Supporting Information for

Diameter Selective Band Structure Modification of Single-Walled Carbon Nanotubes by Encapsulated Phosphorus Chains

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1. Materials and sample preparation

The pristine SWNTs samples was synthesized by arc-discharge method using a catalyst with a 1:1 Y/Ni atomic ratio and puried with recently reported method [1]. To introduce the phosphorus into the channel of pristine SWNTs, 80 mg commercial red phosphorus (80 mg) together with 80 mg SWNTs bucky papers was placed in a quartz tube, sealed in a vacuum of 10^{-3} torr and heated at 440 ^{o}C for 24 h. The quartz tube was allowed to cool naturally to room-temperature and the resulting SWNTs bucky-papers were removed from the quartz tube in an inert atmosphere and dispersed in CS_2 by sonication to remove the exterior unembedded phosphorus, the mixtures were then filtered and washed with CS_2, this protocol was repeated for several times. The product was dried naturally and denoted as P@SWNTs.

2. Characterization methods: High-resolution electronic microscope (HR-TEM) images of the hybrid nanostructure were observed on a JEM-2010 apparatus with an acceleration voltage of 200 kV and its composition was analysed by electronic dispersive X-ray spectroscopy (EDX). The optical absorption studies were recorded at room temperature on a Perkin-Elmer UV-VIS-NIR spectrometer (Lamda900), samples were ultrasonicated dispersed in N,N-dimethylformamide (DMF) for 1 hour and ultracentrifuged at a speed of 5000 rp/min for 3 min for forming supernatant, the spectrum was collected from upper supernatant. Raman spectroscopy (Renishaw 2000, excited at 785 nm) was employed to probe the

modification of electronic structure and vibrational propertie caused by introduction of phosphorus into the core of the pristine SWNTs. X-ray diffraction (XRD) patterns were performed on Rigaku DMAX2500 X-ray diffractometer using a copper target. The differentiated scanned calorimetric (DSC) analysis was carried out on NETZSCH DTA-404PC in a range from 30-600 °C with a heating rate of 10 °C /min in N_2.

3. Supporting data

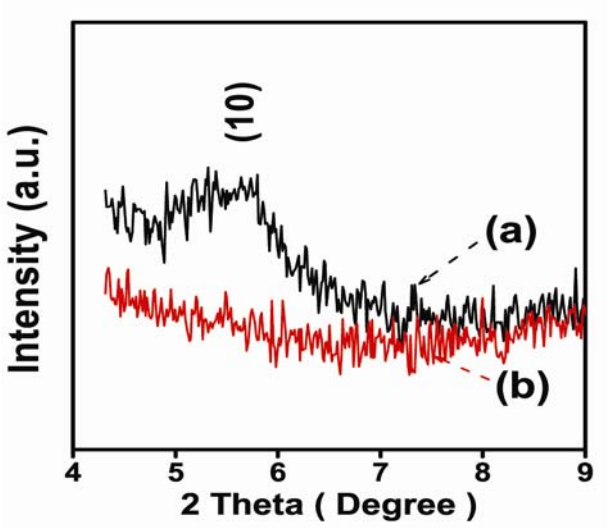

Figure S1. Enlarged XRD patterns of (a) the pristine SWNTs and (b) P@SWNTs

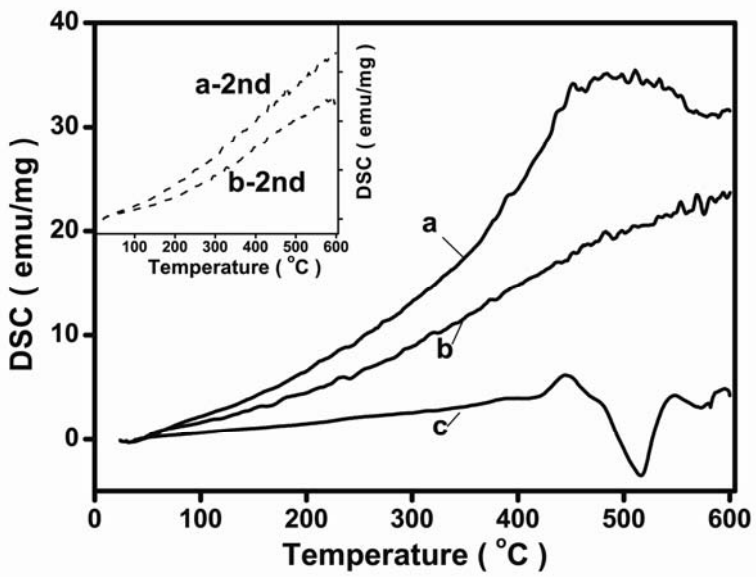

Figure S2. DSC curves of (a) P@SWNTs and (b) the pristine SWNTs and (c) commercial red phosphorus for comparisons. The inset showed the repeated DSC

curves of (a, b).

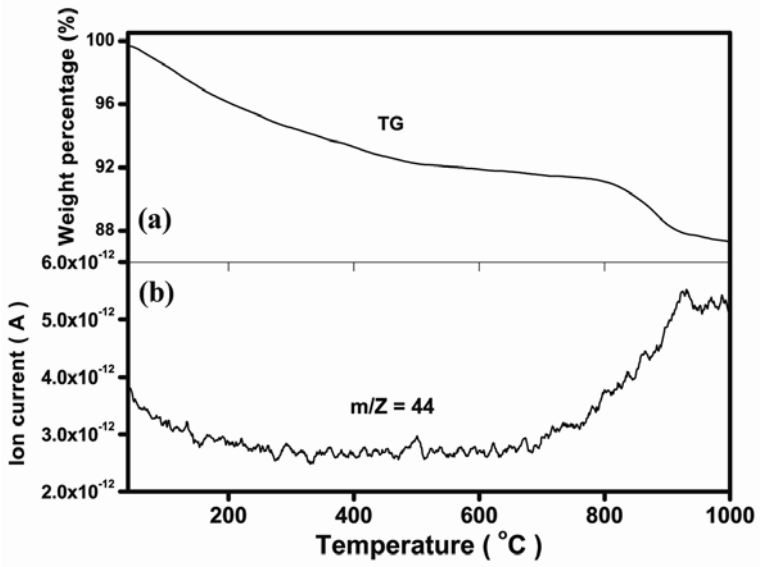

Figure S3. (a) TG curve of P@SWNTs in N_2 atmosphere and (b) Mass spectrum of releasing gas (m/Z = 44).

4. References

[1] Wu, C. X.; Li, J. X.; Dong, G. F.; Guan, L. H. *J. Phys. Chem. C* **2009**, 113, 3612.