Facile synthesis of yolk-shell structured Si-C nanocomposites as anode for lithium-ion battery

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1. Experimental

1.1 Chemicals

Silicon nanoparticles (an average diameter about 100 nm) was purchased from Shanghai ST-Nano science and technology Co. Ltd. Dopamine hydrochloride was purchased from Aladdin Industrial Corporation. Battery-grade dimethyl carbonate (DMC), ethylene carbonate (EC), vinylene carbonate (VC) and LiPF₆ were purchased from Shenzhen Capchem Chemicals Co., Ltd., China, and used without further purification.

1.2 Synthesis of Si@void@C composites

Typically, 180 mg Si nanoparticles were dispersed in 100 mLTris-buffer (10 mM, pH: ~8.5) by ultrasonication for at least 10 min to form a suspension. Subsequently, 180 mg dopamine was added to the mixture under stirring at room temperature for 24 h. Afterwards, the precipitates were collected by centrifugation, washed three times with deionized water, and then dried at 80 °C for 24 h. To carbonize the polydopamine (PODA) coating, the dried powders were placed in a tube and heated to 400 °C at a rate of 1 °C/min under Ar atmosphere and kept this temperature for 2 h, and then heated to 800 °C with a heating rate of 5 °C min⁻¹, and kept at 800 °C for 3 h. The obtained composites were donated as Si@C. Finally, to get the Si@void@C, the Si@C powders were immersed in 0.5M NaOH aqueous solution and etched for 10 min at 60°C, followed by centrifugation and washing three times with deionized water.

1.3 Characterization

X-ray diffraction (XRD) measurements were taken on a X-ray diffractometer (XRD, D/max-2200/PC, Japan) by continuous scanning in the 2θ range of 10-80°. Transmission electron microscopy (TEM) analysis was carried out with a Tecnai G220S-Twin equipment operating at 200 kV. The weight content of Si and carbon in the Si@void@C composites was determined from the weight loss curve measured

under simulated air atmosphere on a TG/DTA instrument (PerkinElmer) with a heating rate of 20 °C/min. The chemical composition of the polydopamine coated Si nanocomposites was analyzed by Fourier transform infrared spectroscopy (ATR-FTIR, Spectrum 100, Perkin Elmer, Inc., USA).

1.4 Electrochemical measurements

Electrochemical experiments were carried out via CR2016 coin-type test cells assembled in an argon-filled glove box with lithium metal as the counter and reference electrodes. The working electrodes were prepared by mixing Si, Si@C or Si@Void@C nanocomposites, carbon black, and sodium carboxymethyl cellulose (CMC) at a weight ratio of 65: 20: 15. After stirred for 8 h to ensure thorough mixing, the resulting slurry was cast onto a thin copper foil and dried in vacuum oven at 80 °C for at least 4 h, and then left at room temperature overnight. Circular electrodes with a diameter of 12 mm were punched and subsequently dried at 80 °C under vacuum oven for 24 h. A Celgard 2400 membrane was used as a separator. The loading silicon on the testing electrodes is about 1 mg/cm². The electrolyte consisted of a solution of 1M LiPF₆ in a 1:1 (w/w) EC/DMC with 10 vol% VC added to improve the cycling stability. The discharge-charge measurements were performed on Land CT2001A tester (Wuhan, China) at the constant current mode over the range of 0.01-1.5 V.



Fig S1. Optical images of bare Si nanoparticles, Si@C and Si@void@C nanocomposites.



Fig S2. SEM image of bare Si nanoparticles.



Fig. S3 FTIR spectra of Si and Si@polydopamine nanocomposites.



Fig. S4 TG curve of Si@void@C nanocomposites.



Fig. S5 TEM image of Si@void@C nanocomposites after 50th cycle.