

LITHIUM-ION BATTERY

What is a lithium-ion battery and how does

The lithium-ion (Li-ion) battery is the predominant commercial form of rechargeable battery, widely used in portable electronics and electrified transportation. The rechargeable battery was invented in 1859 with a lead-acid chemistry that is still used in car batteries that start internal combustion engines, while the research underpinning the Li-ion battery was published in the 1970s and the first commercial Li-ion cell was made available in 1991. In 2019, John B. Goodenough, M. Stanley Whittingham, and Akira Yoshino received the Nobel Prize in Chemistry for their

contributions to the development of the modern Li-ion battery.

During a discharge cycle, lithium atoms in the anode are ionized and separated from their electrons. The lithium ions move from the anode and pass through the electrolyte until they reach the cathode, where they recombine with their electrons and electrically neutralize. The lithium ions are small enough to be able to move through a micro-permeable separator between the anode and cathode. In part because of lithium's small atomic weight and radius (third only to hydrogen and helium), Li-ion batteries are capable of having a very high voltage and charge storage per unit mass and unit volume.

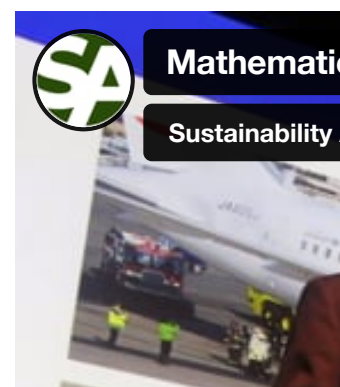
Li-ion batteries can use a number of different materials as electrodes. The most common combination is that of lithium cobalt oxide (cathode) and graphite (anode), which is used in commercial portable electronic devices such as cellphones and laptops. Other common cathode materials include lithium manganese oxide (used in hybrid electric and electric automobiles) and lithium iron phosphate. Li-ion batteries typically use ether (a class of organic compounds) as an electrolyte.

Lithium ions are stored within graphite anodes through a mechanism known as **intercalation**, in which the ions are physically inserted between the 2D layers of graphene that make up bulk graphite. The size of the ions relative to the layered carbon lattice means that graphite anodes are not physically warped by charging or discharging, and the strength of the carbon-carbon bonds relative to the weak interactions between the Li ions and the electrical charge of the anode make the insertion reaction highly reversible.

Battery Applications



Mathematical





What are some advantages of Li-ion batteries

Compared to other high-quality rechargeable battery technologies (nickel-cadmium, nickel-metal-hydride, or lead-acid), Li-ion batteries have a number of advantages. They have one of the highest energy densities of any commercial battery technology, approaching 300 watt-hours per kilogram (Wh/kg) compared to roughly 75 Wh/kg for alternative technologies. In addition, Li-ion cells can deliver up to 3.6 volts, 1.5-3 times the voltage of alternatives, which makes them suitable for high-power applications like transportation. Li-ion batteries are comparatively low maintenance, and do not require scheduled cycling to maintain their battery life. Li-ion batteries have no memory effect, a detrimental process where repeated partial discharge/charge cycles can cause a battery to 'remember' a lower capacity. Li-ion batteries also have a low self-discharge rate of around 1.5-2% per month, and do not contain toxic lead or cadmium.

High energy densities and long lifespans have made Li-ion batteries the market leader in portable electronic devices and electrified transportation, including electric vehicles (EVs) like the Nissan Leaf and the Tesla Model S as well as the hybrid-electric Boeing 787. In terms of decarbonizing our economy's energy use, Li-ion technology has its greatest potential in EVs and electrified aviation.

What are some disadvantages of Li-ion batteries

Despite their transformative effect on technology, Li-ion batteries still have a number of disadvantages, particularly related to safety. Li-ion batteries have a tendency to overheat, and can be damaged at high voltages. They are also flammable, so damaged batteries can experience thermal runaway and combustion. Be

batteries, a number of shipping companies **refuse to perform bulk shipments of batt** mechanisms to limit voltage and internal pressures, which can increase weight and lim batteries are also subject to aging, meaning that they can lose capacity and frequently cost, and safety make Li-ion batteries a poor fit for grid-scale energy storage. And desp compared to other kinds of batteries, they are still around a hundred times less energy Wh/kg by mass or 8760 Wh/L by volume.

CEI Research Highlights

A major focus of CEI energy storage research is the development of novel materials to i researchers develop substitutes for the components of a conventional Li-ion battery, s graphite. Others work to improve upon well-developed battery components by building can improve the speed and efficiency of charge cycles, with physical features that are s researchers are also exploring alternative chemistries to Li-ion that might be suitable f

For example, chemical engineering (ChemE) professor **Vincent Holmberg** and **his rese** alloying materials for Li-ion batteries. Materials like silicon, germanium, and antimony results in greater capacities than graphite anodes that rely on intercalating Li ions betw materials experience greater changes in physical volume that can deform the electrode But by introducing a nanostructure into the alloying material, the Holmberg group can from the charge and discharge reactions. The physical morphologies of the electrodes transfer charge, as can any chemical interactions between the lithium ions and the sur

Developing a deeper understanding of reversible “conversion” charge-discharge reactio chemistries with higher theoretical energy densities, such as lithium-sulfur. With sulfur weight, Li-S batteries could be cheaper and lighter than Li-ion batteries with graphite a simultaneously with long cycle life remains a grand challenge for energy storage scient often fail due to the formation of “dendrites” of lithium metal growing on the anodes li

Materials science & engineering professor **Jun Liu** investigates the degradation mecha cobalt (NMC) cathodes in pouch cells, and has presented fundamental linkages among structural evolution of solid–electrolyte interphase layers. Meanwhile, CEI director and **group** are working on computational models of Li-S systems that can be corroborated **of the Battery500 Consortium** — led by the Pacific Northwest National Laboratory (PN

committee — which aims to develop next-generation EV batteries with energy densities double the industry standard.

With technological progress in mobile electronics driving demand for denser batteries, dimensional (3D) electrode architectures and additive manufacturing methods to rapid improved performance. Research led by mechanical engineering (ME) professor **Corie** focuses on how 3D electrode architectures can improve many aspects of battery performance and prototyping and testing capabilities at the **Washington Clean Energy Testbeds**, ME professor **J. Devin MacKenzie's** group and the Holmberg group are collaborating to structure electrodes. Special inkjet printers allow these engineers to build 3D electrode architectures, one of the only open-access, high-throughput roll-to-roll electronics printers in the world at this scale. The Testbeds, at which MacKenzie is technical director, also house top-of-the-line equipment to validate new electrode designs.

CEI researchers are also creating physical, mathematical and computational models to simulate battery performance. These models can help optimize battery performance and charge/discharge cycles and predict failure. The Schwartz group is advancing diagnostics for Li-ion batteries to obtain data on day-to-day battery health as an alternative to a physical “autopsy” at the end of the device’s use. Along with physics-based diagnostic tools can detect signs of degradation in real time, allowing users to modify their driving habits. Furthermore, researchers in the Schwartz group use these models to project second life EV performance standards, **such as in solar-powered microgrids.**

With the **UW “Hyak” supercomputer**, researchers can simulate molecules and their kinetics to better understand electrochemistry from a perspective that is not afforded to experimental techniques.

CEI researchers also use direct imaging techniques like x-ray spectroscopy to understand battery degradation. **Jerry Seidler's lab** has developed a method to perform X-ray absorption near edge structure (XANES) measurements on benchtop. The technique provides relatively detailed measurements of certain characteristics of the battery without having to open it and thus disrupt the system. Previously, XANES could only be accomplished from instruments such as a synchrotron. These are extremely large and expensive facilities not available to the public via federal labs with months-long waiting lists. But as optoelectronics lab spun out a company to prototype a \$25,000 benchtop instrument that can mimic the capabilities of a synchrotron, **EasyXAFS** already enables scientists to obtain XANES measurements in hours, which can be used to study batteries and other energy-related materials and devices.

Meanwhile, chemistry professor Cody Schlenker and his group investigate the funda storage systems with the goal of gaining a deeper understanding of electrochemical pr with spectroscopy, the lab can identify changes in vibrational frequencies and in the dy specific chemical phenomena at key interfaces between electrodes, separator membra

Explore More

- Website on batteries and battery reuse created by Clean Energy Bridge to Resear

Background

Lithium-air batteries were first discovered in the 1970s and since then they have attracted a lot of attention from academia and research. They're considered the future of energy storage because of their extremely high theoretical energy density which is comparable to that of gasoline. The max energy density was calculated around ~12 kWh/kg which is close to the specific energy of gasoline (~13 kWh/kg).

Figure 1: Li-air energy and power density compared with other systems.

The battery usually contains a lithium metal anode and open air cathode that will allow oxygen in the air get inside. Both are constructed by a non-aqueous electrolyte to allow the transport of lithium ions. The mechanism behind the secondary Li-air battery is the oxygen reduction reaction (ORR) and oxygen evolution reaction (OER) at the tri-phase boundary between oxygen, lithium ions, and conductive air cathode. During discharge the lithium ions from the anode, dissolved oxygen in the electrolyte, along with two electrons from the cathode will react to produce lithium peroxide (Li₂O₂). The process will take the opposite direction and release oxygen when the battery is recharged.

$$2Li^+ + 2e^- + O_2 \leftrightarrow Li_2O_2 \quad (E^0 = 2.96 \text{ V})$$

Figure 2: Schematic of Li-air battery during discharge.

Challenges

Practical Li-air cells suffer limited capacity, high overpotentials, and short cycle life due to factors including sluggish ORR and OER kinetics, insoluble discharge product, and decomposition of carbon cathode and electrolyte. The discharge product, lithium peroxide is also electrically insulating which poisons the cathode. Additionally, some carbon based cathodes and electrolytes can decompose into irreversible lithium carbonate that will lead to severe capacity fading. The instability of these products can dig pores, preventing further diffusion of lithium ions and oxygen.

Figure 3: Clinging of porous cathode material by formation of insoluble Li₂O₂ and Li₂CO₃.

Objective

Different air cathode materials and catalysts help mitigate the additional problems. The objective of the following research in progress is to investigate how the addition of catalytic Co₃O₄ nanoparticles grown on a carbon fiber cathode can improve its performance as an air cathode for Li-air batteries. Carbon fiber felt could be an optimal material for Li-air batteries due to its light weight, ease of manufacturability and low cost. Its open structure can prevent clogging and allow for open diffusion of oxygen and lithium ions. Co₃O₄ is a well studied bifunctional catalyst for the ORR and OER due to its mixed valence spinel structure. The morphology of the catalyst can be adjusted through different synthesis techniques that can affect the performance of the cathode.

Figure 4: Co₃O₄ on PAN carbon fiber.

Methods

Synthesis of Co₃O₄: We are using the hydrothermal process to directly grow cobalt oxide nanostructures on pyrolyzed polyacrylonitrile (PAN) fibers. The process involves preparing a 0.05 M cobalt(III) nitrate precursor solution at a pH of 9. The solution's pH is adjusted by adding ammonium hydroxide. The addition of hydroxide changes the color of the cobalt(III) nitrate solution from light red to blue, and also precipitated green particles after an hour of stirring. The color change is associated with the formation of insoluble cobalt hydroxide, which acts as the seed crystal for nanoparticle growth. Hydrothermal synthesis was performed with PAN felt submerged in the cobalt solution at 180°C for 12 hours with a heating rate of 0°C/min. After washing with water and allowing to dry the sample is annealed at 350°C for 2 hours in air. XRD characterization was performed on precipitated particles at the bottom of the hydrothermal crucible.

Electrochemical Testing: Li-air batteries using as-received PAN felt and Co₃O₄ grown on PAN felt (Co₃O₄/PAN) were made in an argon glove box using CR2032 coin cells modified for metal-air batteries. Glass fiber paper soaked in electrolyte was used to separate the lithium metal anode from air cathode. The electrolyte was 1M LiTFSI dissolved in 1:1:1:1 EC:DMC. The Li-air batteries were tested in an air tight box under 1 atm 99.999% O₂ gas. The batteries were allowed to sit in oxygen for 10 hours before testing. Linear sweep voltammetry was done on the batteries at a rate of 0.5 mV/s from 3.1 and 1.8 V for the cathodic sweep and between 2.9 and 4.05 V for the anodic sweep. The batteries were held at 2.5 V for one hour before the anodic sweep. Galvanostatic cycling was performed at a current rate of 0.02 mA/cm². The cyclic batteries were opened in air and rinsed with acetonitrile in order to perform SEM.

Figure 5: PAN carbon felt felt and coin cell assembly (right).

Figure 6: No-light box for Li-air battery testing.

Improving Lit

Anatomy of a batter

Lithium (Li) batteries are power the Li oxidation reaction:

$$Li \rightarrow Li^+ + e^- \quad (E_0 = 3.0 \text{ V})$$

The oxidation potential (E_0) produces electrons (e^-) generated at the through external circuitry, delivering energy to electrical devices (⚡).

Solid Li anodes give the highest capacities:

$$\text{Anode} = Li_{(s)}$$

For rechargability and safety, it must be dispersed in a "cage" ma

$$\text{Anode} = \text{Cage} + Li_{(s)}$$

TAT MATERIALS SCIENCE & ENGINEERING

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