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13TH INDES 2024
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THE 13TH INTERNATIONAL INNOVATION, INVENTION & DESIGN COMPETITION 2024

EXTENDED ABSTRACTS

e-BOOK

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POWERING THE FUTURE: INNOVATIONS OF NITROGEN-DOPED ACTIVATED CARBON-CATHODE SULFUR HOSTS FOR HIGH PERFORMANCE LITHIUM-SULFUR BATTERIES

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ABSTRACT

Lithium-sulfur (Li-S) batteries have emerged as a promising solution owing to their high theoretical energy density. However, practical implementation has been hindered by the dissolution of lithium polysulfide (LiP) between electrodes, resulting in decreased discharge capacity performance. Thus, this innovation aims to address this challenge by developing an efficient sulfur-cathode host from nitrogen-doped activated carbon (NDAC) derived from palm kernels for the inhibition of LiP. Through nitrogen heteroatom incorporation, the weak interaction between nonpolar carbon surfaces and polar LiP terminals is enhanced, improving the chemical binding capability. Following the sulfur loading, the sulfur composite cathode (NDAC/S) demonstrated stable electrochemical performance, with an initial discharge capacity of 1054.96 mAh/g at 0.1C and retaining a capacity of 686.52 mAh/g after 100 cycles. This capacity is approximately five times higher than commercial nickel manganese cobalt oxide (NMC) Li-ion batteries, which typically offer 278 mAh/g capacity. Owing to its distinctive porous structure and surface nitrogen functionalization, NDAC/S effectively suppressed the formation of lithium polysulfide, resulting in remarkable electrochemical performance.

Keyword: Nitrogen doping, activated carbon, sulfur-host cathode, palm kernel shell, lithium-sulfur batteries

1. INTRODUCTION

The proliferation of portable electronic devices has significantly surged in recent years. This has garnered the interest of researchers and industrial players in developing stable, reliable, and high-energy storage. Although lithium-ion batteries have dominated the market for several decades, their practical energy densities have reached their theoretical limits. Lithium-sulfur (Li-S) batteries have arisen as a favorable alternative for energy storage due to their impressive theoretical specific capacity of 1675 mAh/g and high energy density of 2600 Wh/kg (Cheng et al. 2019). However, the practical implementation of Li-S batteries still have its challenges, such as the shuttle effect resulting from the dissolution, diffusion, and movement of lithium polysulfide intermediates (LiP) between electrodes, which lead to low coulombic efficiency and shuttle effect (Wang et al. 2021).

Significant efforts have been dedicated to improve the electrochemical performance of batteries by inhibiting LiP through adsorption into the activated carbon cathode. However, the interaction between nonpolar activated carbon surface materials and highly polar polysulfides is weak enough to effectively suppress LiP. Nitrogen-doped activated carbon (NDAC) is a promising approach to enhancing the adsorption capacity of carbon materials for polysulfides. This is achieved by improving the electrostatic potential distribution of carbon compounds through the formation of a strong lithium nitrogen chemical bond.

2. METHODOLOGY

The mixture of palm kernel shell, KOH and urea was placed into a quartz tube horizontal split tube furnace and activated up to 800°C for 1 hour. The activated carbon (AC) was then encapsulated with sulfur to produce AC-sulfur composite. The cathode was fabricated by mixing AC-sulfur composite with a carbon black (Super-P) and polyvinylidene fluoride (PVDF) binder in N-methyl-pyrrolidone (NMP). Next, the cathode was coated with the slurry on an aluminum foil. The CR2032-type coin cells were assembled in a glovebox filled with high-purity argon. The nitrogen-doped AC is designated as NDAC while controlled AC is denoted as CAC.

3. FINDINGS

Table 1 indicates the successful introduction of nitrogen onto the surface of AC through the activation reaction with urea. NDAC exhibited high nitrogen content, while CAC had low levels due to the poor stability of the inherent nitrogen-containing functional groups.

Table 1 Elemental analysis

Sample	C	N	H	S	O
NDAC	68.70	3.26	0.87	0.00	27.17
CAC	51.13	0.01	1.63	0.00	47.23

Table 2 BET surface area and total pore of ACs

Sample	BET surface area (m ² /g)	Total pore volume (cm ³ /g)
NDAC	2303.28	1.27
CAC	1188.35	0.82

Table 2 summarizes the BET surface areas and total pore volumes of all samples. NDAC demonstrated a surface area of 2303.28 m²/g and a total pore volume of 1.27 cm³/g, which is approximately twice that of CAC. Nitrogen doping plays an important role in enhancing the specific surface area and porosity of the activated carbons (Singh et al. 2022).

Figure 1a) shows that the NDAC recorded a high LiP adsorption capacity of 12.94 mmol/g, surpassing CAC which has a capacity of only 0.73 mmol/g. The superior LiP adsorption in NDAC can be attributed to its well-developed porosity. Moreover, the substantial nitrogen content within NDAC significantly contributes to enhanced LiP adsorption. The high LiP adsorption is favorable to enhance the batteries performance by reducing shuttle effect (Zhang et al. 2023).

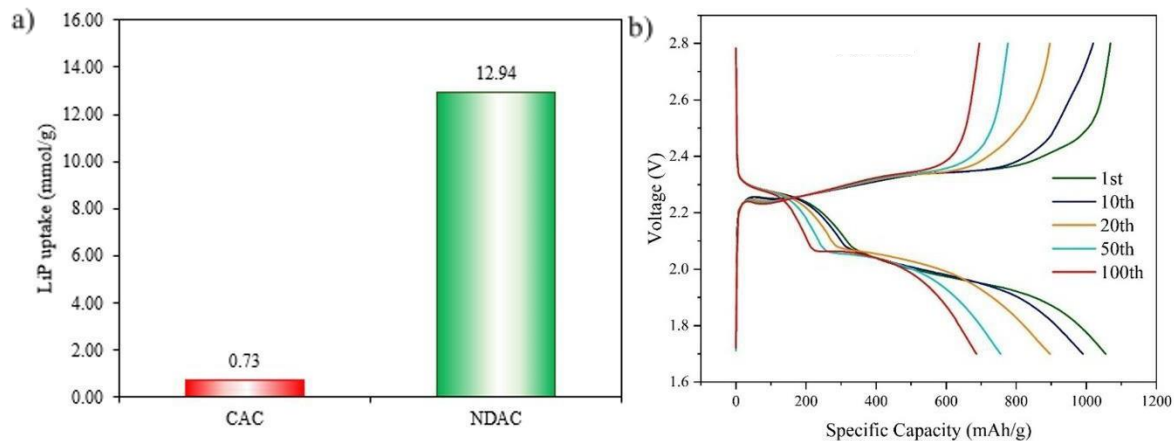


Figure 1 a) Lithium polysulfide adsorption uptake, b) Galvanostatic charge/discharge curves of NDAC/S electrodes at a current density of 0.1C

NDAC was further analyzed for battery performance. Following the sulfur loading, the sulfur composite cathode (NDAC/S) demonstrated stable electrochemical performance, with an initial discharge capacity of 1054.96 mAh/g at 0.1C and retaining a capacity of 686.52 mAh/g after 100 cycles (Figure 1b). This capacity is approximately five times higher than commercial nickel manganese cobalt oxide (NMC) Li-ion batteries, which typically offer 278 mAh/g capacity (Figure 2). Owing to its distinctive porous structure and surface nitrogen functionalization, NDAC/S effectively suppressed the formation of lithium polysulfide, resulting in remarkable electrochemical performance.

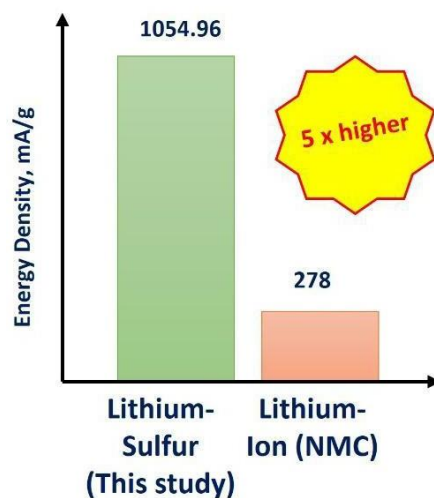


Figure 2 Comparison of energy density.

4. CONCLUSION

These innovations shed light on the production of high-end activated carbon cathodes using cost-effective palm kernel shells as promising sulfur cathode materials for Li-S batteries.

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