Coupling Adsorption and Catalytic Sites for High-performance Lithium-sulfur Batteries

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Lithium-sulfur (Li-S) batteries, boasting an ultrahigh theoretical energy density of 2600 W·h·kg^{-1} along with the low cost and natural abundance of elemental sulfur cathodes, are regarded as a highly promising next-generation energy storage technology.[1] However, the extremely sluggish redox kinetics of lithium polysulfide (LiPS) intermediates persistently impedes the practical deployment of Li-S batteries.[2,3] To overcome the above bottleneck, conventional strategies typically introduce substantial amounts of cathode host materials or catalysts to promote LiPS conversion *via* physical confinement and chemical catalysis.[4−6] Nevertheless, while these approaches enhance electrochemical performance, they simultaneously introduce a significant amount of inactive mass, leading to a drastic decay in the overall energy density of the battery at the device level.[7,8] Therefore, achieving high electrochemical performance while minimizing the fraction of inactive materials remains a grand challenge in rechargeable battery field.

Recently, a joint research team led by Prof. Dan WANG and Prof. Ranbo YU from Shenzhen University, Prof. Jiangyan WANG from the Institute of Process Engineering, Chinese Academy of Sciences, Prof. Zheng LIANG from Shanghai Jiao Tong University, and Prof. Liang LI from Soochow University published an inspiring work in *Nature Sustainability* regarding the integration of adsorption and catalytic sites to construct high-performance Li-S batteries.[9] Breaking away from the long-standing design paradigm of conventional sulfur host materials, the team employed an *in-situ* synthesis technique to ingeniously construct *sp*-hybridized nitrogen-doped graphdiyne hollow multi-shelled structures (*sp*-N GDY HoMSs) through a pericyclic reaction[10] as a novel high-efficiency sulfur cathode host material (Fig. 1, A and B).

This work systematically uncovers the fundamental impact of the electronic structure of doping sites on the synergistic adsorption-catalysis effect. *In-situ* spectroscopic characterizations and density functional theory (DFT) calculations demonstrate excellent *sp* orbital overlap between the nitrogen atom and its adjacent carbon atoms, resulting in a significant alteration of charge distribution compared to conventional carbon and nitrogen atoms (Fig. 1C). Furthermore, the above highly polarized design induces local dipoles between the highly negatively charged nitrogen atoms and the highly positively charged adjacent carbon atoms. Driven by these dipole interactions, these well-defined sites not only strongly anchor LiPSs but also serve as robust catalytic centers to remarkably lower the

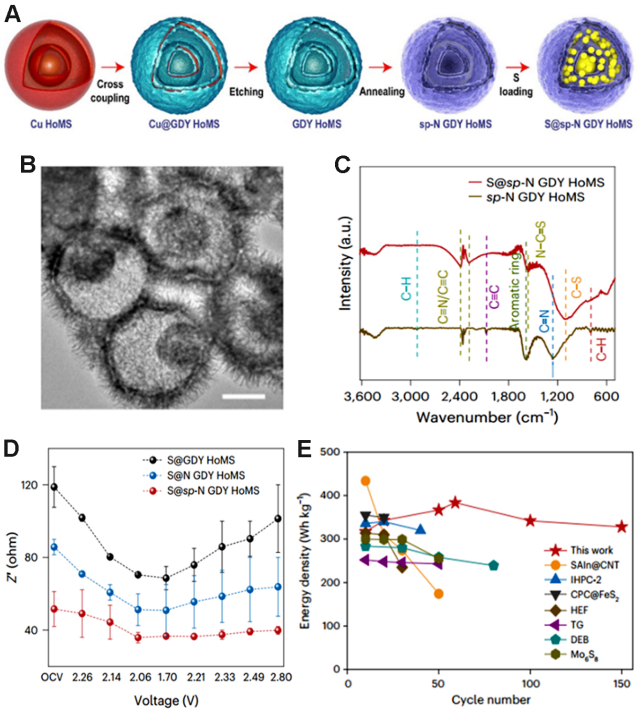

Fig. 1 Synthesis, characterization of *sp*-N GDY HoMSs and their applications in practical lithium-sulfur batteries

(A) Schematic illustration of the synthetic process of S@*sp*-N GDY HoMS; (B) TEM image of *sp*-N GDY HoMSs (scale bar: 500 nm); (C) FTIR curves of *sp*-N GDY HoMSs and S@*sp*-N GDY HoMSs; (D) resistance variation of *in-situ* EIS for different cathodes; (E) gravimetric energy density comparison of S@*sp*-N GDY HoMS pouch cells with reported Li-S batteries.
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reaction energy barriers of the multi-step LiPS redox conversion, especially the rate-limiting liquid-solid phase transition from LiPSs to solid Li_2S_2/Li_2S products (Fig. 1D).

Beyond unprecedented adsorption-catalysis bifunctionality, the multi-shelled network assembled from graphdiyne nanosheets also provides strong physical confinement. Enabled by the rational coupling of the physical confinement and chemical catalysis effects, the composite cathode achieved striking breakthroughs in electrochemical performance. With an ultrahigh sulfur content of 93.9%, the coin cells achieved a high specific discharge capacity of 1462 $mA{\cdot}h{\cdot}g^{-1}$, and it can also deliver stable cycling for over 600 cycles at a high rate of 10 C (1 C=1675 $mA{\cdot}g^{-1}$). Under practical evaluation conditions featuring lean electrolyte and limited lithium adoption, the Ah-level pouch cells realized an outstanding performance of 160 cycles at a high energy density of 400 $W{\cdot}h{\cdot}kg^{-1}$ (Fig. 1E), and maintained excellent electrochemical stability even after multiple physical bending cycles.

In summary, by minimizing the inactive mass fraction while maximizing the bifunctional activity of the host material, this work successfully breaks the long-standing trade-off between electrochemical performance and practical energy output, bridging the critical gap between the molecular design of advanced energy materials and device-level applications, providing a pioneering and universal paradigm for the development of novel battery systems with high energy density and high-rate capability.

Conflicts of Interest

ZHANG Qiang is an editorial board member for *Chemical Research in Chinese Universities* and was not involved in the editorial review or the decision to publish this article. The author declares no conflicts of interest.

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