

Electronic Supplementary Information

Free-standing MoO₂/Mo₂C Imbedded carbon fibers for Li-ion batteries

Hongqin Li,^a Haijun Ye,^a Zheng Xu^a, Chuanyi Wang^c, Jiao Yin^{c*}, Hui Zhu^{a,b*}

^aCollege of Chemistry, Nanchang University, 999 Xuefu Avenue, Nanchang 330031, China

^bState Key Laboratory of Electroanalytical Chemistry, Changchun Institute of Applied Chemistry, Chinese Academy of Sciences, Changchun, Jilin, P. R. China.

^cKey Laboratory of Functional Materials and Devices for Special Environments, Xinjiang Technical Institute of Physics & Chemistry, Chinese Academy of Sciences, 40-1 South Beijing Road, Urumqi, Xinjiang 830011, China

*Corresponding author. Tel.: 86-991-3835879. E-mail address: yinjiao@ms.xjb.ac.cn (Jiao Yin)

*Corresponding author: Tel.: +86-791-83969565. E-mail: huizhu@ncu.edu.cn (Hui Zhu)

1. Experimental Section

1.1 Preparation of MoO₂/Mo₂C ICFs derived from different concentration of phosphomolybdic acid

10% PAN solutions were achieved with 1 g PAN and 10 ml DMF to form a homogeneous polymeric solution after vigorous stirring. Subsequently, 0.2 g and 0.3 g phosphomolybdic acid ($\text{H}_3\text{PO}_4 \cdot 12\text{MoO}_3$) were respectively dissolved in above polymeric PAN solution under vigorous stirring, and then the as-prepared liquid was transferred to spin into fibers, which were subsequently experienced heat treatment in the muffle furnace at 280 °C for 2 h at a heat rate of 2 °C /min. Afterwards, the fibers placed in boat were transferred into tube furnace and carried out calcination at 800 °C for 2 h with the heating rate of 5 °C /min under the protection of hydrogen and argon (10% ppm) mixture. The resultant MoO₂/Mo₂C DCFs were respectively washed by ethanol and water. The two samples were referred as F-0.2P and F-0.3P. To investigate the effect of reaction temperature, the F-0.4P precursor and F-0.4P precursor also treated at 600 °C and 700 °C.

1.2 Preparation of MoO₂/Mo₂C ICFs derived from different concentration of ammonium molybdate

In addition, 0.2322 g and 0.3483 g ammonium molybdate (1:1 by mole of Mo) were respectively used as Mo precursor. 0.2322 g and 0.3483 g $(\text{NH}_4)_6\text{Mo}_7\text{O}_{24} \cdot 4\text{H}_2\text{O}$ were respectively added into 10% PAN solution. And then the mixture was heated in water bath (40 °C) with violent stirring until homogeneous solution was formed. Finally, the uniform solution was executed to electro-spin. The resultant MoO₂/Mo₂C ICFs were also respectively calcinated with same procedures of F-0.2P and F-0.3P followed by washing with ethanol and water. The two swamples were denoted as F-0.2A and F-0.3A.

1.3 Preparation of pure carbon fibers without adding any Mo precursor

Furthermore, the blank sample was prepared via the same procedure as described above without adding any Mo resource, the sample was named as F-0P.

1.4 Preparation of MoO₂/Mo₂C composites

Glucose and $(\text{NH}_4)_6\text{Mo}_7\text{O}_{24} \cdot 4\text{H}_2\text{O}$ (1.5:1 by mass) was dispersed into distilled water (10 mL) under magnetic stirring until a homogeneous solution appeared. The mixture was dried

at 60 °C, and then annealed at 800 °C for 2 h in argon flow.

2. Figures and Tables

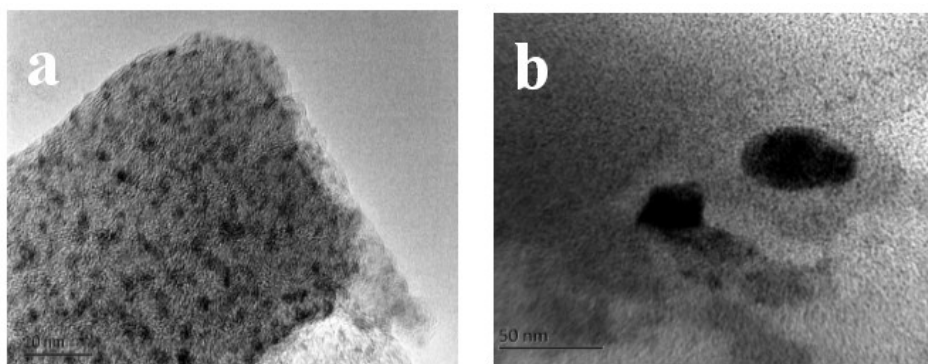


Figure S1 TEM images of F-0.4P with different magnification.

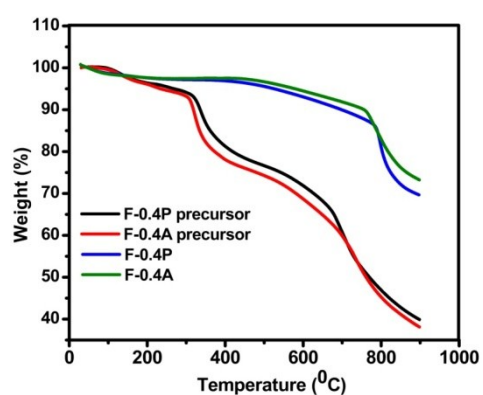


Figure S2 TGA curves of $\text{MoO}_2/\text{Mo}_2\text{C}$ ICFs and correlated precursors for synthesis

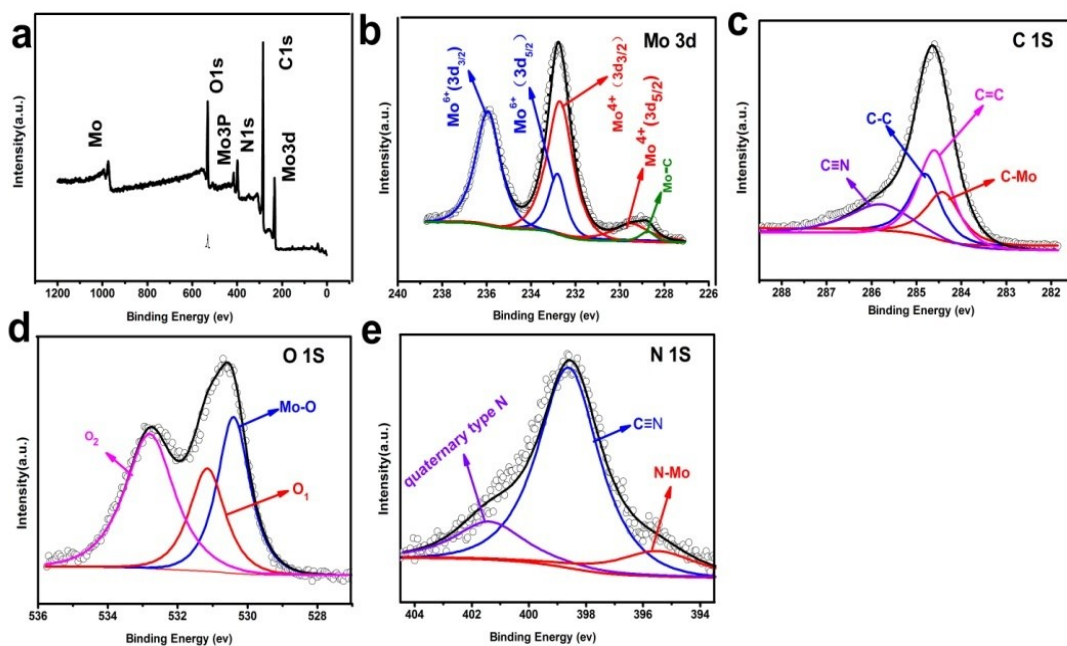


Figure S3 XPS spectrum of MoO_2 ICFs: overall spectrum (a); high-resolution of Mo 3d (b), C 1s (c), O 1s (d) and N 1s (e) spectrum for F-0.4A.

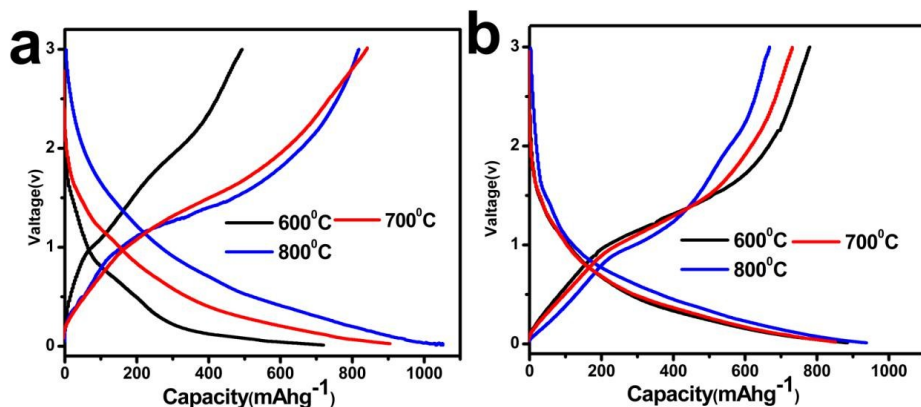


Figure S4 The 2nd cycle charge/discharge curves of F-0.4P (a) and F-0.4A (b) in the potential range of 0.01-3 V (vs. Li/Li⁺) at a current density of 0.1 A g⁻¹ of 600 °C, 700 °C and 800 °C.

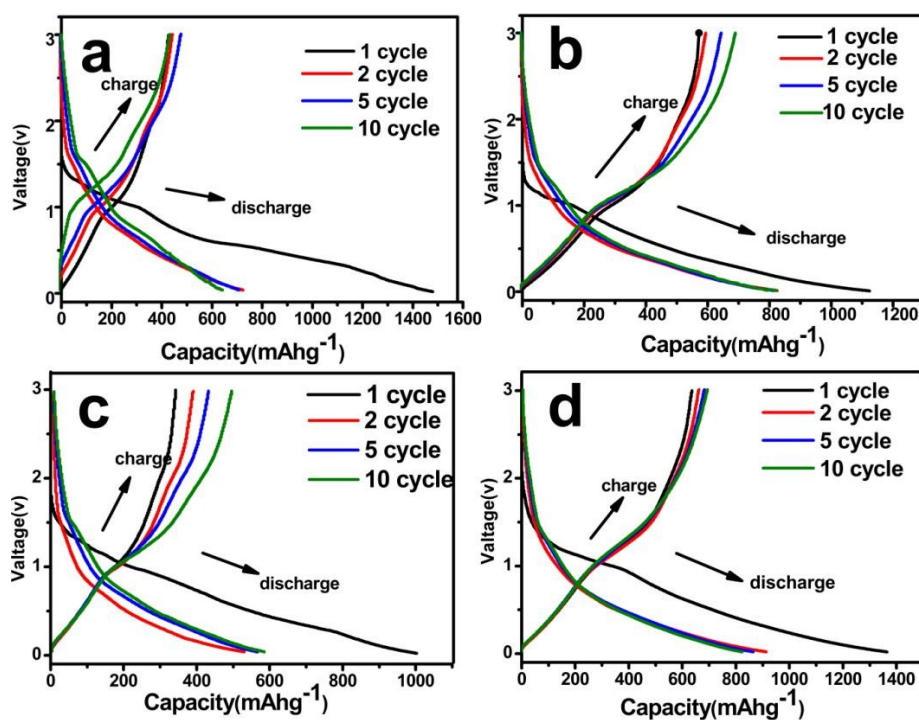


Figure S5 The discharge-charge curves determined over the potential range of 0.01-3 V (vs Li/Li⁺) at a current density of 0.1 A g⁻¹ for F-0.2P (a), F-0.2A (b), F-0.3P (c) and F-0.3A (d), respectively.

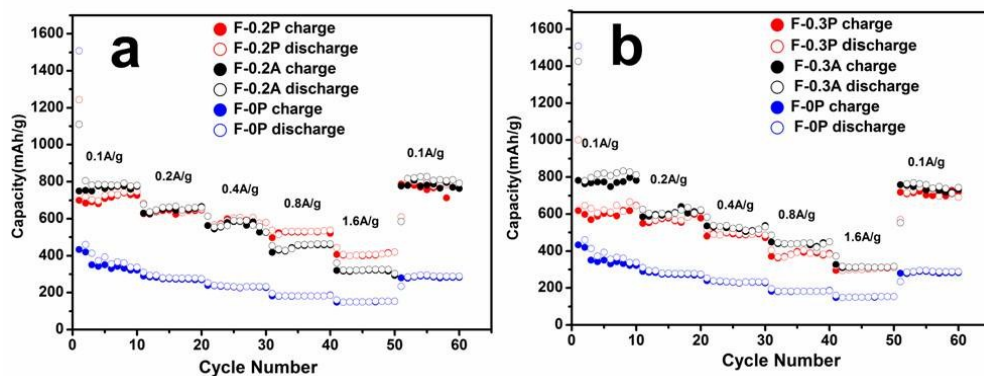


Figure S6 Comparison of rate performance of as-prepared fibers: (a) F-0.2 and F-0P; (b) F-0.3 and F-0P at current density from 0.1 to 1.6 A g⁻¹.

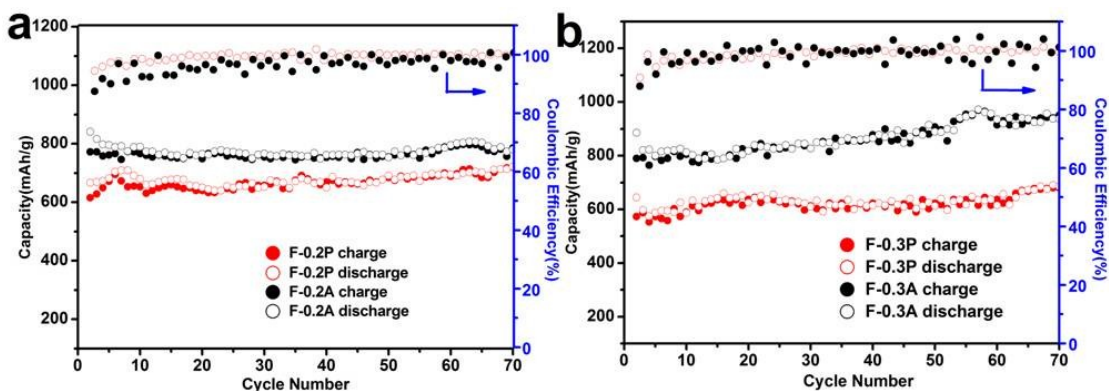


Figure S7 Cyclic stability and Coulombic efficiency of F-0.2 (a) and F-0.3 (b) with a charge-discharge rate of 0.1 A g⁻¹ from the 2nd to the 70th cycle

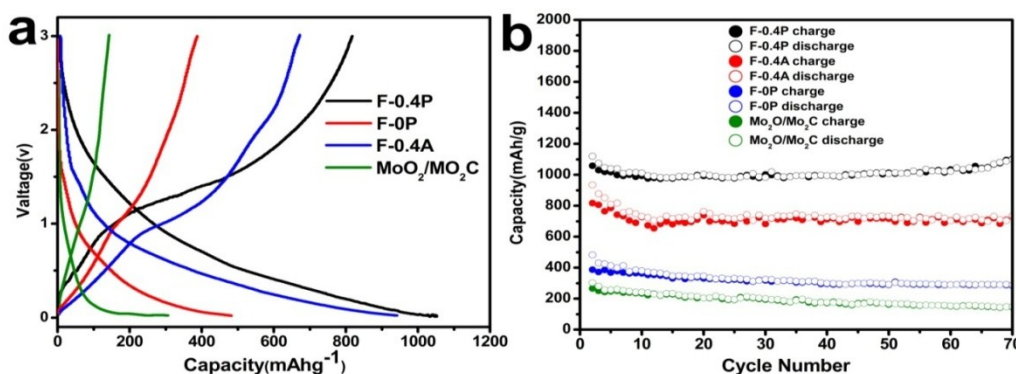


Figure S8 Comparison of electrochemical performance of F-0.4P, F-0.4A, F-0P and MoO₂/Mo₂C: (a) The 2nd cycles discharge-charge curves determined over the potential range of 0.01-3 V (vs Li/Li⁺) at a current density of 0.1 A g⁻¹. (b) Cyclic stability at a current density of 0.1 A g⁻¹ from the 2nd to the 70th cycles.

Table S1. The element weight percentage of MoO₂/Mo₂C ICFs text by EDX.

Weight percentage(%) Element	Materials	F-0.4P	F-0.4A	F-0.3P	F-0.3A	F-0.2P	F-0.2A
C		15.97	10.44	19.39	12.83	18.19	18.05
O		40.33	43.43	38.15	35.31	55.65	50.82
Mo		43.70	46.13	42.56	51.86	26.16	31.13

Table S2. Comparison of MoO₂/Mo₂C ICFs with reported MoO₂/carbon composite in terms of electrochemical performance.

Samples	Mo precursor	Initial CE (%)	Cycle s	Reversible capacities (mAh/g)	Rates mA/g	Rate capacity (mAh/g)	Flexibility	Ref.
MoO₂/Mo₂C ICFs	H₃PO₄·12MoO₃	63.3	70th	889	1600	445	YES	Our work
MoO ₂ -OMC	(NH ₄) ₆ Mo ₇ O ₂₄ ·4H ₂ O	63.6	50th	1049.1	1600	600	NO	4
MoO ₂ -OMC	H ₃ PO ₄ ·12MoO ₃	61.4	50th	784	2000	401	NO	5
MoO ₂ @C nanofibers	(NH ₄) ₆ Mo ₇ O ₂₄ ·4H ₂ O	56.3	50th	~520	200	430.6	YES	8
MoO ₂ /C hybrids	H ₃ PO ₄ ·12MoO ₃	~55	600th	602	800	409	NO	10
MoO ₂ -Mo ₂ C-C	(NH ₄) ₆ Mo ₇ O ₂₄ ·4H ₂ O	67.8	50th	1050	2000	445	NO	34
MoO ₂ /Mo ₂ C Heteronanotubes	MoO ₃	85.8	140th	410	1000	510	NO	37
MoO ₂ @C nanospheres	(NH ₄) ₆ Mo ₇ O ₂₄ ·4H ₂ O	76	30th	570	3 C	410	NO	38
MoO ₂ Nanorods	H ₃ PO ₄ ·12MoO ₃	~71	30th	512	1 C	260	NO	39