Synthesis and high-rate capability of quadrangular carbon nanotubes with one open end as anode materials for lithium-ion batteries

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Supplemental Data:

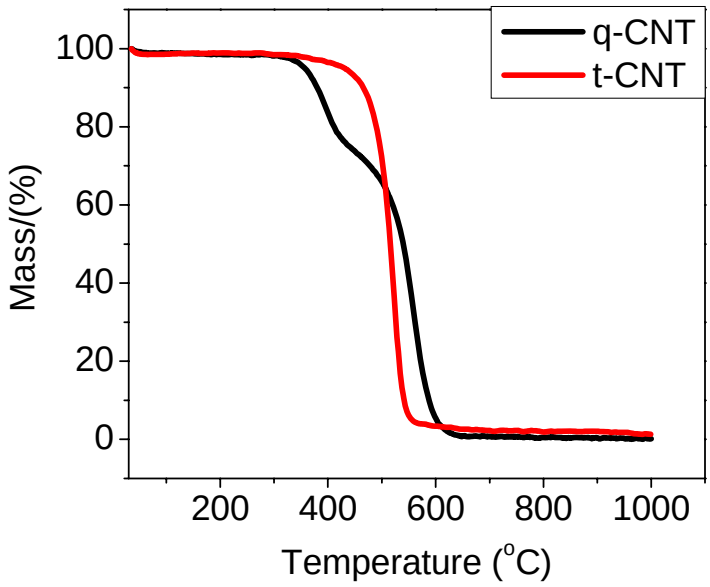

Fig. S1. TG curves at the oxygen gas atmosphere for two CNTs.

Table S1 Data for Raman spectra

Sample	C_D/cm^{-1}	C_G/cm^{-1}	I_D/a.u.	I_G/a.u.	I_D/I_G
t-CNT	1340	1578	2866	5206	0.55
q-CNT	1347	1587	5071	3853	1.32

Note: C_D and C_G stand for the center wave numbers of D- and G-peak, respectively. And I_D and I_G are the intensities of D- and G-peak, respectively.

Table S2 Kinetic parameters of q-CNT and t-CNT electrodes

	q-CNT		t-CNT	
X in Li_xC_6	R_f/(Ω cm^2)	R_{ct}/(Ω cm^2)	R_f/(Ω cm^2)	R_{ct}/(Ω cm^2)
0.025	4.6	9.8	5.3	12.9
0.100	5.3	13.4	5.3	14.0
0.175	5.4	14.1	5.5	16.4
0.250	5.4	15.4	6.1	20.8
0.325	5.1	14.7	7.3	30.4
0.400	4.3	11.1	6.1	24.0
0.475	5.7	17.9	8.4	36.9
0.550	6.1	20.3	9.4	49.3
0.625	6.9	26.1	--	--
0.700	6.6	24.9	--	--
0.775	6.9	26.5	--	--
0.850	7.9	25.9	--	--

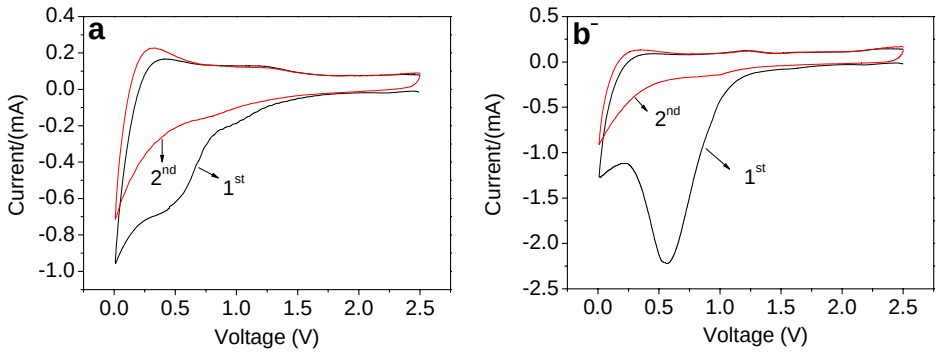

Fig. S2 The cyclic voltammograms of (c) q-CNTs and (d) t-CNTs electrodes.

Calculation of lithium-ion diffusion coefficient:

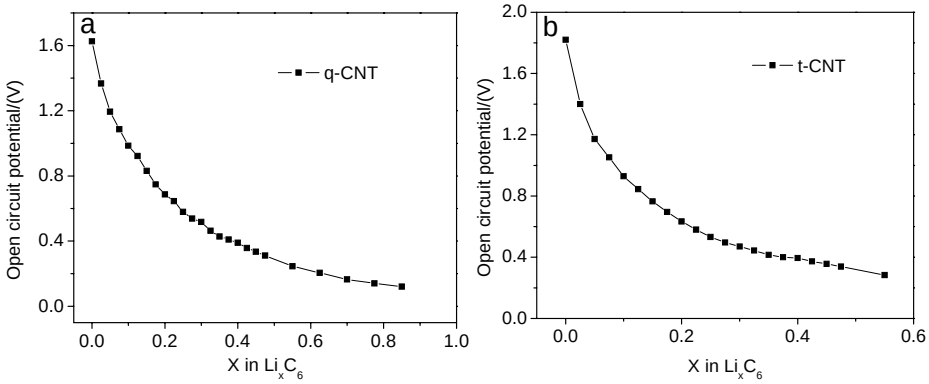

Fig. S3 Open circuit potential vs Li+/Li in $LixC_6$ of (a) q-CNTs and (b) t-CNTs electrodes as function of lithium content x during the second discharge process at the current density of 50 mAg^{-1}.

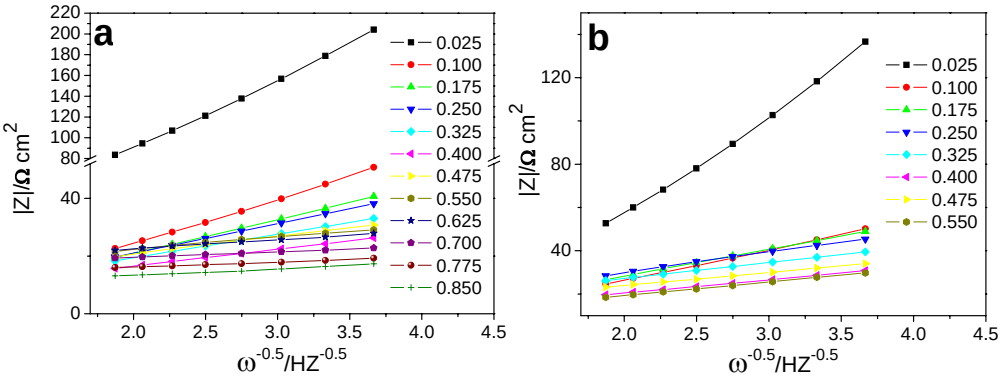

Fig. S4 impedance modulus |Z| as a function of the inverse of square root of angular frequency, $\omega^{-0.5}$ for (a) q-CNTs and (b) tCNTs at various x values in Li_xC_6.

The diffusion coefficient of lithium-ion, D_{li}, can be calculated by the model proposed by Ho et al. [C. Ho, I. D. Raistrik, and R. A. Huggins, *J. Electrochem. Soc.*, 1980, **127**, 343.], according to the following equation:

$$\sigma = V_m(dE/dx)/\{nFA(2D_{li})^{1/2}\} \quad (1)$$

where

(1) V_m is the molar volume of lithiated carbon (6×5.45 cm^3mol^{-1}).

(2) The dE/dx is the slope of open circuit potential (E) vs. x values in Li_xC_6, which can be obtained in Fig. S3. To exclude an effect of irreversible reaction at the firs cycle, the electrode was discharged and charged one time prior to the experiment for the open circuit potential data. Then, the cell was discharge to various x values (in Li_xC_6) at the current density of 50 mAg^{-1} and held for over 10 h at the open circuit conditions, repectively. The open circuit potential was recorded at various x values until the equilibrium was considered to be reached (the variation of voltage was smaller than ± 1 mV).

(3) The Warburg prefactor, σ, can be obtained from the Warburg part in the EIS. The EIS measurement was carried out, after the open circuit potential was measured. And σ is calculated by the plot slope of imaginary resistance (Z") vs. inverse square root of angular frequency ($\omega^{-1/2}$), because the $Z"=-\sigma\omega^{-1/2}$. Fig. S4 shows the linear variation of the modulus of impedance (Z") versus the inverse of the square root of angular frequency ($\omega^{-1/2}$) for two CNTs electrodes at various x values.

(4) The value of n is determined to be 1 obtained from the valence of Li^+.

(5) F is the Faraday constant (96,486 C mol^{-1}).