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A general comparison on energy density between Li-Ion, Li-S and Li-O_2 batteries

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Abstract. Today, under the situation of the rapid development of EVs. Li-ion batteries is the first choice to power EVs than any other energy storage system. Many researches are done on various types of batteries with different theoretical and practical energy density and specific energy, where Li-O_2 and Li-S battery are considered ultimate alternatives to Li-ion battery, mainly due to their high energy density. Basic mechanisms of these three types of batteries are introduced, and some of the recent researches being done on components of Li-ion battery is briefly discussed. Comparisons on energy density between these three types of batteries are made in the article, where Li-O_2 battery has a highest theoretical and practical energy density, followed by Li-S battery, and finally Li-ion battery. By applying a high energy density storage system in EV can further expand the EV market, and hence tend to be potentially beneficial to the global environment.

Keywords: lithium-ion battery, lithium sulphur battery, lithium oxygen battery, energy density, specific energy.

1. Introduction

Under the current circumstance of the rapid expansion of the electric vehicle (EV) market, developing the energy density (ED) of batteries becomes one of the major priorities of EV producers. There are several benefits to doing this. First of all, the ED of batteries is highly related to their driving range. Secondly, the high ED of batteries would give the vehicle higher output power, positively influencing vehicle performance. Furthermore, it is also critical because it determines the size and volume of the battery pack in the EV. Hence, it is a reasonable result for EVs with high ED batteries to have better sales. The increasing ED of batteries can contribute to reducing environmental issues, such as carbon emissions.

Overall, the ED of batteries has increased steadily over the past decade, with several breakthroughs in recent years. Nowadays, Li-ion batteries are the most widely used in the EV industry, due to their reasonably high ED and relatively low cost compared to other batteries still under development. The ED of Li-ion batteries can vary with their cell design, component material, and manufacturing process. Some other potential alternatives to Li-ion batteries are Li-S batteries and Li-O_2 batteries, which are both still in the research stage and not yet commercialized. Li-S battery development has advanced significantly in recent years, and experiments conducted in the lab have revealed that Li-S batteries are capable of far higher ED than Li-ion batteries. Besides, the abundance of sulphur results in a low cost of Li-S battery.

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On the other hand, $Li\text{-}O_2$ batteries have the potential for very high ED, which is much higher than traditional Li-ion batteries. The theoretical ED of a $Li\text{-}O_2$ battery is estimated to be about 5 to 10 times higher than that of a typical Li-ion battery. $Li\text{-}O_2$ battery is often considered the ultimate alternative to Li-ion batteries with its high ED which is almost the ED of diesel or gasoline used in an internal combustion (IC) engine. Due to their potential for high ED and cheap cost, Li-S batteries and $Li\text{-}O_2$ batteries generally hold tremendous promise for the future of energy storage; nevertheless, more work has to be done on research and development before they can be extensively applied in commercial applications [1].

In the article, the mechanism of Li-ion, Li-S, and $Li\text{-}O_2$ batteries will be briefly introduced respectively. In terms of Li-ion batteries, the relationship between their ED and the material of anodes, cathodes, and electrolytes will be discussed. The theoretical and practical ED of each battery will then be discussed with some of the latest research being done. Furthermore, comparisons will be made between the difference between their theoretical and practical ED. Finally, the future development potential of each type batteries will be mentioned.

2. Lithium-ion battery (LIB)

2.1. Basic mechanisms and structure

Lithium ions (Li^+) from the cathode go through the electrolyte and are stored in the anode during charging. Li^+ is irreversibly inserted into the crystal structure of the anode material during this procedure, which is known as intercalation. When a battery is drained, the process is reversed, and the Li^+ migrate from the anode back to the cathode. In contrast, the electrons are halted by the separator and pushed to proceed through the circuit, creating a flow of electrons that may be used to power external devices. The electrolyte, which is commonly a lithium salt mixed in an organic solvent, facilitates the passage of Li^+ in a Li-ion battery. The electrolyte also plays an essential role in preventing short circuits and ensuring the safety of the battery [2]. The chemical reaction of this whole process is given by Equation (1) [3]:

$$C_6 + Li^+ + e^- \rightleftharpoons LiC_6 \tag{1}$$

which is a reversible reaction indicating the battery is rechargeable.

The Li-ion battery structure consists of several key components, including the anode, cathode, electrolyte, separator, and current collectors. It is worth noticing that a battery's performance and ED are highly related to the design and material of these components. A typical cathode serves as a source of Li-ions in the batteries, which is made of metal oxide material, such as $LiCoO_2$, $LiFePO_4$, or $LiMn_2O_4$. Most of the anode in a commercialized battery is made of graphite, which functions as a host material to intercalate Li-ions during charging. In recent years, new anode materials, such as silicon nanotubes, are being developed and getting closer to the stage of commercializing [2]. In terms of electrolyte, conventionally it is a liquid or a type of polymer gel, which allows the flow of Li-ions back and force between the anode and the cathode [4]. The separator is a porous, non-conductive, and partially permeable membrane made of polyethene or polypropylene that physically separates the anode and cathode which only allows Li-ions to go through, and stop the flow of electrons (prevent short-circuits between the two electrodes) [5]. The current collectors are conductive materials that facilitate the flow of electrons between the electrodes and external circuitry. The anode current collector is typically made of copper foil, while the cathode current collector is made of aluminium foil.

2.2. Relations between energy densities and material of components

2.2.1. Anode. The components, as previously discussed, are one of the key elements that affect the ED of batteries. The ED of a Li-ion battery may be enhanced relatively dramatically by modifying the anode material. The use of a high-capacity anode material is one of the prevalent strategies nowadays. The ED increases as the anode's area capacity increases.

Graphite and lithium metal anodes are the two anodes that are most frequently utilized in Li-ion batteries. Lithium-ion batteries with lithium metal anodes have a comparatively high specific capacity of 3861 mAh g^{-1}compared to those with graphite anodes, which have a specific capacity of 372 mAh g^{-1}.

Silicon anodes have been a focus of research, as they are capable of storing about 10 times more Li-ions per unit mass than conventional graphite anodes. The fundamental problem with silicon anodes is the significant volume contraction and expansion that takes place during the discharge process, which causes extremely high mechanical stress and, as a result, a reduction in storage capacity. To tackle the problem, there exist several approaches, with using silicon nanotubes being the main focus, which has significantly larger strength than normal material, allowing them to exhibit good stability and cycle life with a high ED. Recently, Amprius Technologies has developed an ultra-high ED Li-ion battery by applying silicon nanowires anode. The battery has a fast-charging capability and is not far from being widely spread in the market and commercialized [6]. Meanwhile, other approaches, such as porous silicon anode, silicon array, silicon nanosheets, and silicon hollow nanospheres, are also potential alternative solutions to the issue [7].

Another recent research was on Co_2VO_4. The Li-ions diffusion coefficient (6.95×10^{-10} cm^2 s^{-1}) of Co_2VO_4 has been evaluated and rated to be high, which makes it a promising choice of the anode in fast-charging Li-ion battery. A hexagonal porous Co_2VO_4 nanodisk (PCVO ND) is created with a lot of pores and a high specific surface area (74.75 m^2 g^{-1}). With a large capacity of about 1000 mAh g^{-1} and a low capacity loss each cycle (just about 0.024% capacity loss per cycle at 10 C for 1000 cycles), this produces outstanding quick charging [8].

2.2.2. Cathode. Cathode is also a significant factor determining a Li-ion battery's ED. One of the major capacities that dictate the ED of the battery is the discharge capacity which is related to the cathode, as the electrical energy is obtained from the battery during the process of discharging. Lithium metal compounds like $LiCoO_2$, $LiFePO_4$, or $LiMn_2O_4$ are frequently used as cathodes.

2.2.3. Electrolyte. The ED of a Li-ion battery can be significantly influenced by the electrolyte used. For the Li^+ to move through the electrolyte efficiently, they must have a high ionic conductivity. However, the electrolyte also needs to have a low viscosity to reduce internal resistance and boost the battery's power output. A broad electrochemical stability window for the electrolyte is also necessary to prevent side reactions that could eventually impair the performance of the battery.

The ED of Li-ion batteries is significantly impacted by the electrolyte solvent used. Since they can dissolve the lithium salt and offer strong ionic conductivity, solvents with high dielectric constants like ethylene carbonate (EC) and dimethyl carbonate (DMC) are frequently employed in Li-ion battery electrolytes. Some solvents have high molecular weights as well, which can lower the battery's ED [9].

The use of alternate solvents, such as low molecular weight esters and nitriles, that can give high ionic conductivity while simultaneously decreasing the overall weight of the electrolyte has been investigated by researchers as a solution to this problem. For instance, it has been demonstrated that Li-ion batteries utilizing an ethyl methyl carbonate (EMC) and diethyl carbonate (DEC) solvent mixture have better ED than those using EC/DMC electrolytes [10].

3. Lithium sulphur battery (Li-S battery)

3.1. Basic mechanisms and structure

The Li-S battery stores and releases energy by operating a redox reaction to transfer electrons and Li-ions between the anode and cathode. It has a similar basic working principle and structure as the Li-ion battery. Similarly, the anode of the Li-S battery is also made of lithium metal, which releases electrons that flow through the external circuit during the process of discharging. However, a typical cathode in a Li-S battery is made of sulphur. While discharging, sulphur reacts with Li-ions to form lithium sulphide

(Li_2S). The electrolyte can be considered the same as in Li-ion batteries with the same function and type of materials.

On the other hand, the Li-S battery is still in the developing stage with a few unsolved problems. One issue with the Li-S battery is the polysulfide shuttle phenomenon that appeared during discharging, where polysulfides are formed as intermediates in the reaction between sulphur and Li-ions. The chemical property of polysulfides makes them soluble in the electrolyte, which enables them to shuttle between the two electrodes, resulting in the amount of active sulphur decrease, and hence the battery capacity decline [11].

3.2. Energy density

A Li-S battery has been estimated to have a potential ED of about 2600 Wh kg^{-1} [12]. This high ED results from the low atomic weight of lithium used as an anode material and the large theoretical capacity of sulphur used as a cathode material. However, due to a number of technical difficulties that must be resolved before large-scale manufacture and commercialization, Li-S batteries' actual ED is far lower. One of the key problems, which leads to subpar battery performance, is the low electrical conductivity of sulphur. The use of conductive additives, the development of innovative sulphur cathodes with enhanced conductivity, and changes to the electrode shape to increase sulphur consumption are a few strategies that have been put out to address this issue.

4. Lithium oxygen battery (Li-O_2 battery)

4.1. The mechanisms and structure

Similarly, as in the other two batteries, the Li-O_2 battery stores and releases energy by capturing Li-ions. However, the way of storing Li-ions is very different. The catalyst of a typical Li-O_2 battery can be thought of as a kind of catalyst, which most of them are made of carbon-based material with a large surface area. For example, carbon nanotubes or graphene which both provide a huge number of active sites for the oxygen reduction reaction to happen. During discharging, the Li-ions are transferred from the anode through the separator and the electrolyte and the electrons through the external circuit arrive at the cathode. They then are enforced to react with oxygen molecules to form Li_2O_2, and hence energy is released. Due to the existence of the high reactivity of Li_2O_2 and the presence of an organic electrolyte, the cathode must be very stable [13].

4.2. Energy density

ED up to 3860 Wh/kg, or around ten times that of traditional lithium-ion batteries, are achievable using Li-O_2 batteries. The high ED of Li-O_2 batteries is largely attributable to the Li_2O_2 that generates upon discharge, which has a high theoretical capacity. Additionally, oxygen is a lighter cathode material since it has a lower atomic weight than other popular cathode components like cobalt and nickel. However, a number of factors make it difficult to actually achieve the theoretical ED of Li-O_2 batteries. One of the main problems is the production and decomposition of lithium peroxide, which can lead to irreversible reactions and poor coulombic efficiency. Poor cell performance can result from the cathode becoming clogged due to the formation of solid lithium peroxide, which also limits oxygen diffusion. The high overpotential needed for oxygen reduction at the cathode, which leads to high energy consumption and restricts the battery's usable ED, is another problem. The low electronic and ionic conductivity of the cathode material and the slow oxygen reduction kinetics are primarily to blame for the high overpotential. Additionally, the use of aprotic organic electrolytes in Li-O_2 batteries may result in problems with cost, stability, and safety. At high potentials, organic electrolytes can easily decompose, resulting in the formation of reactive species that can have unintended side effects and reduce battery performance. The conclusion is that although Li-O_2 batteries have a very high theoretical ED, achieving this ED in practise is difficult due to a number of factors, including the production and deterioration of lithium peroxide, high overpotential, and problems with the stability and safety of the electrolyte. To overcome these obstacles, new cathode materials, electrolytes, and cell architectures must be developed, which will enhance the functionality and stability of $Li\text{-}O_2$ batteries [14,15].

5. Comparisons

Theoretically, Li-ion batteries can store up to 387 Wh/kg and 1,015 Wh/L of energy, which is much more than previous battery technologies [16]. However, depending on the particular design and elements used, the practical ED of Li-ion batteries is often lower, ranging from 100 to 265 Wh/kg and 250 to 660 Wh/L.

Compared to Li-ion batteries, $Li\text{-}O_2$ batteries offer a theoretically greater ED of up to 3,582 Wh/kg and 3,436 Wh/L [16]. However, a number of issues, including as the poor efficiency of the oxygen reduction and evolution processes, the generation of insoluble lithium peroxide during discharge, and the instability of the carbon-based cathodes, are currently limiting the practical ED of $Li\text{-}O_2$ batteries. As a result, the literature reports that the realistic ED of $Li\text{-}O_2$ batteries ranges from 100 to 1,000 Wh/kg and 150 to 3,500 Wh/L.

Li-S batteries have a potential ED that is greater than Li-ion batteries at up to 2,567 Wh/kg and 2,199 Wh/L [16]. The poor conductivity of sulphur and its discharge products, the production of soluble polysulfides during cycling, and mechanical deterioration of the cathode are some of the problems that currently restrict the practical ED of Li-S batteries. Therefore, the realistic ED of Li-S batteries as stated in the literature varies between 200 and 500 Wh/kg and 400 and 1,200 Wh/L.

Although Li-ion batteries are the industry leader at the moment, there is still opportunity for progress in terms of their cost, cost-effectiveness, and ED. New cathode and anode materials, electrolytes, and cell designs are being researched in order to improve the performance of Li-ion batteries.

$Li\text{-}O_2$ and Li-S batteries have shown significant potential for producing higher ED than Li-ion batteries, while being in the early stages of development. Researchers are addressing the technological challenges that these battery systems provide, such as their poor efficiency, limited cycle life, and safety issues.

6. Conclusion

In the current situation, Li-ion battery is still the most commonly used type of battery in EVs, due to its reliability, reasonably high ED, relatively low price and etc. However, Li-S and $Li\text{-}O_2$ batteries are thought to be potential alternatives to Li-ion battery with higher ED. In future perspectives, if the technical challenges are solved, these two types of batteries would replace the current Li-ion battery, which would have a phenomenal impact on the EV market, due to the increase of range caused by the higher ED of batteries.

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