Electronic Supplementary Information (ESI)

Partially Nitrided Molybdenum Trioxide with Promoted Performance as the Anode Material for Lithium-Ion Batteries

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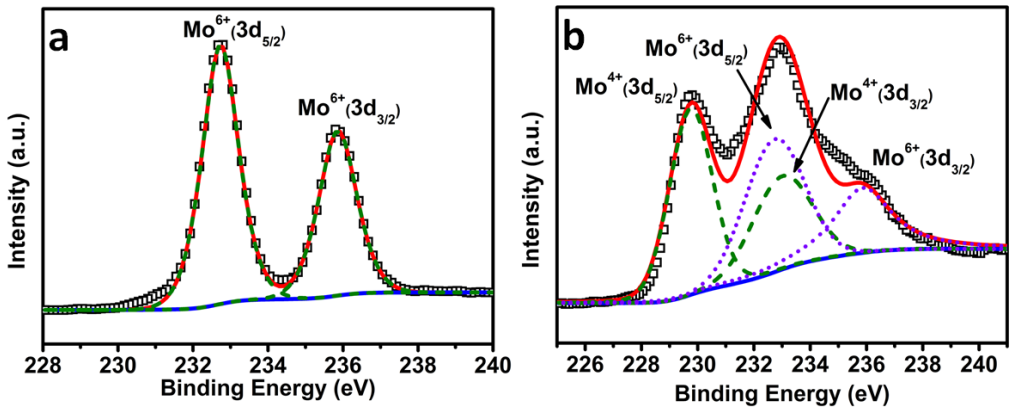

Fig. S1. XPS patterns of MoO_3 in the Mo 3d region: a) before argon ion etching; b) after argon ion etching.

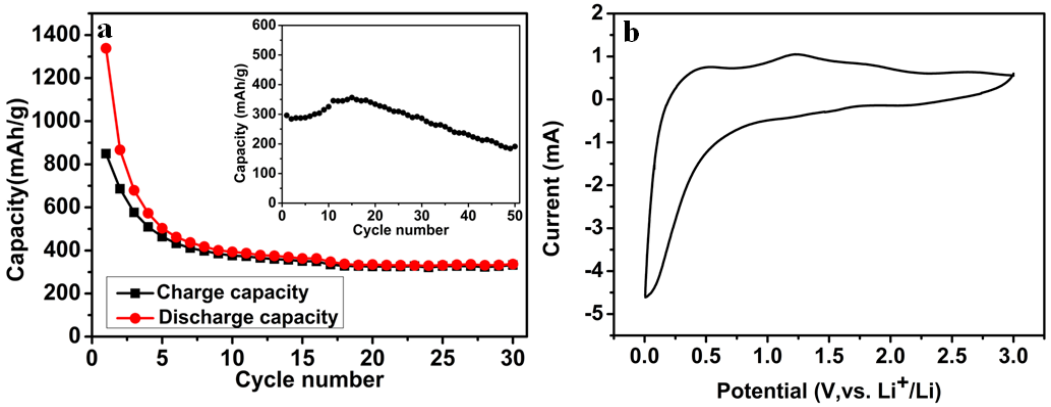

Fig. S2. Electrochemical performance of the bulk MoO_3 and the MoO_2 obtained by heating MoO_3 in NH_3 atmosphere at 450 °C: a) Cycling behavior of the bulk MoO_3 in the range of 0.005-3 V vs. Li^+/Li at a current density of 50 mA/g. The inset shows the cycling behavior of MoO_2; b) Cycling voltammograms of the bulk MoO_3 at a scan rate of 0.2 mV/s in the range of 0.005-3 V vs. Li^+/Li.

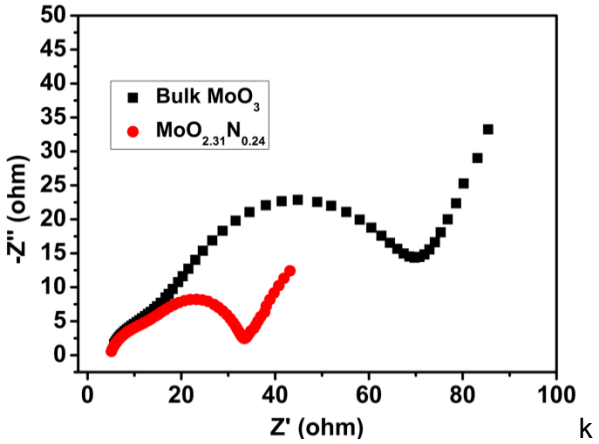

Fig. S3. Electrochemical impedance spectra of the as-synthesized $MoO_{2.31}N_{0.24}$ and bulk MoO_3.

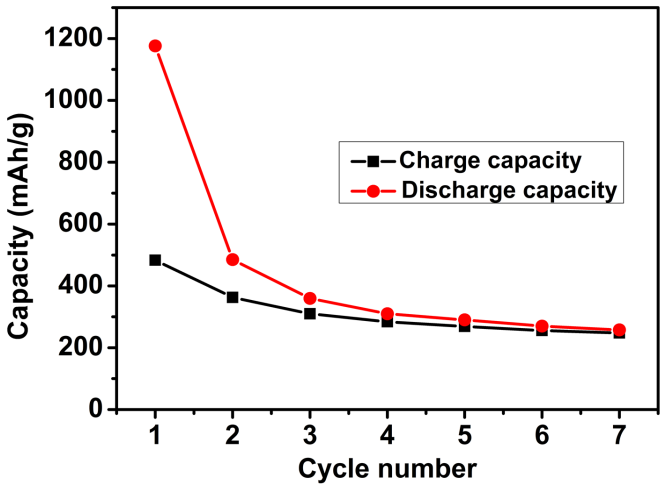

Fig. S4. Cycling behavior of the mixture of MoO_3 (95 wt%) and MoO_2 (obtained by heating MoO_3 in NH_3 atmosphere at 450 °C, 5 wt%) in the range of 0.005-3 V vs. Li^+/Li at a current density of 100 mA/g.

Table S1. Results of peak fitting for the molybdenum oxynitride in the Mo 3d region before argon ion etching.

Peak	Position(eV)	Relative peak Area (%)	FWHM(eV)
$Mo^{4+}(3d_{5/2})$	229.8	24.2	1.45
$Mo^{4+}(3d_{3/2})$	233.0	16.1	1.45
$Mo^{6+}(3d_{5/2})$	232.8	35.8	1.50
$Mo^{6+}(3d_{3/2})$	235.9	23.9	1.50

Table S2. Results of peak fitting for MoO_3 in the Mo 3d region after argon ion etching.

Peak	Position(eV)	Relative peak Area (%)	FWHM(eV)
$Mo^{4+}(3d_{5/2})$	229.8	30.8	1.80
$Mo^{4+}(3d_{3/2})$	233.0	20.5	2.50
$Mo^{6+}(3d_{5/2})$	232.8	29.2	2.50
$Mo^{6+}(3d_{3/2})$	235.9	19.5	2.42

Table S3. Results of peak fitting for the molybdenum oxynitride in the Mo 3d region after argon ion etching.

Peak	Position(eV)	Relative peak Area (%)	FWHM(eV)
$Mo^{4+}(3d_{5/2})$	229.8	40.3	1.58
$Mo^{4+}(3d_{3/2})$	233.0	26.9	2.30
$Mo^{6+}(3d_{5/2})$	232.8	19.7	2.54
$Mo^{6+}(3d_{3/2})$	235.9	13.1	2.60

Table S4. Electronic conductivities of the materials.

Sample	Electronic conductivity (S/cm)
MoO_3	$(1.6\sim1.1)*10^{-5}$
$MoO_{2.31}N_{0.24}$	$5*10^{-2}$
MoO_2 [a]	25
Mo_2N	$> 10^4$

[a] MoO_2 was obtained by heating MoO_3 in NH_3 atmosphere at 450 °C.