

2D layered CrPSe₃-G-MWCNTs@NiB composite as a superior anode for high performance lithium storage



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Introduction

Energy storage based on electrochemical systems has made a surprising contribution to the well-being of our modern society. In particular, with the development of the electric vehicles (EVs) and storage energy stations, lithium-ion batteries (LIBs) due to their advantageous energy storage performance, low weight, and versatility not only have been given an excellent development opportunity but also have encountered a great challenge due to the huge demands of key markets, such as higher capacity [1]. Accordingly, the key solution to these issues is dependent upon the development of the new electrode materials with high energy and power densities [2].

Design

Based on the considerations of attractive Li storage properties of two-dimensional (2D) layered chromium selenophosphate (CrPSe₃), as well as high conductivity and high specific surface area of carbon materials (graphite and multi-walled carbon nanotubes), we synthesized a 2D CrPSe₃ by one step high-temperature solid-phase synthesis [3]. After combining with graphite and multi-walled carbon nanotubes by high-energy ball milling, the novel 2D/2D heterojunction of CrPSe₃-G-MWCNTs@NiB composite was successfully prepared.

Results and Discussion

The XRD data of crushed single crystals of bulk CrPSe₃, CrPSe₃-G-MWCNTs, and CrPSe₃-G-MWCNTs@NiB materials are displayed in **Figure 1**, which exhibit similar diffraction peaks that can be well assigned to the CrPSe₃ phase (PDF no. 00-033-0403). The morphology features of CrPSe₃-G-MWCNTs@NiB material under different magnifications were observed by SEM and SEM-EDX, as can be seen in **Figure 2**. The electron micrograph of **Figure 2a** and **2b** shows the layered cross-linked structure where MWCNTs are embedded into few-layer graphite, which may create channels between the graphite layers and CrPSe₃. Panels **c–h** of **Figure 2** report the elemental mappings of Cr, P, Se, C, Ni and B, which indicate uniform distribution of all elements throughout the specimen. Compared with the bulk CrPSe₃, the CrPSe₃-G-MWCNTs@NiB composite can enhance the electronic conductivity, increase the interface contact area, and ameliorate the volume change during the repeated insertion/extraction of Li, thus contributing to fast ion/electron transport kinetics [4]. Following this trend, promising electrochemical performances in terms of low discharge-charge polarization, reversibility, cycling stability (660 mAh g⁻¹ after 70 cycles), and capacity retention (89%) are observed (**Figure 3a** and **b**). Thus, such a kind of 2D layered CrPSe₃-G-MWCNTs@NiB material is considered as a promising anode for applications in high performance LIBs.

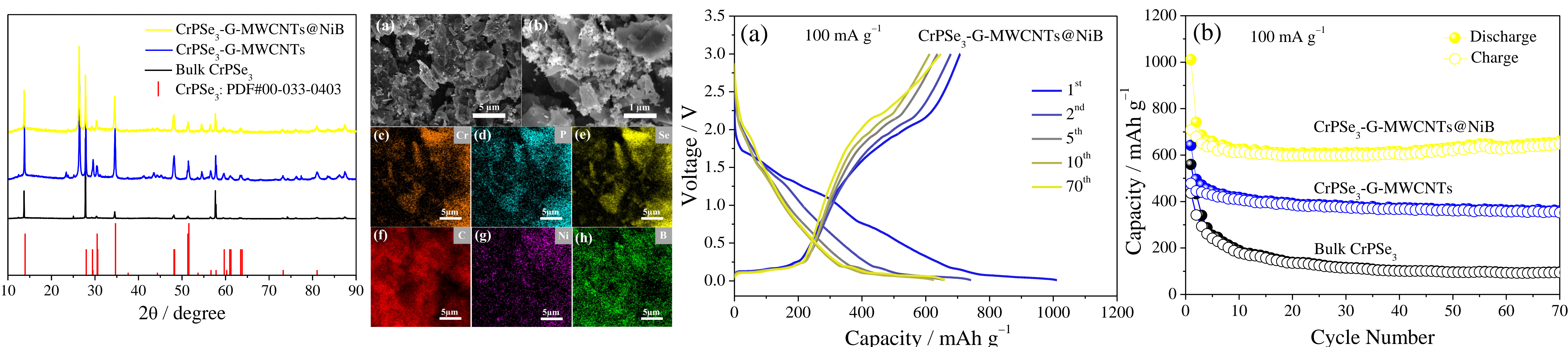


Figure 1. (a) XRD patterns of bulk CrPSe₃, CrPSe₃-G-MWCNTs, and CrPSe₃-G-MWCNTs@NiB.

Figure 2. (a,b) SEM images under two different magnifications of the CrPSe₃-G-MWCNTs@NiB powder; (c–h) SEM-EDS elemental maps of (c) Cr, (d) P, (e) Se, (f) C, (g) Ni, and (h) B in the specimen.

Figure 3. Cycling performance of the as-prepared electrodes in lithium coin cells galvanostatically cycled at a current rate of 100 mA g⁻¹ in terms of (a) voltage profile (CrPSe₃-G-MWCNTs@NiB) and (b) specific capacities (bulk CrPSe₃, CrPSe₃-G-MWCNTs, and CrPSe₃-G-MWCNTs@NiB). Voltage range: 0.01 – 3.0 V.

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Reference

- [1] G. Chen, L. Yan, H. Luo et al., *Adv. Mater.* 28 (2016) 7580–7602.
- [2] S.H. Yu, S.H. Lee, D.J. Lee et al., *Small.* 12 (2016) 2146–2172.
- [3] R. Samal et al., *J. Mater. Chem. A.* 9 (2021) 2560–2591.
- [4] Q.L. Pei, X. Luo, G.T. Lin, et al., *J. Appl. Phys.* 119