Electronic Supplementary Material (ESI) for ChemComm.

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VN and SeS_2 Embedded Porous Carbon-Nanofiber Film as a Free-standing Electrode for Improved Li-SeS_2 Battery

*Yu Shao[1], Fei Chen[1], Naiqing Ren[1], Shuo Wang[1], Junru Wang[1], Zhaoyin Wen[2], Chunhua Chen[1,] **

[1]CAS Key Laboratory of Materials for Energy Conversions, Department of Materials Science and Engineering & Collaborative Innovation Center of Suzhou Nano Science and Technology, University of Science and Technology of China, Anhui Hefei 230026, China. E-mail: cchchen@ustc.edu.cn

[2]Key Laboratory of Energy Conversion Laboratory, Shanghai Institute of Ceramics, Chinese Academy of Sciences, Shanghai 200050, China

Experimental section

Synthesis of VN/CNFs, CNFs, VN/CNFs-2 and VN/CNFs-3 hosts.

All chemicals were analytical grade and used without further purification. Firstly, 9.1 g N,N-dimethylformamide (DMF, SCRC), 0.4 g vanadyl(IV) acetylacetonate, 0.15 g polystyrene (PS, Mw=280000), and 0.85 g polyacrylonitrile (PAN, MW=150 000, Aldrich) were mixed and stirred for several hours. After that, the precursor solution was loaded into a 10 ml syringe with 18-gauge blunt tip for electrospinning. The feeding rate was 15 μl min^{-1}, the positive voltage was 19 kV and the distance between the syringe nozzle and the collector was 15 cm. The as-prepared nanofibers film was then stabilized at 250 °C for 2 h in air and subsequently annealed at 700 °C for 1 h in NH_3 atmosphere to obtain the VN/CNFs. The CNFs was prepared with the same conditions except that no vanadyl(IV) acetylacetonate was added in the precursor solution. Moreover, we carried out the same synthesis process that used to prepare VN/CNFs sample except that reducing the amount of vanadyl(IV) acetylacetonate from 0.4 g to 0.1 g, and obtained the sample with a low VN content (VN/CNFs-2). Similarly, we prepared the sample with a high VN content (VN/CNFs-3) by increasing the amount of vanadyl(IV) acetylacetonate from 0.4 g to 0.7 g.

Synthesis of SeS_2@VN/CNFs, SeS_2@VN/CNFs-2, SeS_2@VN/CNFs-3 and SeS_2@CNFs cathode films.

0.72 g commercial SeS_2 powder was firstly mixed with 0.28 g VN/CNFs. The mixture was then heated at 155 °C for 12 h in an Ar-filled autoclave. After cooling down to room temperature, SeS_2@VN/CNFs was obtained. Similarly, SeS_2@VN/CNFs-2, SeS_2@VN/CNFs-3 and SeS_2@CNFs were prepared with the same process.

Material Characterization

The microstructure morphology of these samples was investigated by filed-emission scanning electron microscopy (FESEM, JEOL, Tokyo, Japan), transmission electron microscopy (TEM, JEOL, Tokyo, Japan) and high-resolution TEM (HRTEM). X-ray powder diffraction (XRD) (Philips X'Pert PRO SUPER X-ray diffractometer with Cu-Kα radiation) and XPS measurement was used to characterize surface chemistry of the samples. The EDX mapping was performed on a Hitachi S-4800 scanning electron microscope equipped with an energy dispersive X-ray analyzer (Horiba EMAX).

Electrochemical Investigation

The SeS_2@VN/CNFs and SeS_2@CNFs films were directly used as the cathode and metallic Li sheet was used as counter and reference electrode to make 2032-type coin cells in an argon-filled glove box. The Celgard 2400 membrane was used as a separator. The average mass loading of SeS_2 in cathode films was around 1 mg cm^{-2}. The electrolyte was composed of 1 M lithium bis(trifluoromethanesulfonyl)imide (LiTFSI) in a solvent mixture of 1,3-dioxolane (DOL) and dimethoxymethane (DME) (1:1 in volume) with 1 wt.% $LiNO_3$ as an additive. The electrolyte/SeS_2 ratio was around 35 μL mg^{-1} for Li-SeS_2 batteries. The galvanostatic charge-discharge measurements were performed on Neware BTS-610 instrument at a voltage window of 1.6-2.8V. The cyclic voltammetry tests and electrochemical impedance spectrum

tests are carried out on CHI 660D workstation.

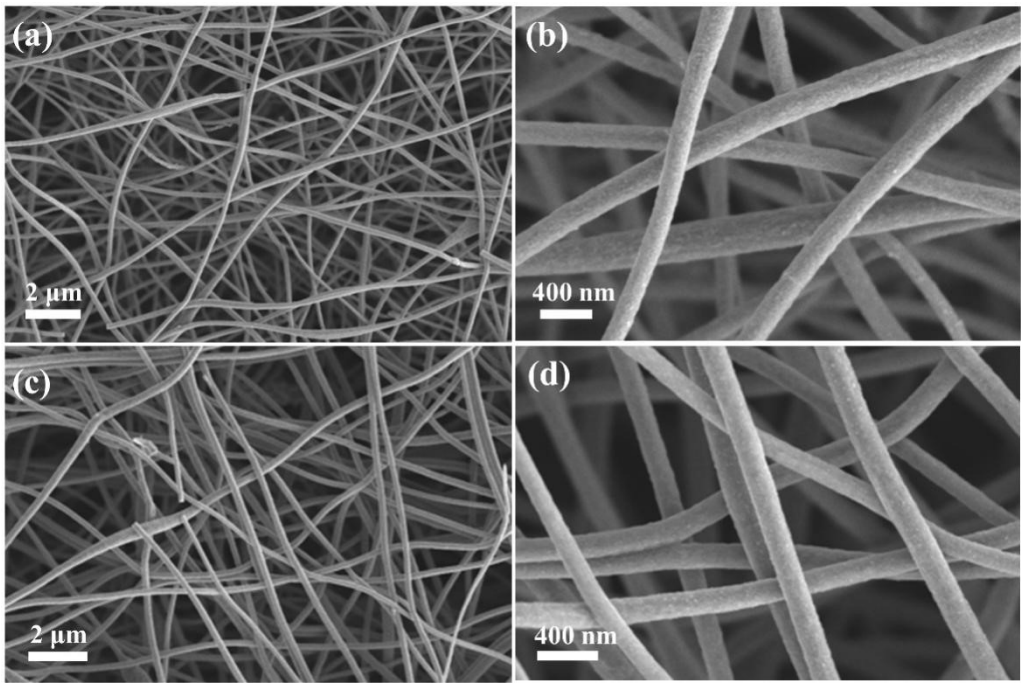

Fig. S1 SEM images of (a and b)VN/CNFs, (c and d) SeS_2@VN/CNFs.

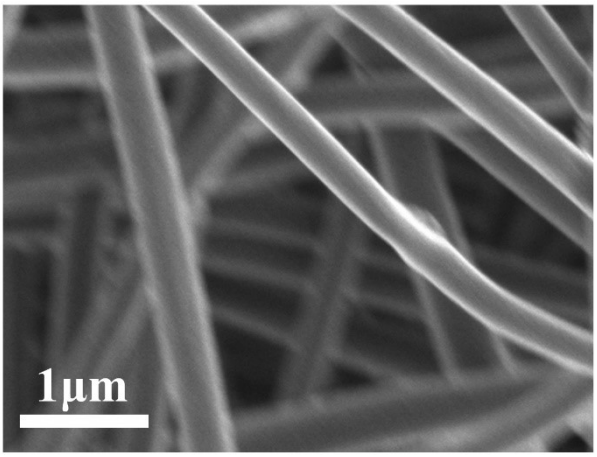

Fig. S2 SEM image of the CNFs.

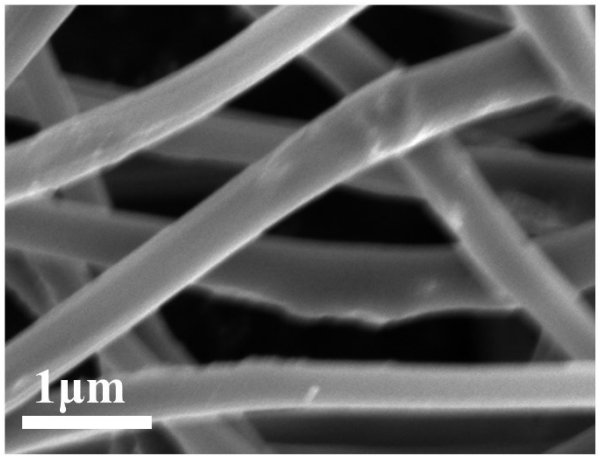

Fig. S3 SEM image of the SeS_2@CNFs

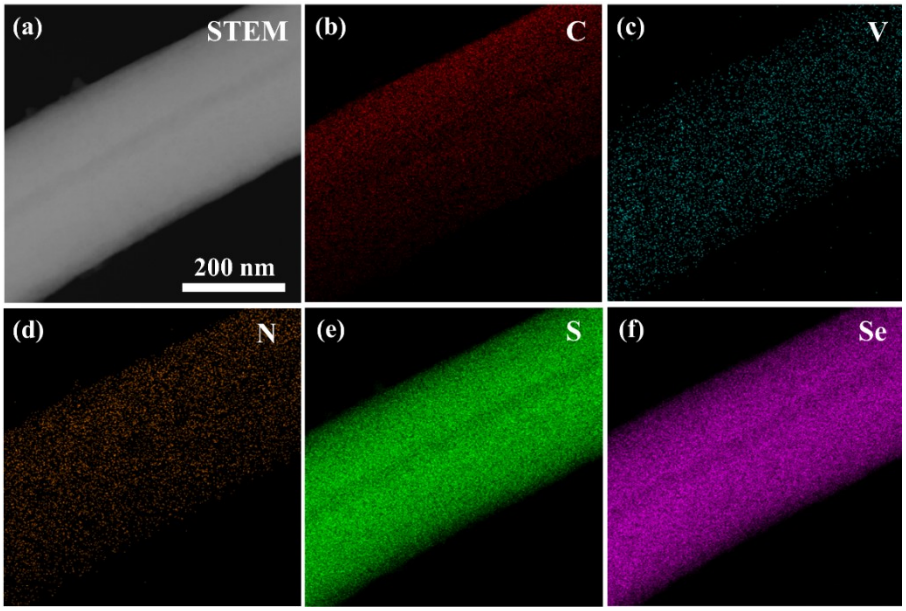

Fig. S4 TEM elemental mapping images of SeS_2@VN/CNFs.

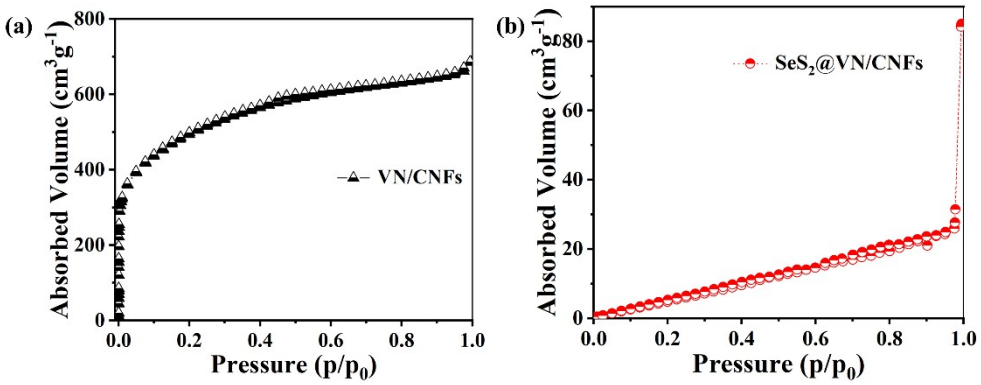

Fig S5. Nitrogen adsorption/desorption isotherm of VN/CNFs and SeS_2@VN/CNFs.

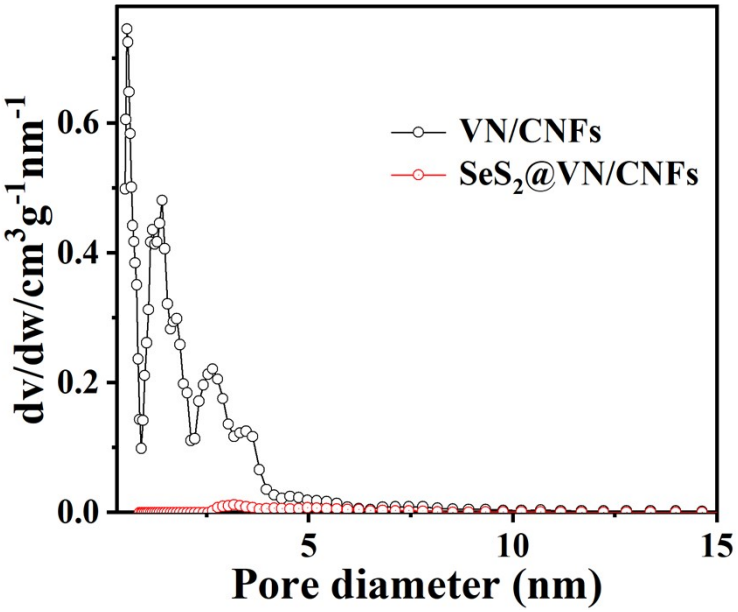

Fig. S6 Pore size distribution of VN/CNFs and SeS_2@VN/CNFs.

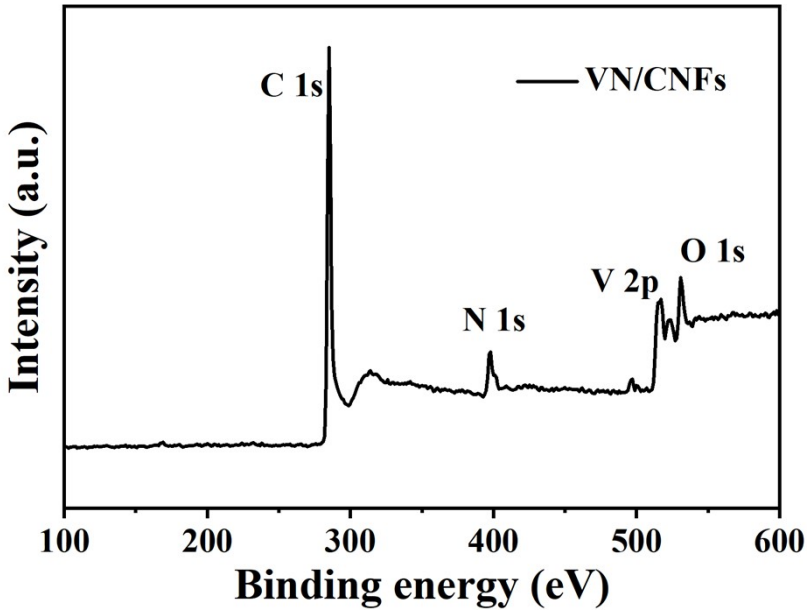

Fig. S7 XPS survey spectrum of VN/CNFs.

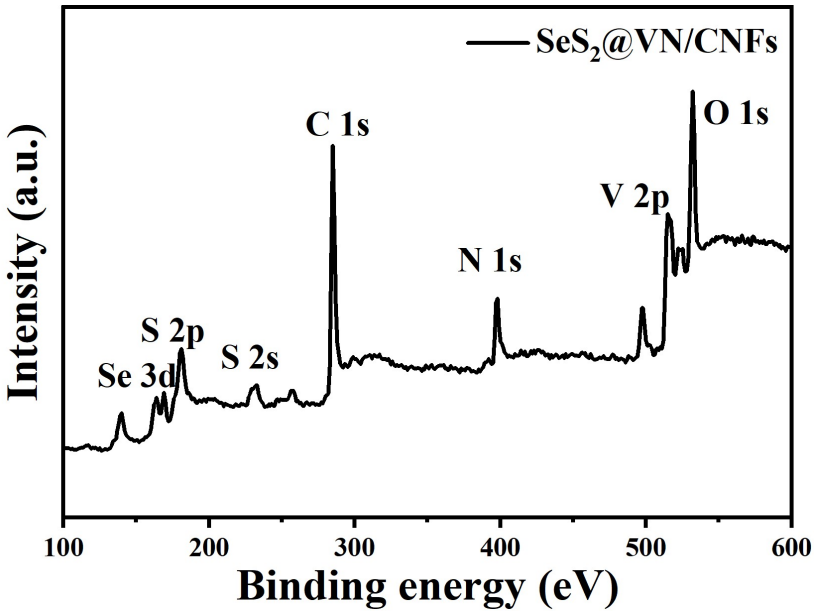

Fig. S8 XPS survey spectrum of SeS_2@VN/CNFs.

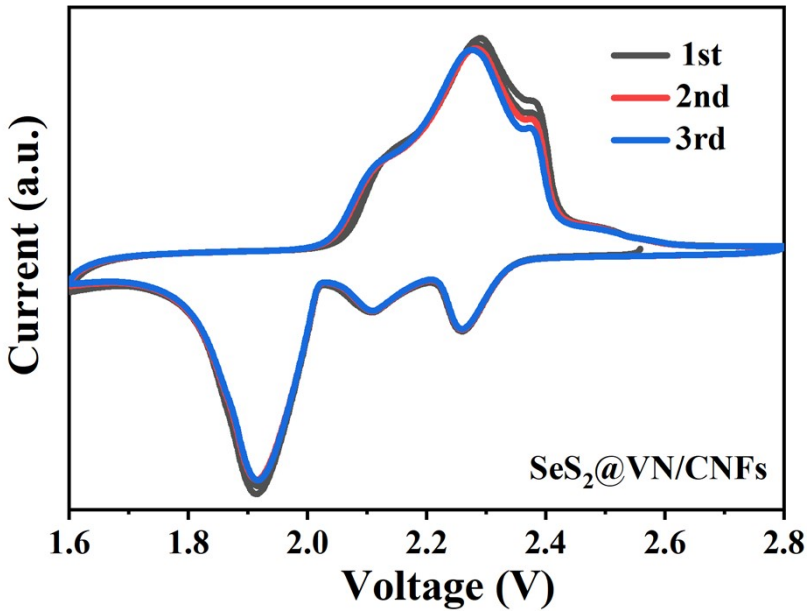

Fig. S9 The CV curves of the SeS_2@VN/CNFs.

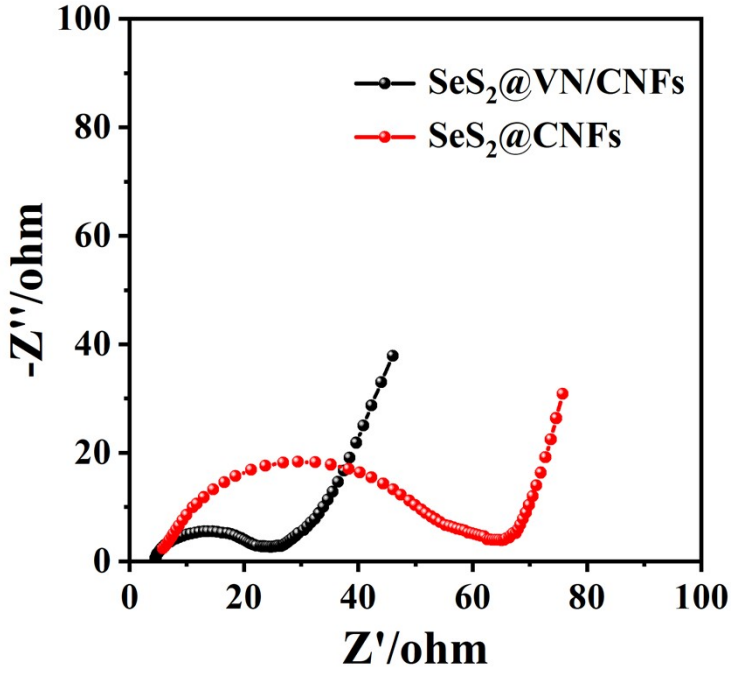

Fig. S10 Nyquist plots for Li-SeS_2@VN/CNFs and Li-SeS_2@CNFs cells after three cycles at 0.2 C.

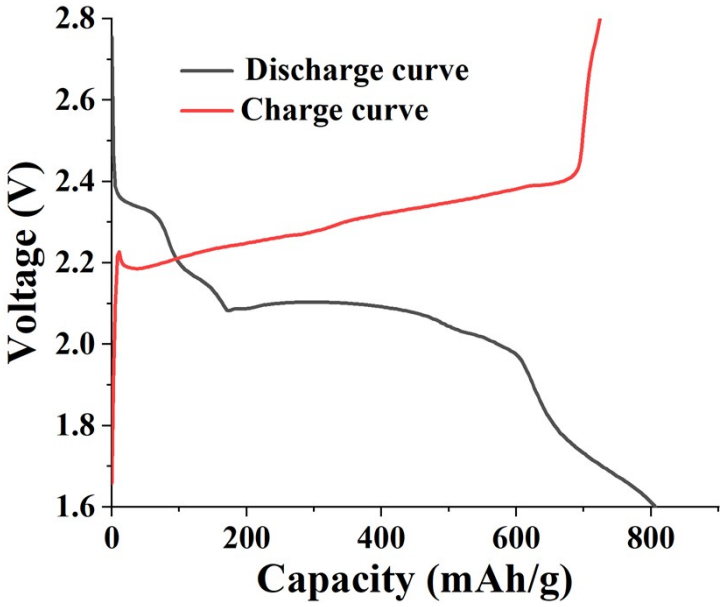

Fig. S11 The first-cycle charge-discharge curve of SeS_2@VN/CNFs.

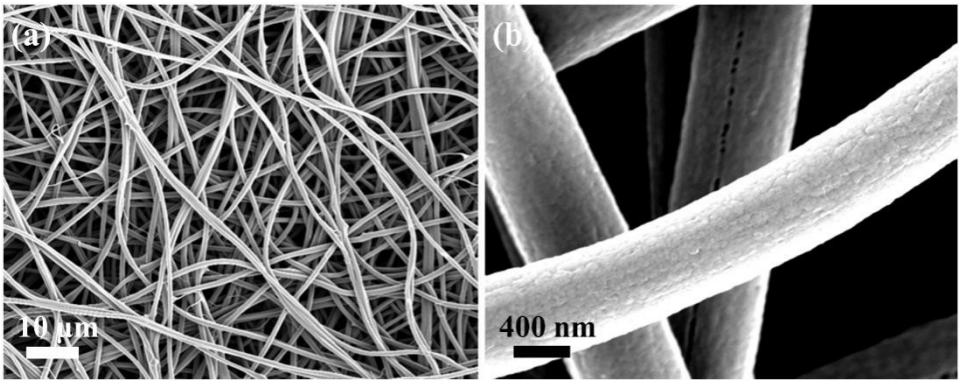

Fig. S12 SEM images of VN/CNFs-2.

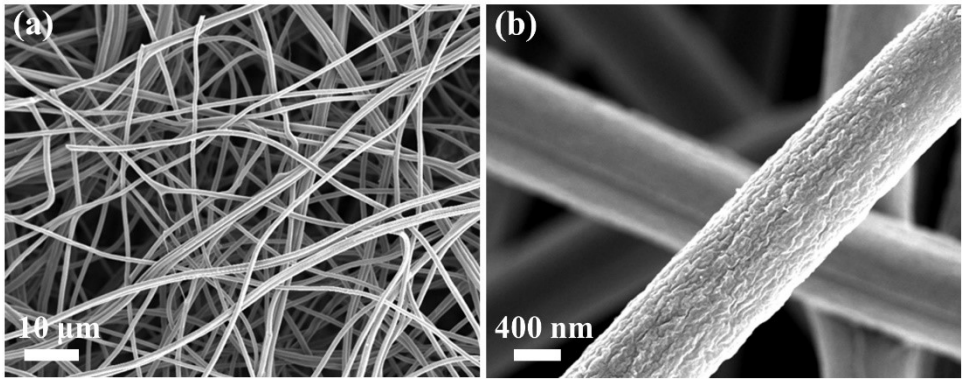

Fig. S13 SEM images of VN/CNFs-3.

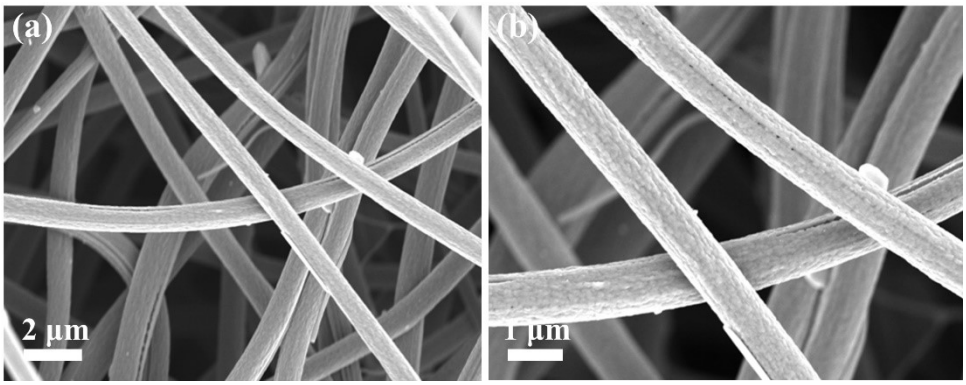

Fig. S14 SEM images of SeS_2@VN/CNFs-2.

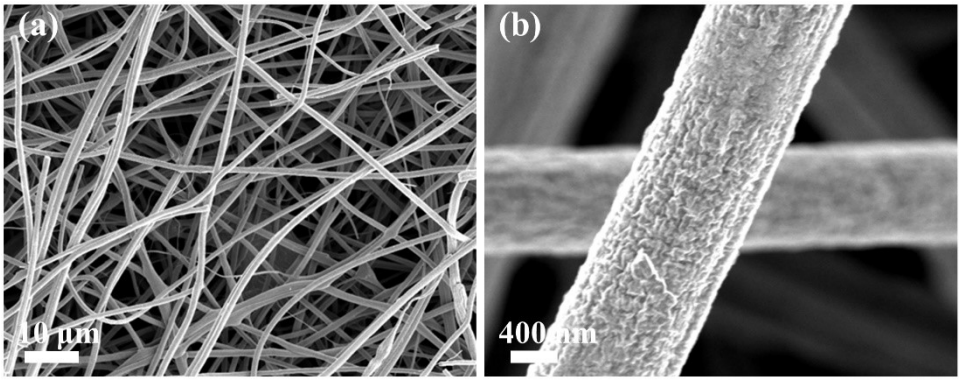

Fig. S15 SEM images of SeS_2@VN/CNFs-3.

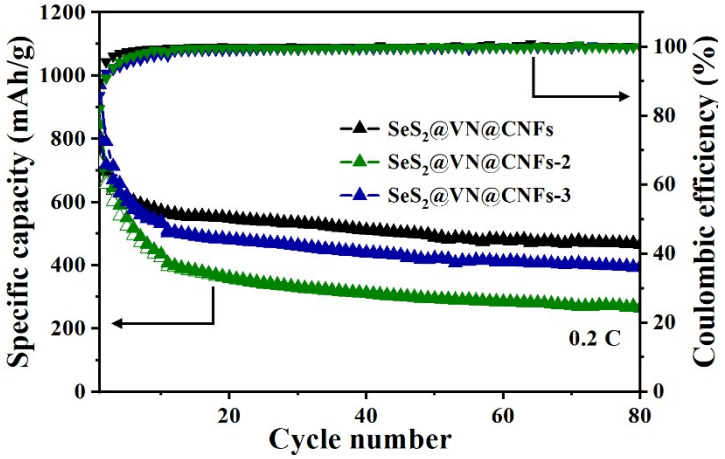

Fig. S16 Cycle performance comparisons of SeS_2@VN/CNFs, SeS_2@VN/CNFs-2 and SeS_2@VN/CNFs-3 at 0.2 C.

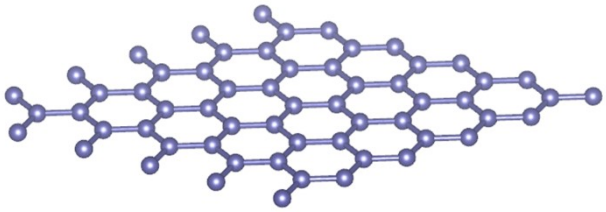

Fig. S17 The model structure of graphite for DFT calculations.