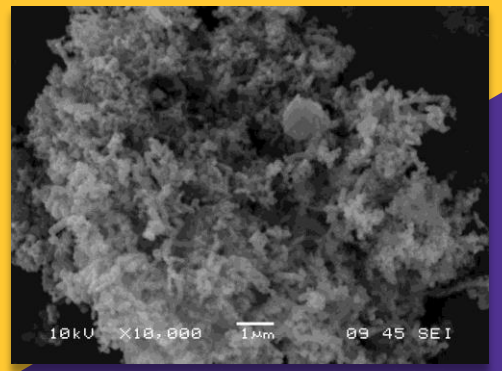
# Battery Material Development

**Wrapping Si particles in porous conductive Polyaniline matrix - Si encapsulated in PANI matrix shows improved cycle life**




**High-performance silicon anode:**

- 100 nm silicon particles in crosslinked conducting polyaniline matrix (#918334)
- 1-micron silicon particles in crosslinked conducting polyaniline matrix (#912409)




Si particles in crosslinked conducting polyaniline matrix

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# Device Prototyping

**Device Prototyping**

- Ultra-high purity materials and battery grades with very low water content
- Electrode powders with particle sizes in nanomaterials
- Ready-to-use premixed electrolyte formulations

**A growing selection of Ready-to-use premixed electrolyte formulations**

Lithium hexafluorophosphate solution #746735

In Ethylene carbonate and Ethyl methyl carbonate, 1.0 M

LiPF6 in EC/EMC=50/50 (v/v), battery grade

$LiPF_6$

Lithium hexafluorophosphate solutions

New!

Preformulated electrolytes with **additives (VC)**

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## Solid Electrolytes for Solid-state batteries

| Electrolyte | Composition | Art. |
|---|---|---|
| Al-doped Lithium Lanthanum Zirconate Oxide (LLZO) powder, battery grade | $Li_{6.24}La_3Zr_2Al_{0.24}O_{11.98}$ | 915874 |
| 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 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 |

**New** solid-electrolytes, **doped** to improve performance (compatibility and ionic conductivity)

New!

| Art | Available | Composition |
|---|---|---|
| 934720 | Now! | Ta-doped LLZO |
| 934763 | Now! | I-doped $Li_6PS_5Cl$ |

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# Recently Introduced R&D Materials

| Name | Composition | Art. |
|---|---|---|
| Ready-to-Cast Slurry for Lithium-Ion battery (NMC111) | $LiNi_{0.33}Mn_{0.33}Co_{0.33}O_2$ | 928003 |
| Ready-to-Cast Slurry for Lithium-Ion battery (LFP) | $LiFePO_4$ | 928011 |
| Ready-to-Cast Slurry for Lithium-Ion battery | $LiCoO_2$ | 928038 |
| Ready-to-Cast Slurry of Graphite Powder for Lithium-Ion battery | MesoCarbon MicroBeads | 928046 |
| Lithium hexafluorophosphate solution 1 M $LiPF_6$ in EC/EMC=30/70 (w/w), battery grade | $LiPF_6$ | 930156 |
| Lithium hexafluorophosphate solution 1.2 M $LiPF_6$ in EC/EMC=30/70 (w/w), battery grade | $LiPF_6$ | 930164 |
| Lithium hexafluorophosphate solution 1 M $LiPF_6$ in EC/DMC=30/70 (w/w), battery grade | $LiPF_6$ | 930172 |
| Sodium Terephthalate Composite, high-capacity anode for sodium ion batteries | Sodium Terephthalate | 932566 |
| Lithium Nickel Manganese Cobalt Oxide (NMC111) Crosslinked Polyaniline Composite | $LiNi_{0.33}Mn_{0.33}Co_{0.33}O_2$ | 932558 |

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# Sodium-Ion battery materials

- Innovating across the workflow from electrolytes to electrodes
- High-performance materials useful for full-cell testing
- More to come!

| Prod. # | Available | | |
|---|---|---|---|
| 936006 | Now | Electrolytes | 1.0M NaTFSI in EC/DMC 1:1 |
| 935999 | Now | | 1.0M NaTfO in diglyme |
| 935972 | Soon! | | 1.0M NaPF6 in EC/DMC/EMC |
| 933953 | Now | Electrolyte salts | NaDFOB |
| 931950 | Now | | $NaClO_4$ |
| 934704 | Now | Electrode active material | $Na_{0.44}MnO_2$ |
| 932566 | Now | | Sodium terephthalate |
| 921378 | Now | | PMDA composite |
| 921386 | Now | | NTCDA composite |
| 921351 | Now | | PAQS composite |
| 934739 | Now | Electrode sheet | $Na_{0.44}MnO_2$ cathode |
| 934666 | Now | | Hard carbon anode |



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## ElectroGreen™ Blends product list

## Sustainable alternatives Bio-based Solvents

# ElectroGreen™ Blends

## Greener Solvents for Electronics & Energy Applications

*A safer switch from harmful solvents without compromising your device performance.*

Our **ElectroGreen™ blends** are made of **bio-based safer alternatives to replace synthetic fossil-based solvents with specifications tailored for electronics and energy applications**.

- ✓ **GC purity >=99%**
- ✓ **Low residue in evaporation**
- ✓ **Metal content by ICP**
- ✓ **Water content (KF)**
- ✓ **Low acidity**
- ✓ **Low toxicity and VOC** (enabling solution-processable techniques outside of fume hood)
- ✓ **Accessible cost** (to help you with the switch!)

**100%** Renewable carbon

**Sustainably** produced

**Low** toxicity

# Battery Recycling

Our Bio-Renewable solvents are sourced from renewable, sustainable biobased materials, significantly lowering their environmental impact.

- **Drop-in Replacements**
- **Bio-Renewable Greener Substitutes**
- **Other Greener Substitutes**

**Battery Recycling**

- Technical Grade Acids, Bases, and Salts for Hydrometallurgy
- Greener Solvents, incl. REACH compliant greener substitutes for DMF/NMP


## Cyrene™

Novel dipolar aprotic solvent substitute for NMP and DMF, REACH compliant. Blends available for reduced viscosity.

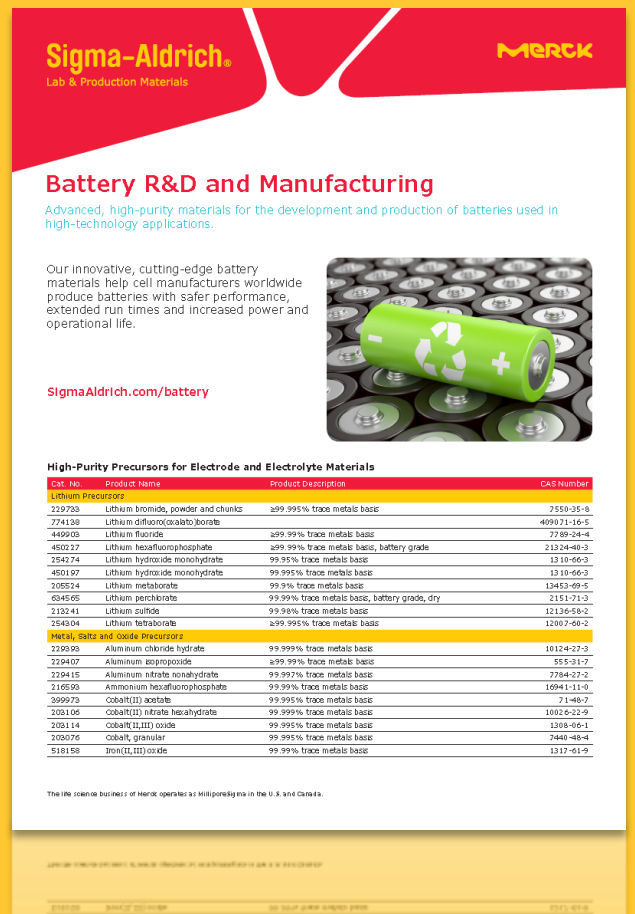
SigmaAldrich.com/biorenewable

SigmaAldrich.com/battery-manufacturing

# Battery Materials for Manufacturing

## Battery Manufacturing

- High-Purity Salts
- Oxides & Ceramics
- Metals & Alloys
- Specialty & Smart Polymers
- Customization
- Custom Manufacturing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Lab & Production Materials

MERCK

Battery R&D and Manufacturing

Advanced, high-purity materials for the development and production of batteries used in high-technology applications.

Our innovative, cutting-edge battery materials help cell manufacturers worldwide produce batteries with safer performance, extended run times and increased power and operational life.

SigmaAldrich.com/battery

High-Purity Precursors for Electrode and Electrolyte Materials

| Cat. No. | Product Name | Product Description | CAS Number |
|---|---|---|---|
| Lithium Precursors | | | |
| 229733 | Lithium bromide, powder and chunks | ≥99.995% trace metals basis | 7550-35-8 |
| 774138 | Lithium difluoro(oxalato)borate | | 409071-16-5 |
| 449903 | Lithium fluoride | ≥99.99% trace metals basis | 7789-24-4 |
| 450227 | Lithium hexafluorophosphate | ≥99.99% trace metals basis, battery grade | 21324-40-3 |
| 254274 | Lithium hydroxide monohydrate | 99.95% trace metals basis | 1310-66-3 |
| 450197 | Lithium hydroxide monohydrate | 99.995% trace metals basis | 1310-66-3 |
| 205524 | Lithium metaborate | 99.9% trace metals basis | 13453-69-5 |
| 634565 | Lithium perchlorate | 99.99% trace metals basis, battery grade, dry | 2151-71-3 |
| 213241 | Lithium sulfide | 99.98% trace metals basis | 12136-58-2 |
| 254304 | Lithium tetraborate | ≥99.995% trace metals basis | 12007-60-2 |
| Metal, Salts and Oxide Precursors | | | |
| 229393 | Aluminum chloride hydrate | 99.999% trace metals basis | 10124-27-3 |
| 229407 | Aluminum isopropoxide | ≥99.99% trace metals basis | 555-31-7 |
| 229415 | Aluminum nitrate nonahydrate | 99.997% trace metals basis | 7784-27-2 |
| 216593 | Ammonium hexafluorophosphate | 99.99% trace metals basis | 16941-11-0 |
| 399973 | Cobalt(II) acetate | 99.995% trace metals basis | 71-48-7 |
| 203106 | Cobalt(II) nitrate hexahydrate | 99.999% trace metals basis | 10026-22-9 |
| 203114 | Cobalt(II,III) oxide | 99.995% trace metals basis | 1308-06-1 |
| 203076 | Cobalt, granular | 99.995% trace metals basis | 7440-48-4 |
| 518158 | Iron(II,III) oxide | 99.99% trace metals basis | 1317-61-9 |

The life science business of Merck operates as MilliporeSigma in the U.S. and Canada.

## In-house Customization and Development Capabilities

- High-purity inorganics (metals, salts, oxides)
- Anhydrous and beaded materials
- Electrode materials



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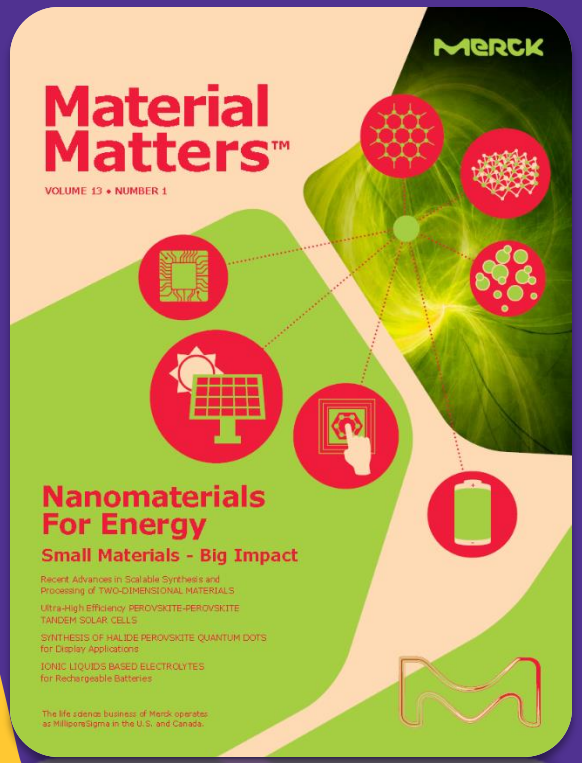
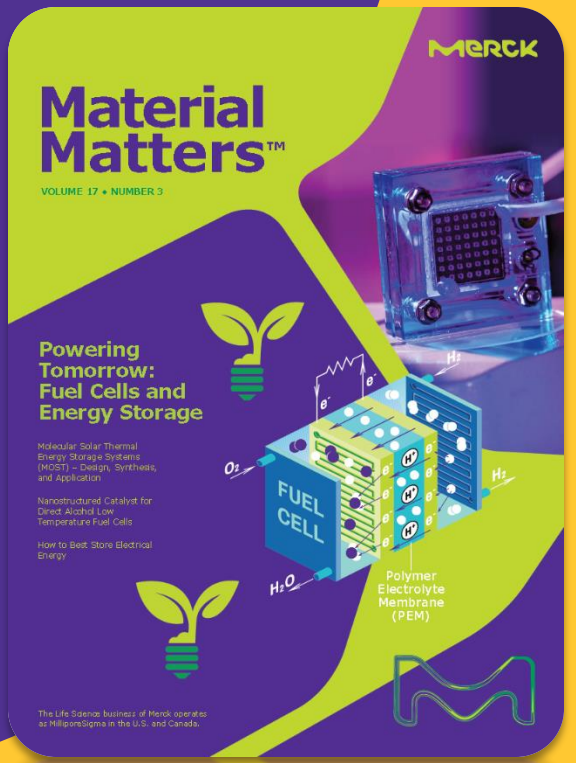
## Material Matters 13.1




## Material Matters 15.2

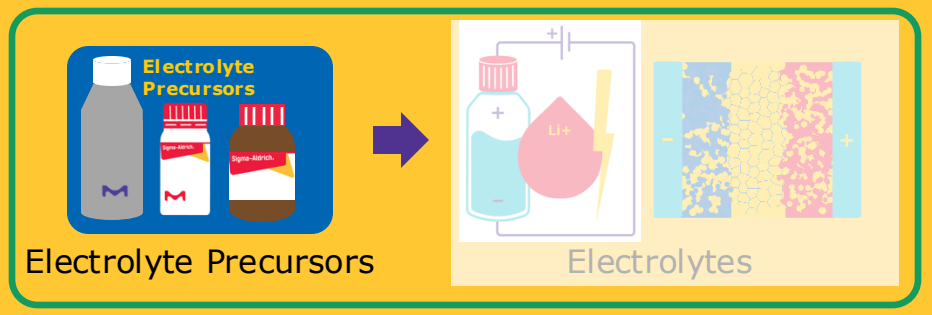

## Material Matters 17.3

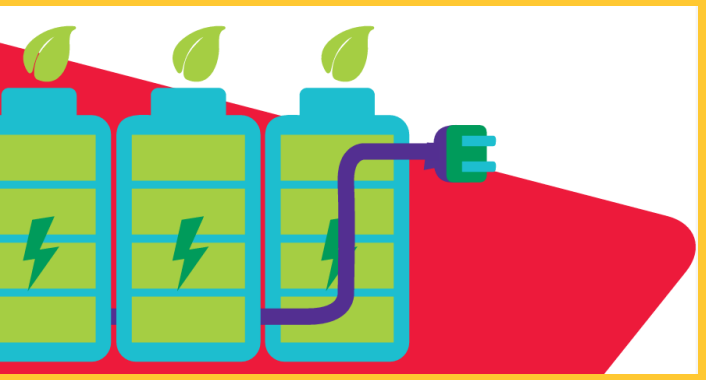



**SigmaAldrich.com/materialmatters**


# Welcome to our Merck booth

# Innovative products
# **Electrolyte Precursors**

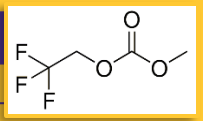


## **Battery grade** fluorinated solvents and additives

High purity (>99%), anhydrous (ppm water), low acid content (ppm HF) for battery applications

- Enhances the electrode-electrolyte interface
- Enables localized high-concentration electrolytes
- Reduces flammability



| Prod. # | Available | |
|---|---|---|
| 934003 | Now | FEMC |
| 935905 | Now | FEC |
| 934038 | Now | HFPM |
| 934046 | Now | ETFE |
| 933961 | Now | TTE |
| 933988 | Now | TFTFE |
| 934011 | Now | DFDEC |

Tech. article: "The Rise of Electrolyte Additives in Advancing Lithium-ion Battery Technology"

- Improved the production capability of our core products
- New compositions that perform better at higher operating temperatures

| Prod. # | Available | |
|---|---|---|
| 920371 | Now | $LiPF_6$ |
| 935913 | Now | $LiBF_4$ |
| 930938 | Now | $LiNO_3$ |
| 931969 | Now | $LiClO_4$ |
| 935832 | Now | LiFSI |