Facile Preparation of Hf_3N_4 Thin Films Directly Used as the Electrodes for Lithium-Ion Storage

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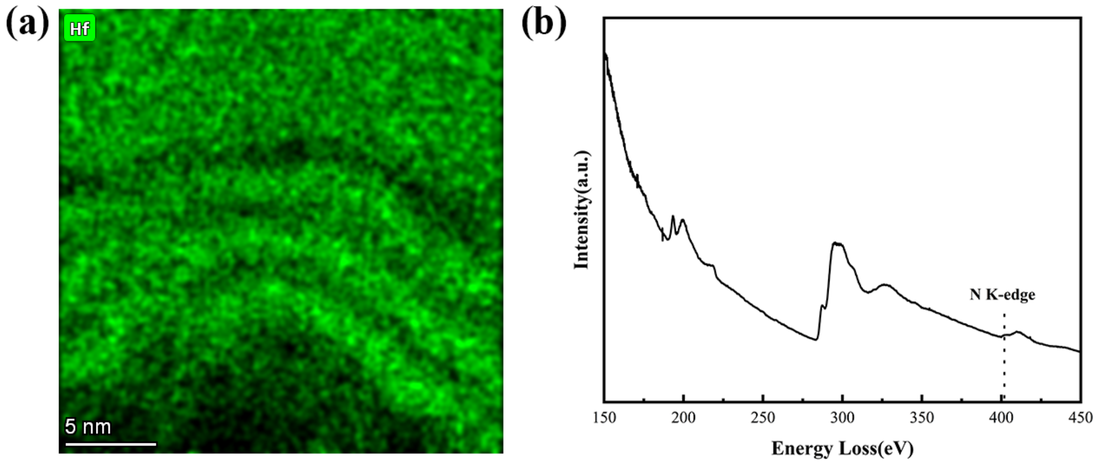

Fig. S1 (a) The EDS mapping image of Hf_3N_4 film transverse; (b) The EELS point scan result of Hf_3N_4 film transverse.

Table S1 Comparison of the crystal plane spacing of Hf_3N_4 thin films with the values from Hf_3N_4-JCPDS.

The work (Å)	Hf_3N_4 (JCPDS 01-083-6354) (Å)	Crystal plane
2.768	2.794	(200)
2.620	2.610	(111)
2.570	2.565	(201)
2.323	2.140	(112)
2.011	2.029	(211)
1.870	1.809	(013)
1.811	1.809	(013)
1.715	1.721	(113)
1.424	1.427	(220)
1.211	1.216	(321)
1.014	1.015	(422)
0.902	0.901	(134)
0.823	0.824	(425)

According to the volume V (1.13×10^{-7} cm^3) of the film and the experimental volume density P (11.59 g/cm^3), the mass *m* is calculated as 0.013 mg according to Eq. S1.

$$m = V \times P$$ .... Eq. S1

According to the total reaction formula (Eq. S2) and the theoretical capacity calculation formula (Eq. S3), the theoretical capacity of the active substance after all reactions can be calculated as **543.7** $mAhg^{-1}$.

$$Hf_3N_4 + 12Li^+ + 12e^- = 4Li_3N + 3Hf$$ .... Eq. S2

$$C_0 = \frac{Fnm}{3600M}$$ .... Eq. S3

Where C_0 is the theoretical capacity, *F* is the Faraday constant, *n* is the charge transfer number, *m* is the mass of Hf_3N_4, and M is the molar mass of Hf_3N_4.

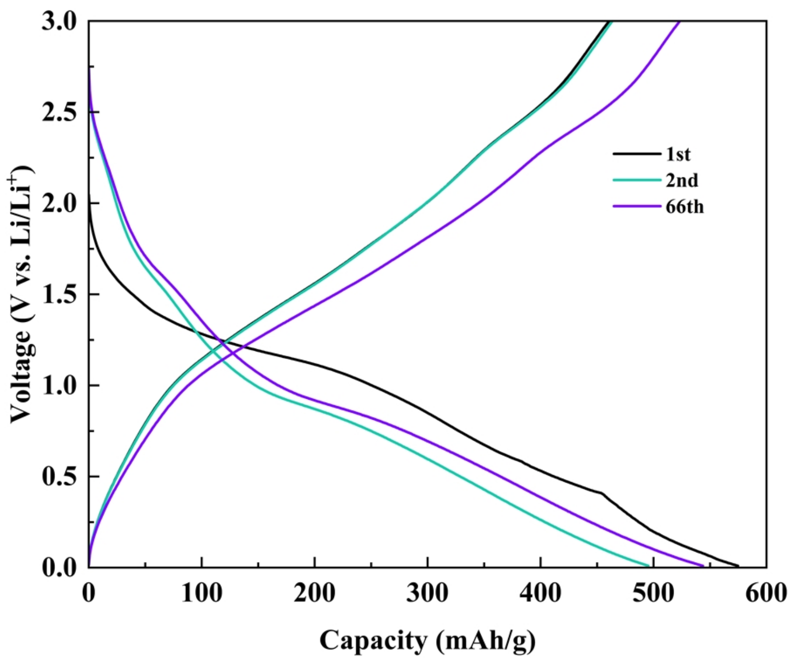

Fig. S2 The galvanostatic charge-discharge curves of the orthorhombic Hf_3N_4 thin film electrode at the current density of 0.1 A g^{-1} in the 1st, 2nd, and 66th cycles.

Table S2 The characteristics and battery performances of TMN thin film electrodes for LIBs.

Materials	Production methods	Rate capability	Cycling performance
TiN[1]	Sputtering deposition at RT	99 mA h g^{-1} at 1 mA cm^{-2}	206 mA h g^{-1} at 25 μA cm^{-2} after 50 cycles
FeN[2]	Sputtering deposition at RT	469 mA h g^{-1} at 10 A g^{-1}	1020.4 mA h g^{-1} at 0.2 A g^{-1} after 100 cycles
Ni_2N[3]	Sputtering deposition at RT	191.7 mA h g^{-1} at 2.24 A g^{-1}	461.9 mA h g^{-1} at 0.12 A g^{-1} after 100 cycles
RuN[4]	Sputtering deposition at 50°C	260 mA h g^{-1} at 1.17 A g^{-1}	330 mA h g^{-1} at 117 mA g^{-1} after 70 cycles
Mo_2N[5]	Sputtering deposition at RT	252 mA h g^{-1} at 2 A g^{-1}	N/A
MoN_x[6]	ALD at RT	N/A	696 mA h g^{-1} at 100 μA cm^{-2} after 100 cycles
Ti_2N[7]	Sputtering deposition at RT	450 mA h g^{-1} at 0.1C	450 mA h g^{-1} at 0.1C after 100 cycles
Mn_3N_2[8]	Sputtering deposition at RT	N/A	~400 mA h g^{-1} at 0.16 A g^{-1} after 300 cycles
Ni_3N[9]	PLD at 200°C	N/A	~325 mA h g^{-1} at 7 μA cm^{-2} after 40 cycles
Co_3N[10]	PLD at 200°C	N/A	~350 mA h g^{-1} at 7 μA cm^{-2} after 40 cycles

RT: room temperature.

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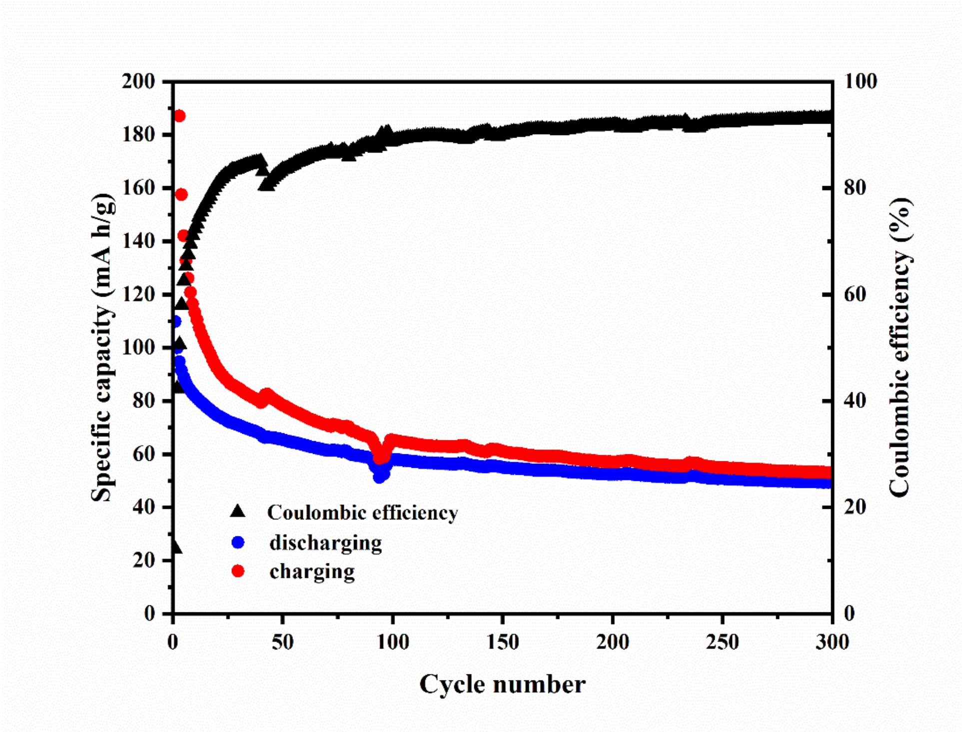

Fig. S3 The cycling performance of full-cells fabricated using the orthorhombic Hf_3N_4 thin film anodes and the $LiFePO_4$ cathodes at the current density of 0.1 A g^{-1}.