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Organic Electrocatalysts in Lithium-Sulfur Batteries: Progress and Prospects

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Perspective

Lithium Sulphur (LiS) batteries are the most attractive candidate for the next-generation energy storage system due to their ultra-high energy density and cost-efficiency. However, their practical uses are plagued by a number of significant disadvantages, the most of which stem from the reactivity and transformation of sulphur intermediates. The study issues in this subject are based on grasping and catalysing these sulphur species. As standard Lithium Polysulfide (LiPS) propellers, carbon dopants with metal/metal-free atoms combined with transition-metal complex displayed considerable electrochemical performance enhancements. These host-accelerators' surface atoms could potentially be employed as active sites. Organic materials with variable structure and composition, on the other hand, can be disseminated as individual molecules on the surface of substrates, making them potentially more efficient electrocatalysts. The well-defined molecular structures also help to clarify the surface-binding mechanisms involved.

Organic electrocatalysts have made significant development as a result of these beliefs. It addresses the structure–activity relationship between the inserted organic molecules and LiPSs and concentrates on the organic electrocatalysts employed in each portion of LiS batteries. The search for high-energy-density secondary batteries is still ongoing, and it has never been slowed by the devastating effects of fossil fuel usage. Beyond typical Lithium-Ion Batteries (LIBs), new upcoming battery systems with ultra-high predicted performance include lithium/sodium-oxygen (Li/NaO_2), lithium/sodium-sulfur (Li/Sul), and zinc-oxygen/sulfur (Zn-O_2/S). Lithium-ion batteries haven't always been easy to develop. Bulk sulphur (S_8) insulation is a priority to address since it will obstruct electron transfer resulting in sluggish sulphur redox reactions and low sulphur utilisation. When electrons were given to the S8 molecules, the S-S bond was broken, resulting in the formation of a long-chain lithium polysulfide (LiPS) molecule. The as-obtained LiPSs are soluble in typical ether electrolyte and can diffuse to the lithium (Li) anode (as known as the "shuttle effect"), resulting in solid Li_2S_2/Li_2S precipitations and low Coulombic efficiency. Various carbon materials have been designed that physically encapsulate LiPSs. Their nonpolar surface, on the other hand, is unable to effectively inhibit the shuttle effects of polar LiPSs. The solution is to make carbonaceous materials more polar, resulting in high chemisorption effects. For example, exposed active sites on carbon materials such as heteroatoms (N, O, S, P, etc.) can adsorb and enrich LiPSs at the electrochemical interfaces by forming chemical interactions. High concentrations of LiPSs collected at highly active interfaces can speed up conversion events and improve reaction kinetics. As a result, LiPSs chemical adsorption favours homogeneous distribution of S and insoluble Li2S2/Li2S on hosts,

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ensuring a strong electrical contact with conductive substrates and efficiently lowering dissolved LiPSsnds. Organic electrocatalysts have two functions in a LiS battery

- Chemically bind LiPSs through active sites to prevent the shuttle effect
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- LiPS redox processes are accelerated
- Regulate the nucleation and growth dynamics of Li2S to optimise the usage of active materials. Traditional LiS batteries use mostly inorganic elements like metal oxides and nitrides as catalysts. Many crystal planes are exposed on their surfaces, which can lead to a variety of intermediate products. As a result, it's difficult to tell which sites operate as catalysts