Neural-network design of Li_3VO_4/NC fibers toward superior high-rate Li-ion storage

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Preparation of LVO/NC Fs: Firstly, 2.5 mmol NH_4VO_3, 7.5 mmol $LiNO_3$, 12.5 mmol $H_2C_2O_4{\cdot}2H_2O$ were added in 10 mL dimethylformamide (DMF) and stirred for 10 min. Then 1.85 g polyvinylpyrrolidone (PVP) with molecular weight of 1, 300, 000 was added and stirred for another 12h. After that, the prepared solution was transferred into a 10 mL syringe with a 0.4 mm stainless-steel nozzle for electrospinning with an ejection rate of 1.5 mL h^{-1}. After the electrospinning process, the resultant membranes were dried (80 ^oC, 12h). Finally, the as-prepared sample was calcined to 250 ^oC for 3 h and then sintered at 600 ^oC for 5h under dynamic N_2 atmosphere.

Preparation of LVP/C Fs: Firstly, 2.5 mmol NH_4VO_3, 3.75 mmol H_3PO_4, 3.75 mmol $LiNO_3$, 12.5 mmol $H_2C_2O_4{\cdot}2H_2O$ were added in 10 mL dimethylformamide (DMF) and stirred for 10 min. Then 1.4 g polyvinylpyrrolidone (PVP) with molecular

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weight of 1, 300, 000 was added and stirred for another 12h. After that, the prepared solution was transferred into a 10 mL syringe with a 0.4 mm stainless-steel nozzle for electrospinning with an ejection rate of 1.5 mL h^{-1}. A high voltage of 15 kV was applied by a high-voltage power supply. After the electrospinning process, the resultant membranes were dried (80 °C, 12h). Finally, the as-prepared sample was calcined to 200 °C for 3 h under air and then sintered at 800 °C for 4h under dynamic N_2 atmosphere.

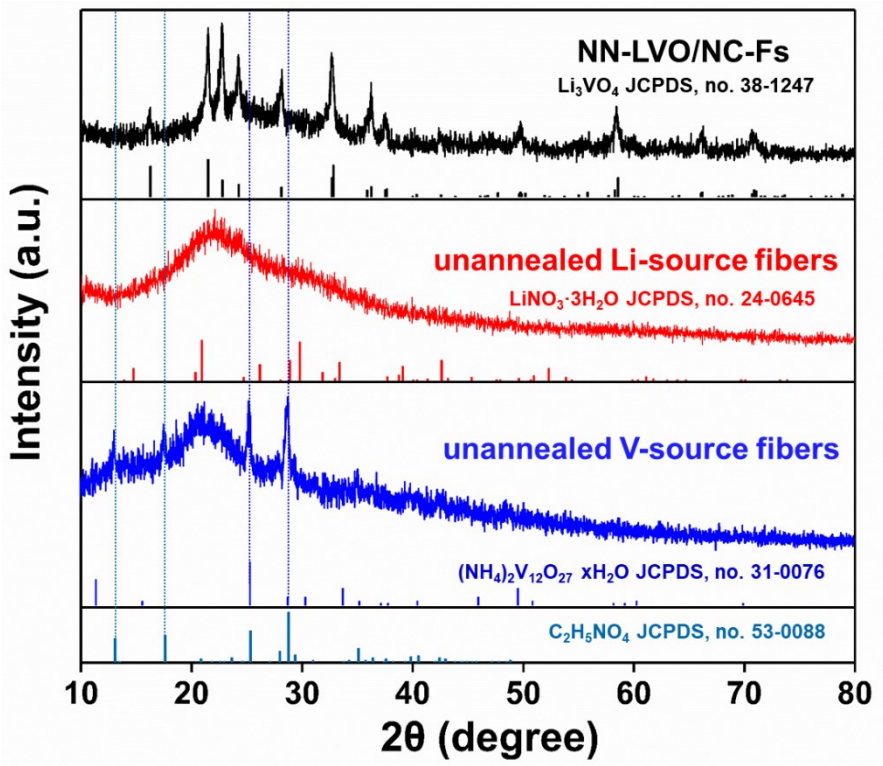

Fig. S1 XRD patterns of the unannealed Li-source ($LiNO_3$) fibers and V-source (NH_4VO_3) fibers and the NN-LVO/NC-Fs.

As shown in Fig. S1, the Li-source fibers show weak crystallinity, and the V-source fibers indicate NH_4VO_3 decomposes to a certain extent during electrospinning and drying. It is clear that the diffraction peaks of the unannealed Li-source and V-source fibers differ much from those of the NN-LVO/NC-Fs. As shown in Tab. S1, the

weight of the final NN-LVO/NC-Fs is 0.5191 g. According to the LVO content in the NN-LVO/NC-Fs (~51.3%, Fig. 2c), it could be deduced that the obtained LVO is 0.2663 g. Compared with the theoretical weight of the LVO (2.5 mmol, 0.34 g), the transformation efficiency from the Li-source ($LiNO_3$) and V-source (NH_4VO_3) fibers to the NN-LVO/NC-Fs is ~78.3%. Consider the fact that a few amount of Li-source ($LiNO_3$) and V-source (NH_4VO_3) fibers stick on Al foil after exfoliation, the practical transformation efficiency from the Li-source ($LiNO_3$) and V-source (NH_4VO_3) fibers to the NN-LVO/NC-Fs may be higher than 78.3%.

Tab. S1 The weight information of the nanofibers containing of Li- and V-source and the NN-LVO/NC-Fs.

Experiment reagent	Solution A	Solution B
	7.5 mmol $LiNO_3$ (0.5171 g) 1.0 g polyvinylpyrrolidone 5 mL dimethylformamide	2.5 mmol NH_4VO_3 (0.2925 g) 12.5 mmol $H_2C_2O_4 \cdot 2H_2O$ (1.5759 g) 0.85 g polyvinylpyrrolidone 5 mL dimethylformamide
Li- and V-source fibers	2.6775 g	
NN-LVO/NC-Fs	0.5191 g	
Transformation efficiency	~78.3 %	

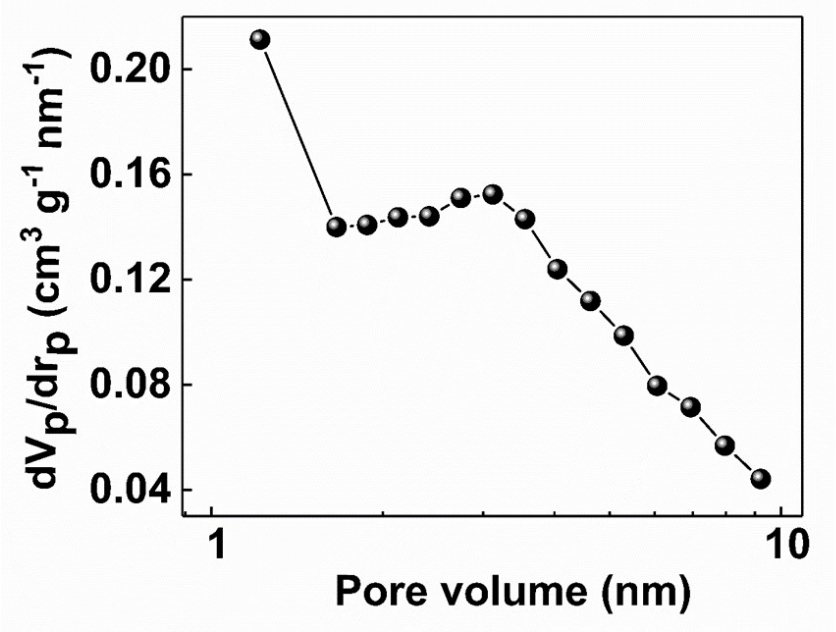

Fig. S2 Pore size distribution of the NN-LVO/NC-Fs.

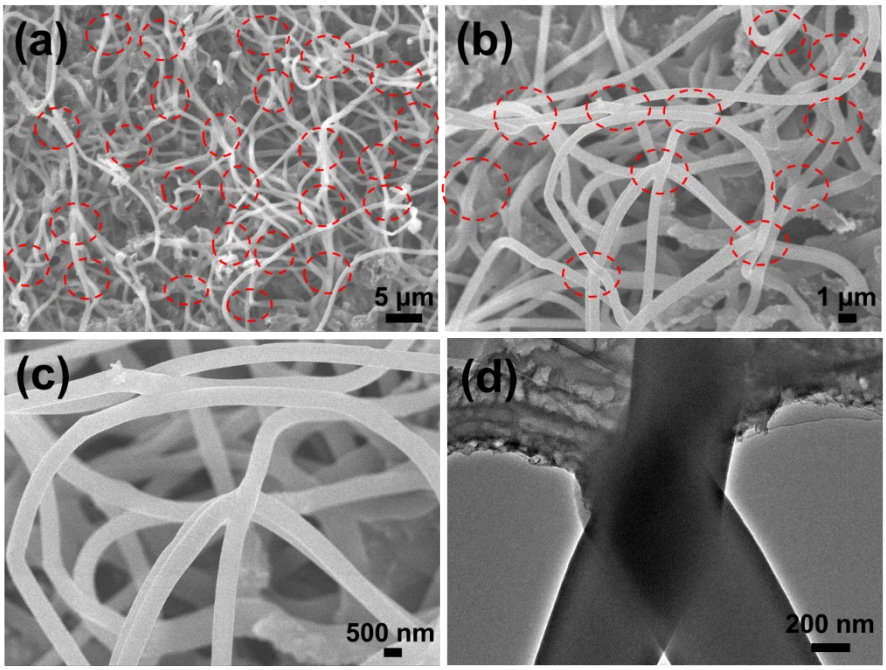

Fig. S3 (a)-(c) SEM and (d) TEM images of the NN-LVO/NC-Fs.

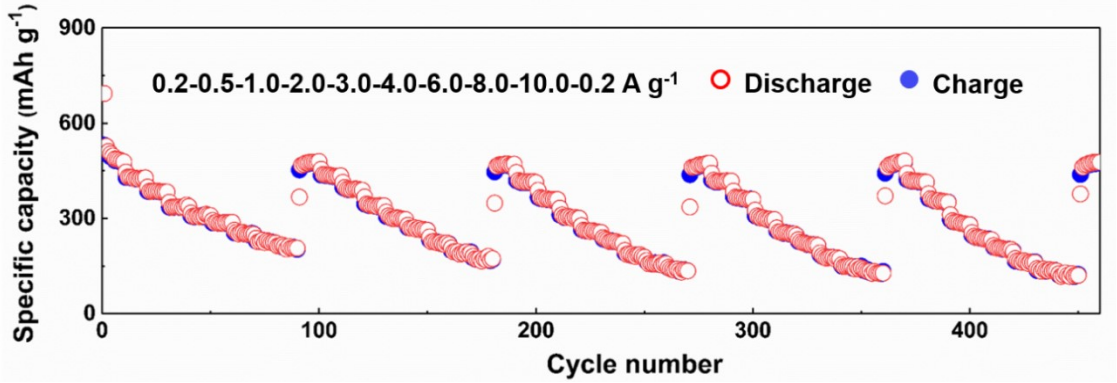

Fig. S4 Rate capability of LVO/NC-Fs electrode obtained via ordinary electrochemical spinning.

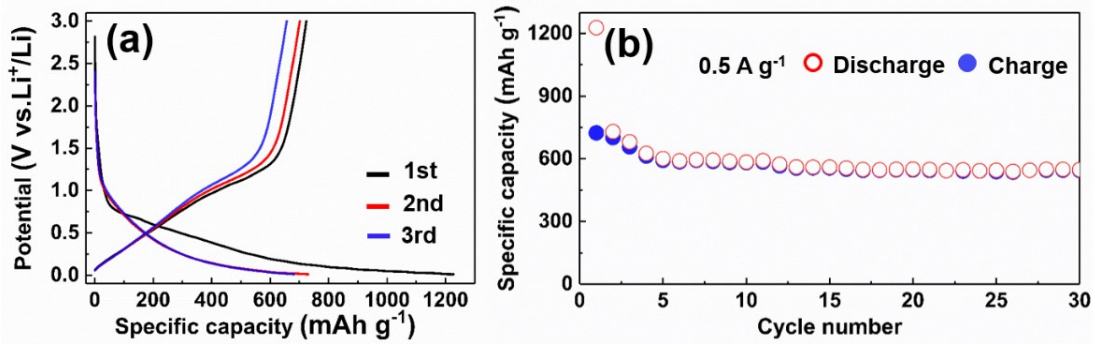

Fig. S5 (a) Charge/discharge curves and (b) capacity retention of N doped carbon fibers obtained without Li- and V-source.

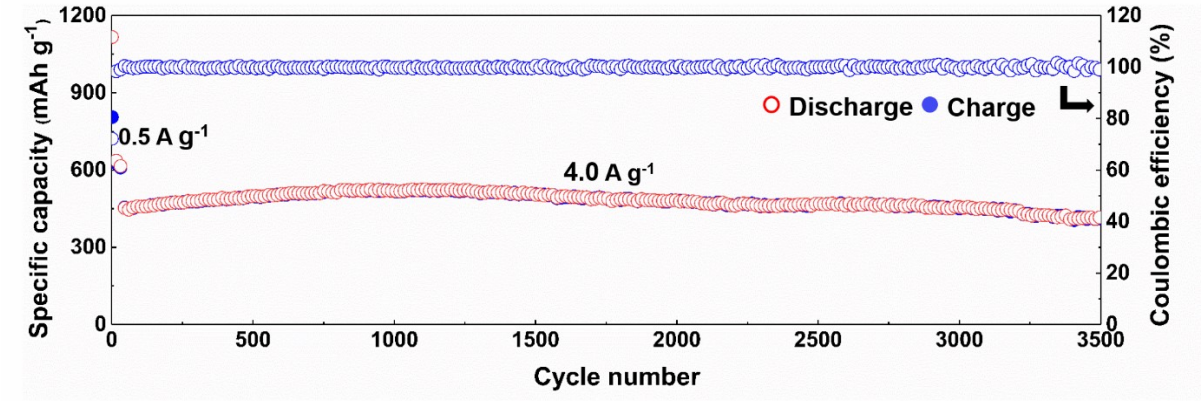

Fig. S6 Long cycle performance of the NN-LVO/NC-Fs electrode.

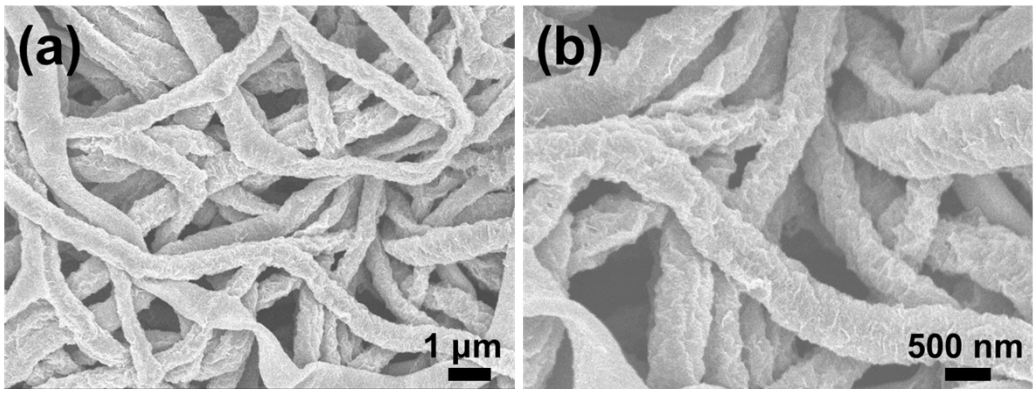

Fig. S7 (a) Low and (b) high magnification SEM images of the LVO/NC-Fs.

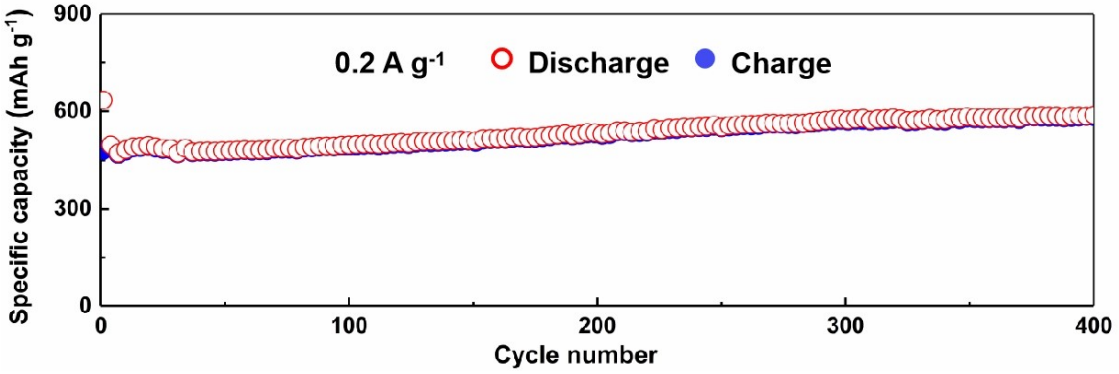

Fig. S8 Capacity retention of LVO/NC-Fs electrode obtained via ordinary electrochemical spinning.

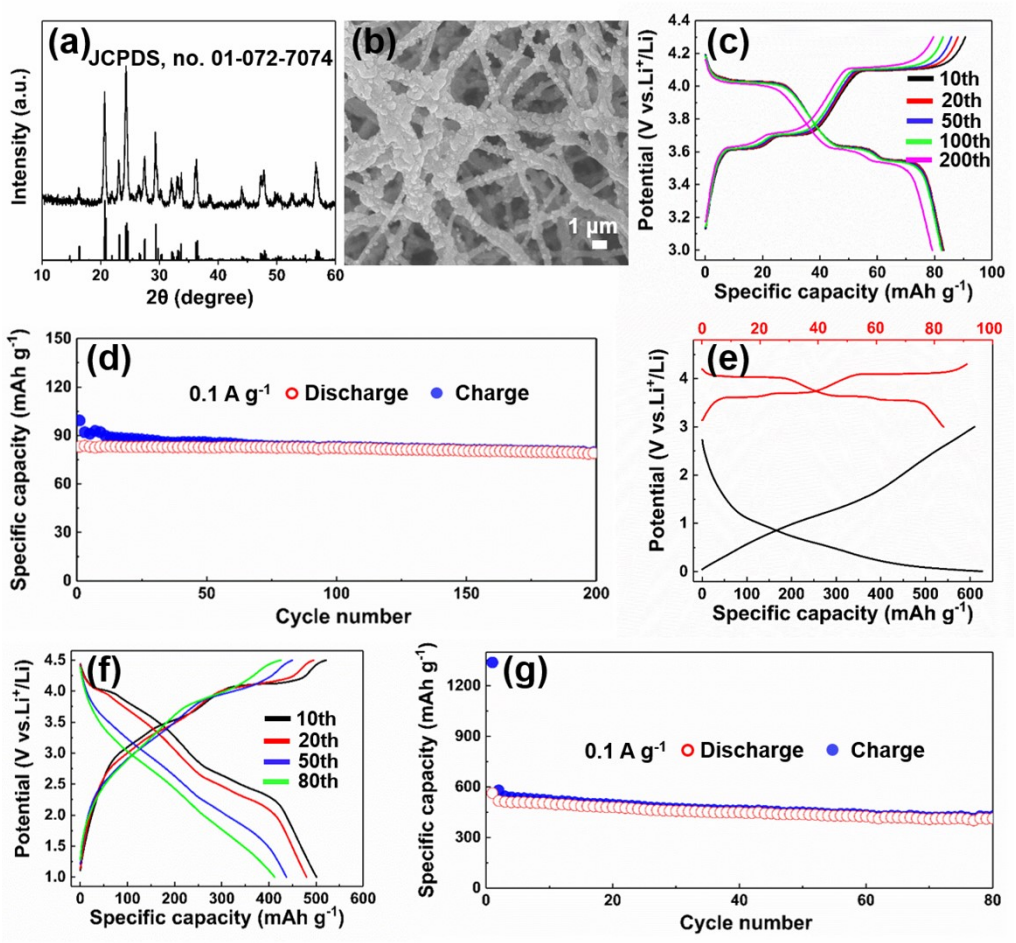

Fig. S9 (a) XRD pattern and (b) SEM image of the LVP/NC Fs. (c) Galvanostatic charge/discharge curves and (d) Cycling performance of the LVP/C Fs electrode at 0.1 A g^{-1}. (e) The comparison of capacity and potential between the NN-LVO/NC-Fs and the LVP/C Fs electrode. (f) Representative charge/discharge curves and (g) Cycling performance of the NN-LVO/NC-Fs//LVP/C Fs full cell.