Electronic Supplementary Information

Vapor Selenization Produced Bi_2Se_3 Nanoparticles in Carbon Fibers 3D Network as Binder-Free Anode for Flexible Lithium-Ion Batteries

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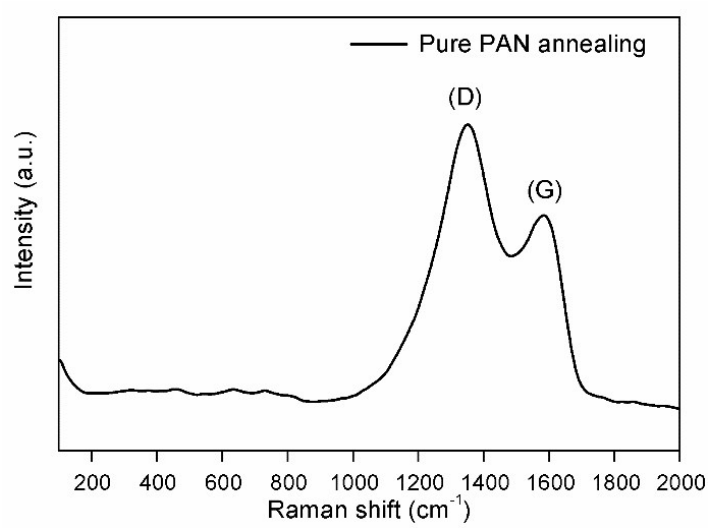

Fig. S1. Raman spectra of the pure PAN after annealing at 700 ˚C for 6 h.

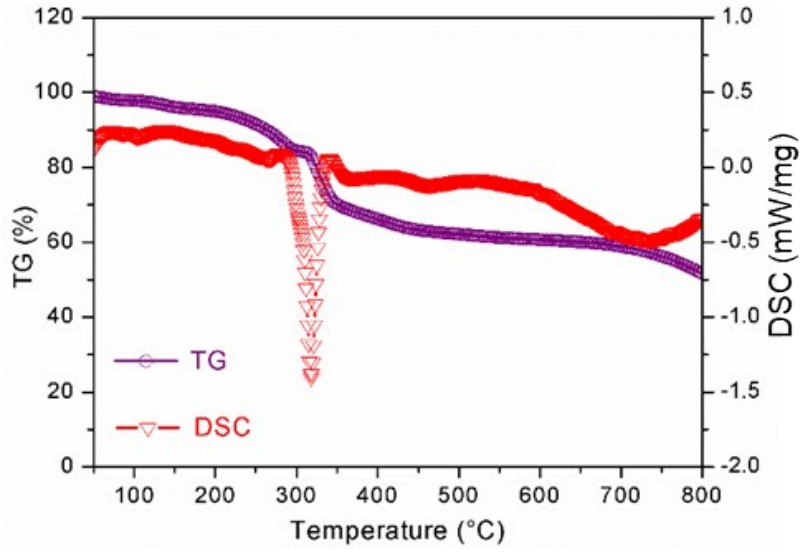

Fig. S2. TGA-DSC curves of the $BiCl_3$/PAN.

Depiction S1

$$2Bi + O_2 \xrightarrow{700\,℃,\ O_2} Bi_2O_3 \quad \text{..... (4)}$$

$$C + O_2 \xrightarrow{700\,℃,\ O_2} CO_2\uparrow \quad \text{..... (5)}$$

$$Bi_2Se_3 + O_2 \xrightarrow{700\,℃,\ O_2} Bi_2O_3 + SeO_2 \quad \text{.....(6)}$$

The content of Bi nanoparticles in Bi/CNFs can be calculated by calculation combining equation (4) and (5). In the same way, the content of Bi_2Se_3 nanoparticles in Bi_2Se_3/CNFs can be calculated by calculation combining equation (6).

$$\text{Bi (\%)} = \frac{\text{Final weight of } Bi_2O_3}{\text{Initial weight of Bi/CNFs}} \times \frac{\text{Molecular weight of Bi} \times 2}{\text{Molecular weight of } Bi_2O_3} \times 100\%$$

$$Bi_2Se_3\ (\%) = \frac{\text{Final weight of } Bi_2O_3}{\text{Initial weight of } Bi_2Se_3/\text{CNFs}} \times \frac{\text{Molecular weight of } Bi_2Se_3}{\text{Molecular weight of } Bi_2O_3} \times 100\%$$

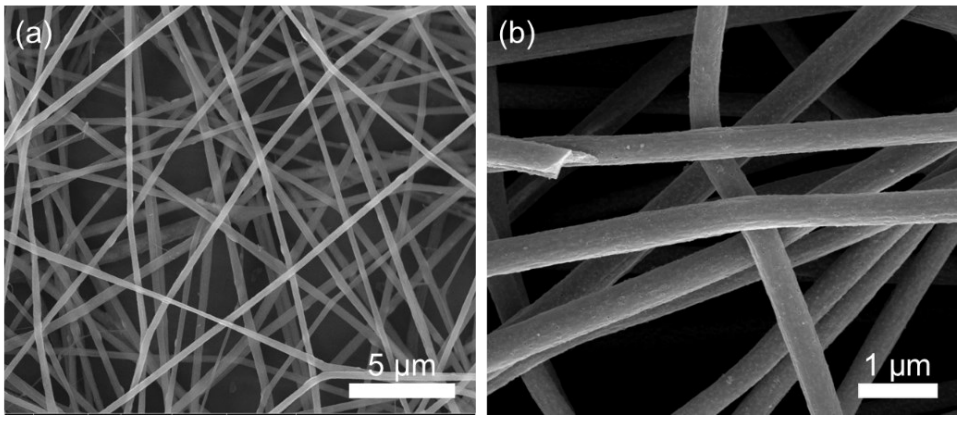

Fig. S3. SEM images of (a) $BiCl_3$/PAN and (b) Bi/CNFs.

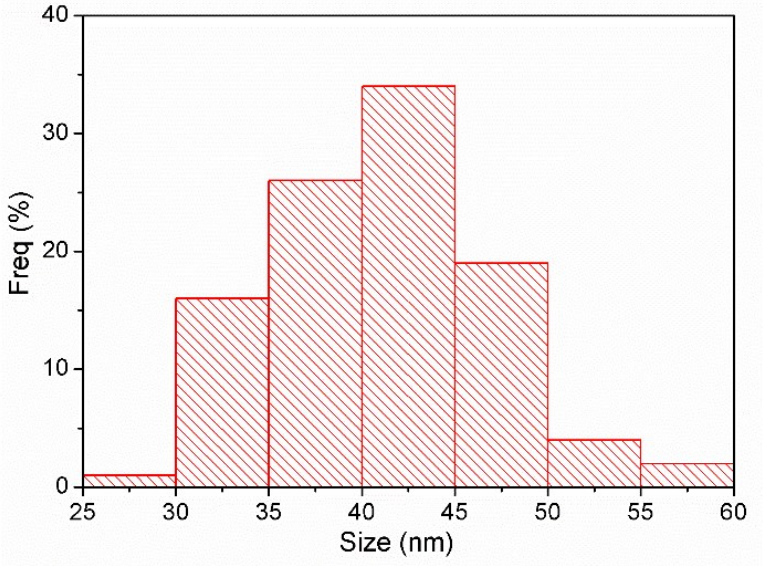

Fig. S4. The particle size distribution of Bi_2Se_3 nanoparticles.

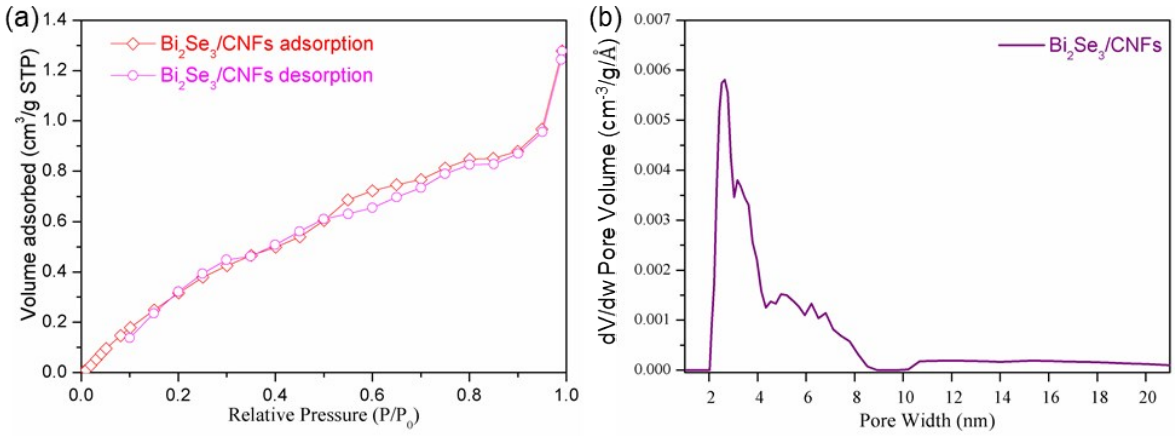

Fig. S5. (a) N_2 adsorption-desorption isotherms and (b) the pore size distribution of the Bi_2Se_3/CNFs.

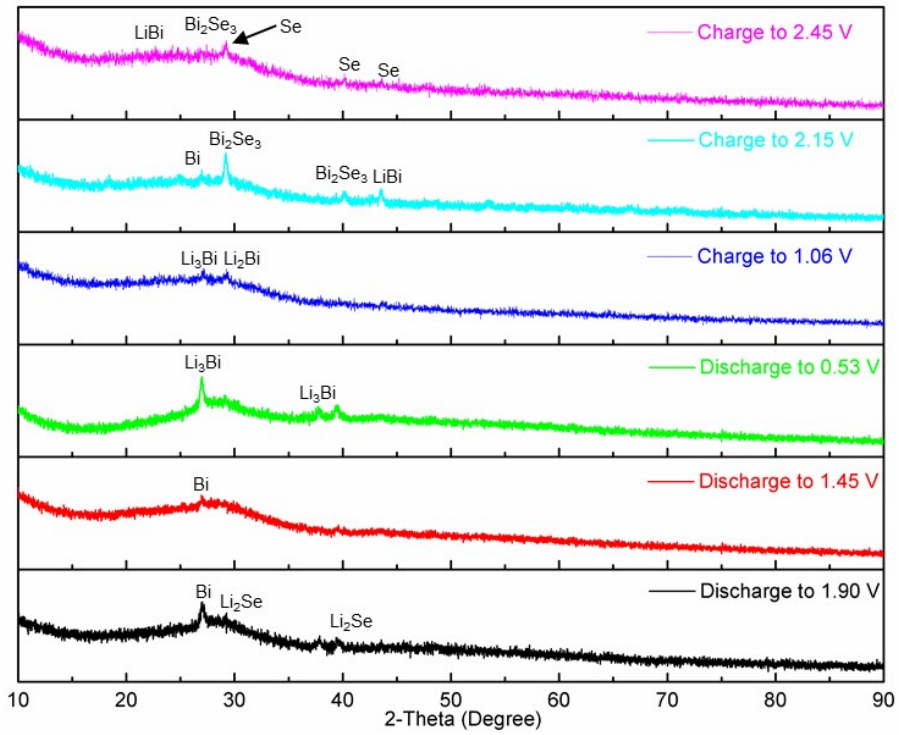

Fig. S6. The *ex*-situ XRD patterns of a new battery discharged and charged to different voltage platforms in the third cycle with Cu Kα1 (40 kV, 40 mA, 10° < 2θ < 90°)

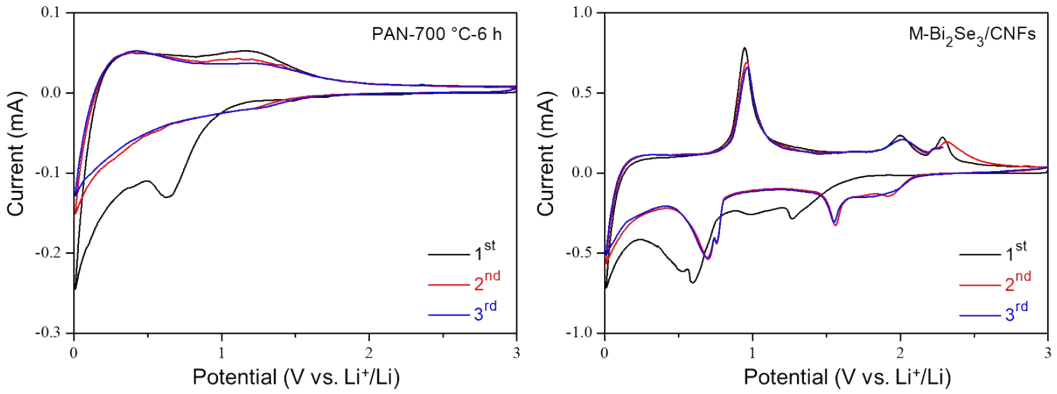

Fig. S7. CV curves of the (a) PAN was annealed at 700 ˚C for 6 h and (b) M-Bi_2Se_3/CNFs electrode from 3.0 V to 0.01 V vs. Li^+/Li at a scan rate of 0.1 mV s^{-1}.

Table S1. The specific capacity of our work for LIBs vs. previous works.

Sample	Current	Cycles	Capacity vs Li^+ ($mAh\ g^{-1}$)	Ref.
Bi_2Se_3 rectangular nanosheets	50 mA g^{-1}	50	34	[1]
Bi_2Se_3 stacking nanosheets	50 mA g^{-1}	50	45	[2]
In-doped Bi_2Se_3	50 mA g^{-1}	50	160.3	[3]
Hierarchical Bi_2Se_3 microrods	50 mA g^{-1}	50	36	[4]
Bi_2Se_3 nanosheets	50 mA g^{-1}	50	66.1	[5]
Bi_2Se_3/Graphene	50 mA g^{-1}	100	203.6	[6]
S-doped Bi_2Se_3	200 mA g^{-1}	100	109.4	[7]
CNTs@C@Bi_2Se_3	100 mA g^{-1}	100	431	[8]
	2 A g^{-1}	100	222	
Bi_2Se_3@NC	100 mA g^{-1}	50	410.6	[9]
	500 mA g^{-1}	400	335.8	
Flexible Bi_2Se_3/CNFs	100 mA g^{-1}	100	443	Our work
	400 mA g^{-1}	100	308	
	2 A g^{-1}	100	189	
	16 A g^{-1}	100	103	

Depiction S2

Synthesis of Bi_2Se_3 nanosheets: 0.75 g $Bi(NO_3)_3 \bullet 5H_2O$, 1.0 g of SeO_2 and 1.0 g of glucose were dissolved in an appropriate amount of deionized water and continuously stirred to obtain the mixed solution A. After continuous stirring to completely dissolve the powders, 20 mL ethanolamine was added to solution A under magnetic stirring, and mixed solution B was obtained after uniform stirring. Transfer the mixed solution B to a 60 mL Teflon stainless steel reactor and add deionized water until it reaches 80% of the total volume. The autoclave reacts for 30 h at 180 ˚C, and after natural cooling, the filtered products are washed several times with distilled water and anhydrous ethanol, and then dried for 6 hours in a vacuum drying oven at 60 ˚C.[10]

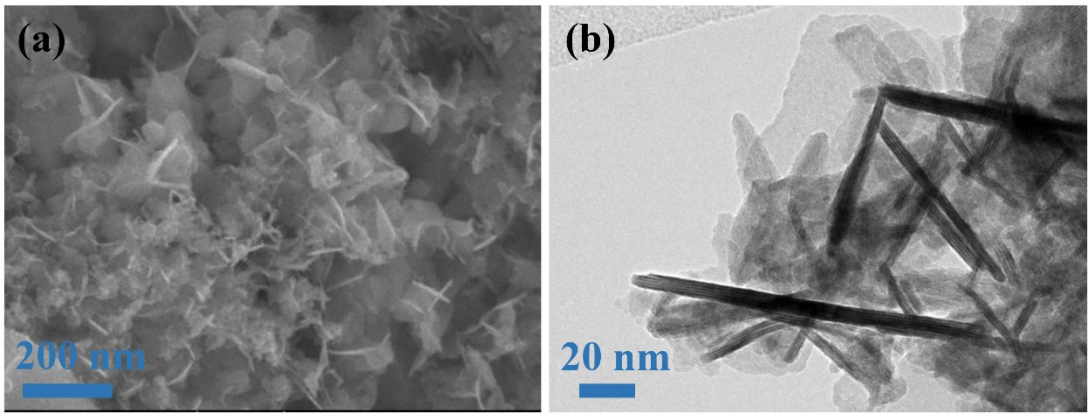

Fig. S8. (a) SEM image of Bi_2Se_3 nanosheets. (b) TEM image of Bi_2Se_3 nanosheets.

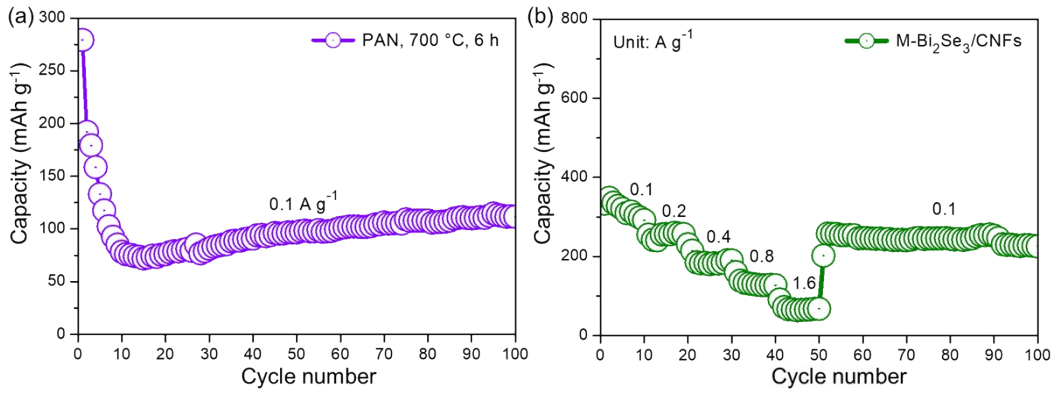

Fig. S9. (a) The specific discharge capacity of pure carbon nanofibers at a cycling rate of 0.1 A g^{-1}. (b) Rate capability of the M-Bi_2Se_3/CNFs electrode at various current rates from 0.1 A g^{-1} to 1.6 A g^{-1}.

Depiction S3

The diffusion coefficient of lithium ions and electric conductivity in open circuit state are calculated by the following formula：

$$D = R^2T^2/2A^2n^4F^4C^2\sigma^2 \cdots\cdots (1) \qquad Z_{Re} = K + \sigma\omega^{-1/2} \cdots\cdots (2)$$

where *D* is the diffusion coefficient (cm^2 s^{-1}), *R* is the gas constant (8.31 J mol^{-1} K^{-1}), *T* is the absolute temperature (298 K), *A* is the surface area of the cathode (0.5 cm^2), *n* is the number of electrons transferred in the half-reaction for the redox couple, *F* is the Faraday constant (96485 C mol^{-1}), *C* is the is the molar concentration of Li-ions in Bi_2Se_3/CNFs electrode, *K* is a constant, *ω* is frequency, and *σ* is the Warburg factor which corresponds to the slope of the curve shown in **Fig. 6**b.[11,12]

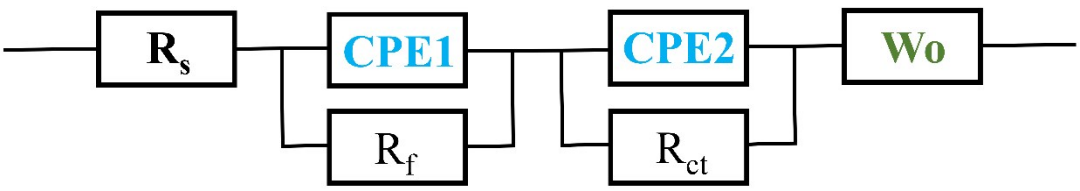

Fig. S10. Equivalent circuit diagram of Electrochemical Impedance Spectroscopy

Table S2. The linear correlation fitting results of Bi_2Se_3/CNFs, M-Bi_2Se_3/CNFs and Bi_2Se_3 nanosheets electrodes, respectively.

Sample	Bi_2Se_3/CNFs	M-Bi_2Se_3/CNFs	Bi_2Se_3 Nanosheets
Intercept	67.6	111.2	84.8
Slope	***17.6***	***60.3***	***250.3***

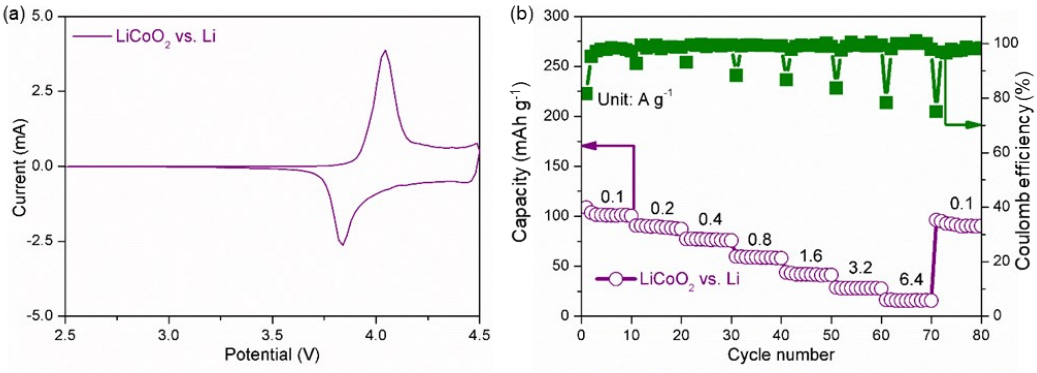

Fig. S11. (a) The CV curve with a sweep speed of 0.1 mV s^{-1} and (b) rate performance of $LiCoO_2$ cathode with current density from 0.1 A g^{-1} to 6.4 A g^{-1}.

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