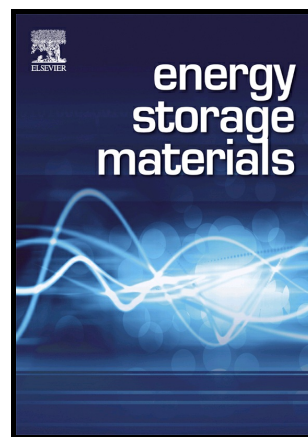


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Cobalt-Embedded Nitrogen-Doped Hollow Carbon Nanorods for Synergistically Immobilizing the Discharge Products in Lithium-Sulfur Battery

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Abstract: Hollow nanostructured carbon materials served as host scaffolds for sulfur cathode in lithium-sulfur (Li-S) battery can effectively promote electronic conductivity, physically confine sulfur and polysulfide, and offer enough space to accommodate volume expansion. However, the capacity decay induced by the detachment of discharge products ($\text{Li}_2\text{S}_2/\text{Li}_2\text{S}$) still remains a great challenge due to the weak interaction between the lithium sulfides and carbon host. Herein, cobalt-embedded nitrogen-doped hollow carbon nanorods (Co@NHCRs) were reported to be employed as sulfur hosts. Density functional theory calculations reveal that the doping of nitrogen atoms and incorporation of metal cobalt nanoparticles can modulate the electron structure of hollow carbon nanorods, thus synergistically helping to enhance chemical adsorption of lithium sulfides on the surface of hollow carbon nanorods. Such a strongly anchored $\text{Li}_2\text{S}_2/\text{Li}_2\text{S}$ prevents the loss of active mass and maintains good electrical contact with conductive carbon matrix. Benefiting from these combined advantages, the as-made Co@NHCRs and sulfur composite (Co@NHCRs/S) possesses high rate capability and excellent cycling stability. The present strategy that metal nanoparticles embedded in hollow nanostructured carbon materials can modulate and immobilize the deposition of discharge products paves one's new way for the development of high-performance Li-S battery.

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