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Novel 3D flower-like micro/nano-structure FeS/N-doped-C composites as advanced cathodes with high lithium storage performances

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Abstract

Due to their merits of high capacity, abundant resources and environmental benignity, Fe monosulfides are considered as attractive electrode materials for Li-ion batteries. However, inferior cyclability and rate performances resulted from inherent low conductivity limit their applications. Herein, we present novel 3D flower-like micro/nano-structure FeS/N-doped-C composites which are directly synthesized from low-cost organosulfur compounds through facile precipitation and subsequent calcination and for the first time applied as cathodes for lithium storage. The FeS nanoparticles are coated by highly conductive N-doped-C shells. Such a confinement of coating microstructures, especially outer N-doped-C, is highly beneficial for the conversion reactions ($FeS+2Li^{+}+2e^{-}\leftrightarrow Fe + Li_2S$), and could strengthen conductivity and simultaneously better protect FeS from electrolyte corrosions, ensuring stable conductive frameworks. Also, such N-doped-C anchor FeS, Fe, and Li_2S effectively, as confirmed by density functional theory calculations. Thus, the FeS/N-doped-C cathodes exhibit remarkable cycling stability (621 mAh g^{-1} at 200th cycle at 1C, with a decay of 0.07%/cycle), and high rate performances (600 mAh g^{-1} even at 10C), delivering higher energy density than commercial $LiCoO_2$ cathodes. This work discloses a novel and paramount route to exploit transition metal sulfides for lithium storage and helps us further understand the key role of N-doping in electrochemical energy storage.