Novel hard carbon/graphite composites synthesized by a facile in-situ anchoring method as high-performance anode for Lithium ion batteries

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Experimental

Thermogravimetric analysis (TGA) was carried out on a NETZSCHSTA449 F3 instrument from room temperature to 1000 °C at a heating rate of 5 °C/min under the nitrogen atmosphere. Particle size distribution was determined with a Malvern 2000 Instruments. The particle morphology was observed using a scanning electron microscope (Ultra-high Resolution SEM S-4800, Hitachi

Company) and transition electron microscope (JEOL 2100F, Japan), and EDS mapping analysis was used to analyze the composition and element distribution of the particle surface.

Results

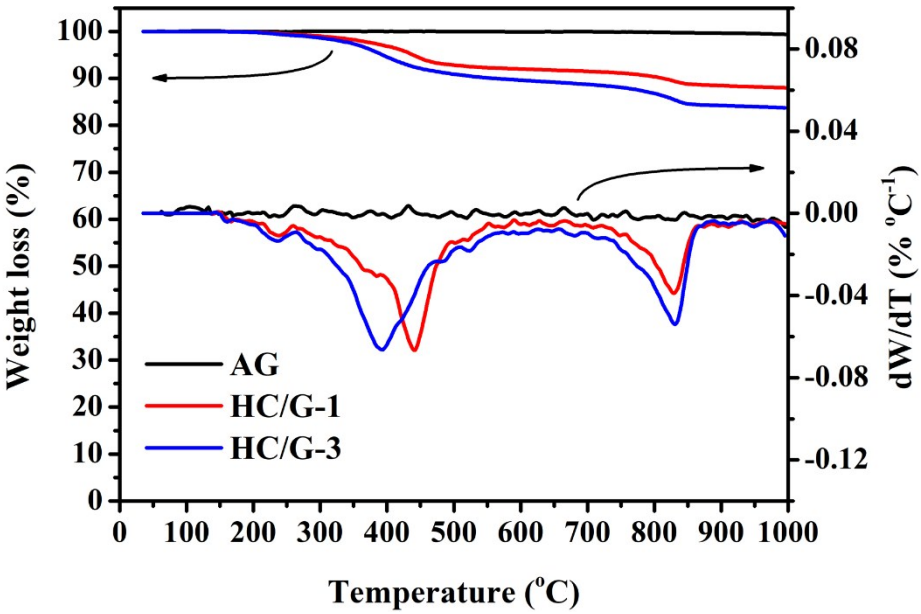

Fig. S1 TG and DTG curves of the samples after drying process

The pyrolysis behavior of the samples were first determined by thermogravimetric (TG) analysis under nitrogen atmosphere, as shown in Fig. S1. The obtained TG-DTG curves revealed a two-stage weight loss process.

Table S1 Types of phosphorus and oxygen functional groups and their binding energies based on the P2p and O1s XPS peaks [1]

Region	Peak	Position (eV)	Assignment
P2p	C_3-P	130.2±0	C_3-P
	C_3-P=O	132.3±0.2	C_3-P=O
	C-P-O	133.1±0.3	C-P(O)$(OH)_2$, C_2-P(O)(OH), $(CO)(C)_2$-PO, $(CO)_2$(C)-PO, and (CO)(C)-P(O)(OH)
	C-O-P	134.0±0.3	CO-P(O)$(OH)_2$, $(CO)_2$-P(O)(OH), and $(CO)_3$-PO
O1s	O-I	530.8±0.4	C=O in carbonyl, quinine or carboxylic acids and P=O
	O-II	532.6±0.1	C-O in phenol, ethers, or C-O-P
	O-III	534.0±0.1	C-O in lactone or carboxylic anhydride

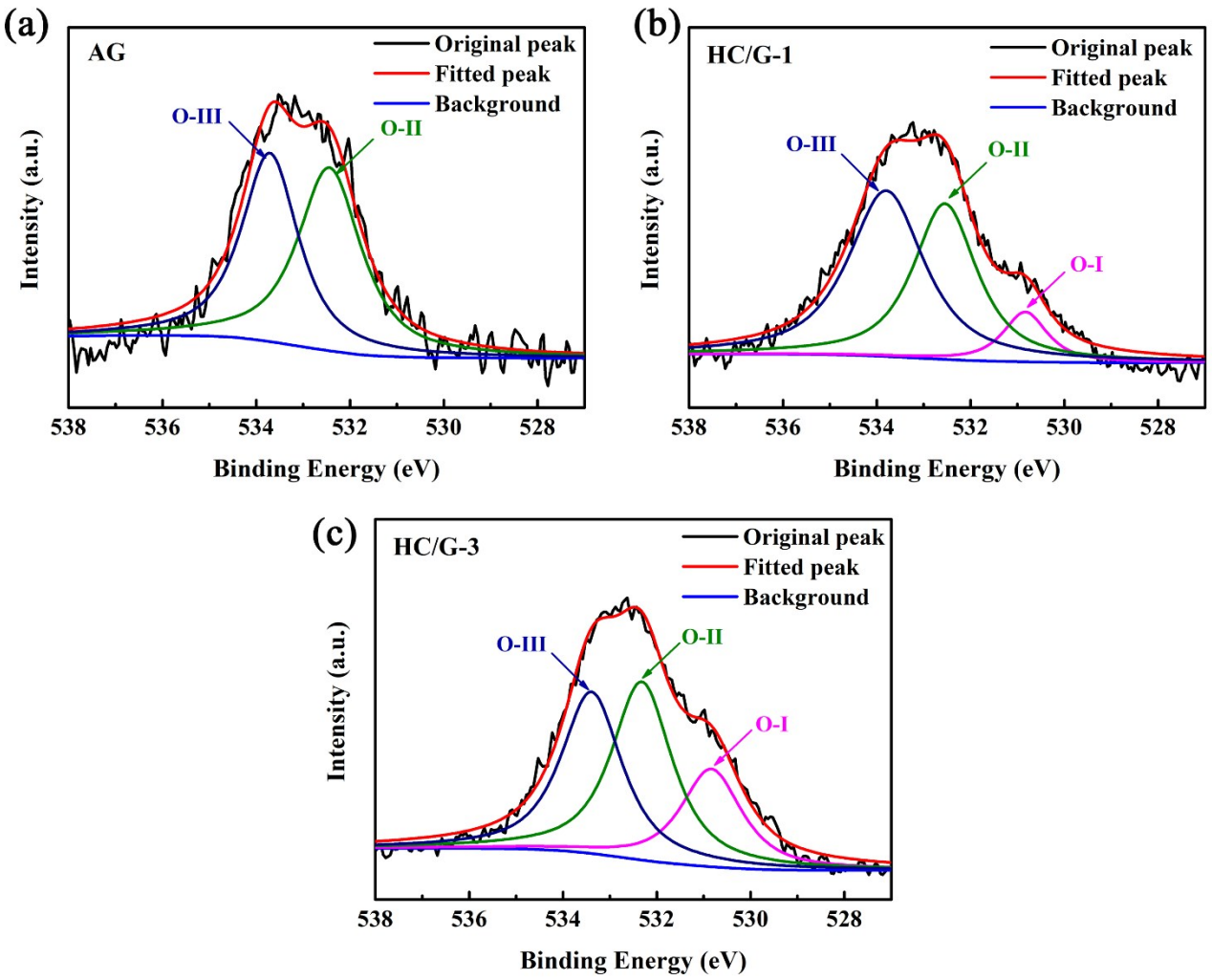

Fig. S2 O1s XPS spectra of the samples after carbonization

Table S2 Results of deconvolution of the P2p and O1s XPS Peaks of the samples after carbonization

Sample	Elemental content (wt.%)			P2p peak (%) Relative contents of phosphorus species				O1s peak (%) Relative contents of oxygen species		
	C	O	P	C-O-P	C-P-O	C_3-P=O	C_3-P	O-I	O-II	O-III
AG	97.1	2.9	0	0	0	0	0	0	52.0	48.0
HC/G-1	89.8	7.0	3.2	18.7	30.0	45.7	5.6	9.0	40.2	50.8
HC/G-3	88.8	7.6	3.6	24.9	22.1	31.0	22.0	22.4	40.6	36.9

Table S1 summarizes the types of phosphorus and oxygen functional groups and their binding energies, obtained by deconvoluting the P2p XPS spectra and O1s XPS spectra of the samples. Table S2 lists the deconvolution results of the high-resolution P2p and O1s core-level peaks in the XPS spectra (Fig. 2 and Fig. S2) of the composites. To be noted, the relative contents of O-I species corresponding to C=O and P=O bonding are remarkably increased with the increase of PO addition, indicating a higher degree of oxidation for HC/G-3.

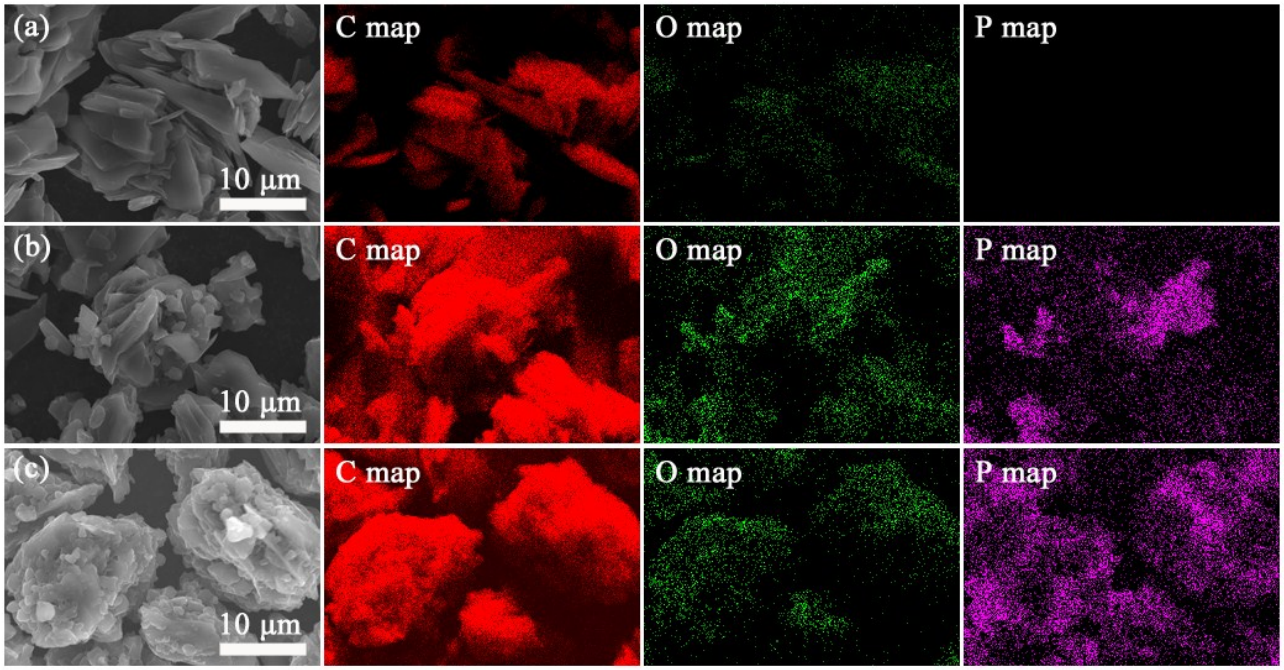

Fig. S3 SEM mapping of (a) AG, (b) HC/G-1, (c) HC/G-3

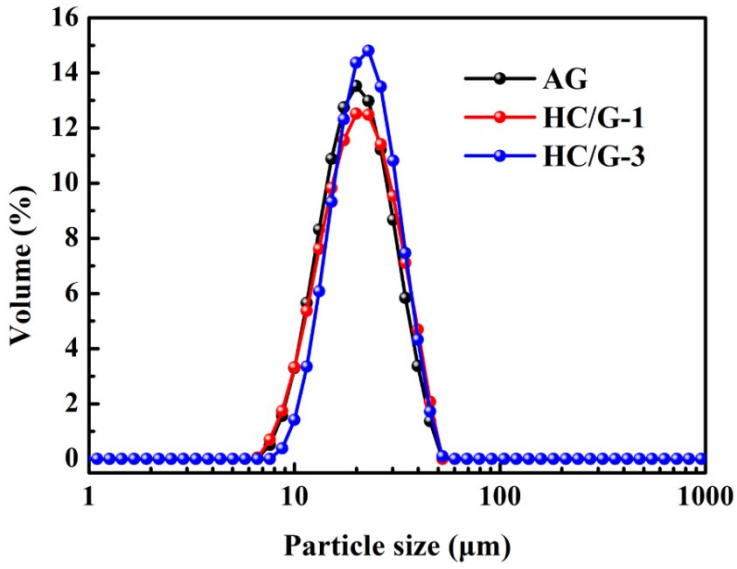

Fig. S4 Particle size distributions of the samples

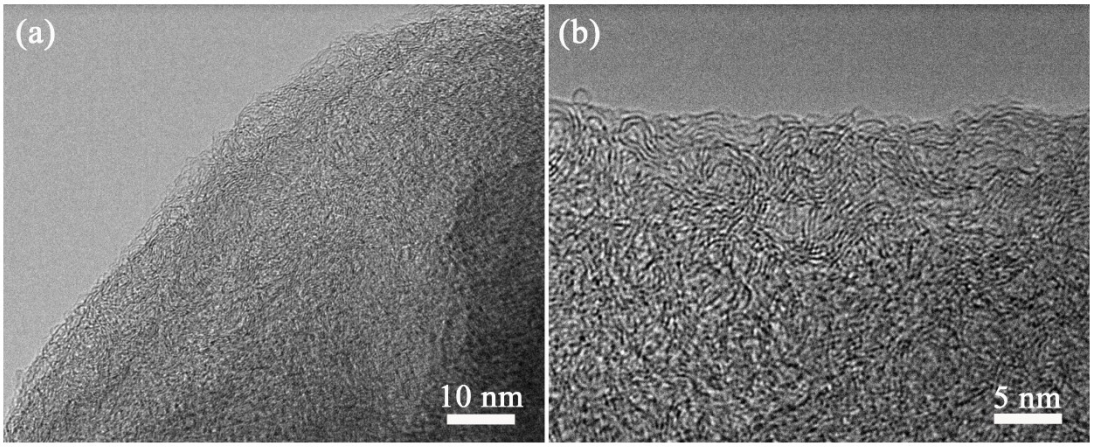

Fig. S5 TEM images of the hard carbon particle in the composite

Fig. S5 gives the TEM image of the hard carbon particle in the composite. It is found that the hard carbon component is poorly crystallized and the short-range parallel stacking of small and curved graphene layers gives rise to nanoporosity in the carbon material. Only turbostratic graphitic structure can be observed, which close to the typical “house of cards” model for hard carbons.

References

[1] Wang, Y., Zuo, S., Yang, J. and Yoon, S. H. (2017). Evolution of phosphorus-containing groups on activated carbons during heat treatment. Langmuir, 33(12), 3112-3122.