High Performance Potassium Ion Batteries based on Hollow Ternary (Bi-Sb)₂S₃@N-C Nanocube

Hui Ying Yang*

Singapore University of Technology and Design

*E-mail: yanghuiying@sutd.edu.sg

The utilization of metal sulfide anodes has been a promising boost to potassium ion batteries (PIBs) owing to their high theoretical capacities. However, the sluggish kinetics and inferior cycling performance caused by severe volumetric change and particle pulverization greatly hinder their further development. In our work, we discovered robust hollow structure design together with phase structure engineering endow (Bi-Sb)2S3@N-C anode with superior (de)potassiation kinetics and excellent electrochemical performances in PIBs. Specifically, in situ X-ray diffraction combined with density functional theory calculations and ex situ X-ray photoelectron spectroscopy and highresolution transmission electron microscopy (TEM) analyses indicated a fresh reaction mechanism of (Bi-Sb)2S3 anode with a distinctive multistep (de)potassiation route along (003) plane of (Bi,Sb) alloy thanks to the Bi-Sb phase regulation in (Bi-Sb)2S3 anode, ensuring it with superior reaction kinetics. Moreover, in situ TEM characterization revealed the advantages of the hollow nanostructure with carbon shell, facilitating fast ion transport kinetics and high tolerance of volume change as well as enabling the structural integrity of electrode material during (de)potassiation. As a result, the (Bi-Sb)2S3 hollow nanocube with N-doped carbon shell ((Bi-Sb)2S3@N-C) delivers a high initial Coulombic efficiency of 66.3%, a great rate performance of 289 mAh g-1 at 2.0 A g-1, and an ultralong cycling life (89% retention after 220 cycles at 0.1 A g-1 and 85% retention after 1600 cycles at 2.0 A g-1) in PIBs. This work combines structural design and in situ techniques, proving a successful nanostructure engineering strategy to rationalize alloy-type electrode materials for PIBs.