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Supporting Information

Revealing the role of NH_4VO_3 treatment on Ni-rich cathode materials with improved electrochemical performance for rechargeable lithium-ion batteries

Congcong Zhang,[a] Siyang Liu,[b] Junming Su,[a] Chunguang Chen,[b] Mengmeng Liu,[a] Xiang Chen,[a] Jianhua Wu,[c] Tao Huang[a] and Aishui Yu*[ab]

[a] Laboratory of Advanced Materials, Shanghai Key Laboratory of Molecular Catalysis and Innovative Materials, Collaborative Innovation Center of Chemistry for Energy Materials, Institute of New Energy, Fudan University, Shanghai 200438, China

[b] Department of Chemistry, Fudan University, Shanghai 200438, China

[c] Jiangmen KanHoo Industry Co. , Ltd., Jiangmen City, Guangdong 529040, China

E-mail: asyu@fudan.edu.cn; Phone: +86-21-51630320; Fax: +86-21-51630320;

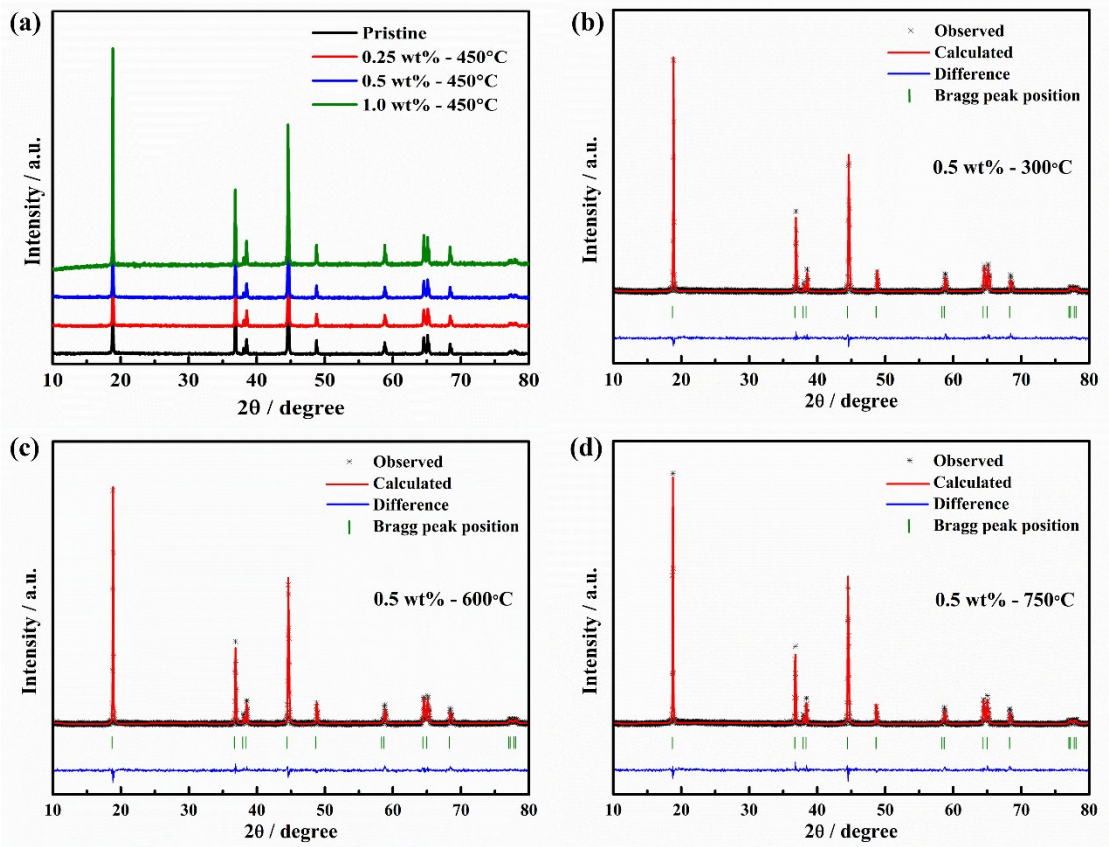

Fig. S1 (a) XRD patterns of the pristine and 0.25, 0.5, 1.0 wt% NH_4VO_3 treated NCM622 materials at 450 ºC; Rietveld refinement of (b) 0.5 wt%–300 ºC, (c) 0.5 wt%–600 ºC and (d) 0.5 wt%–750ºC.

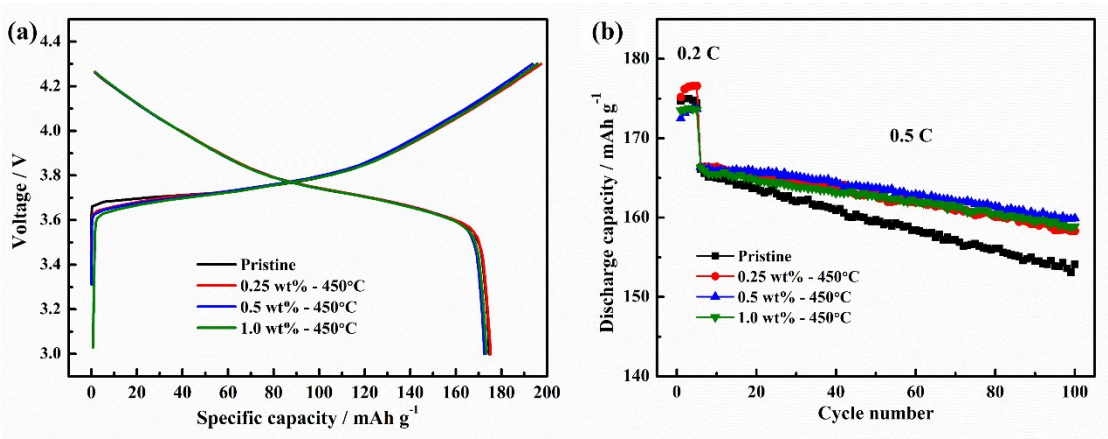

Fig. S2 (a) the first charge-discharge curves at 0.2 C and (b) cycling performance of the pristine and 0.25, 0.5, 1.0 wt% NH_4VO_3 treated NCM622 sintered at 450 ºC.

Table S1 Detailed values of discharge capacity and capacity retention for pristine and different amount of NH_4VO_3 treated NCM622 sintered at 450 ºC

Samples	Discharge capacity (mAh g^{-1})			Capacity
	1st	6th	100th	retention (%)
Pristine	174.7	166.1	154.1	92.8
0.2 wt%–450ºC	175.2	166.4	158.3	95.1
0.5wt%–450ºC	172.5	166.4	159.9	96.1
1.0wt%–450ºC	173.5	166.3	158.9	95.6

The effect of NH_4VO_3 amount on electrochemical performance of NCM622 is investigated and shown in Figure S2 and Table S1. There are no difference in the shape of first charge-discharge curves for all samples and all samples have the similar initial discharge capacity (174.7, 175.2, 172.5, and 173.5 mAh g^{-1} for the pristine, 0.25 wt%, 0.5 wt%, and 1.0 wt% NH_4VO_3 treated samples, respectively), indicating that NH_4VO_3

treatment has no harm to the inherent electrochemical capability of active materials. For the pristine NCM622, the discharge capacity decays to 154.1 mAh g^{-1}, with a capacity retention of 92.8 %. In case of the NH_4VO_3 treated samples, the discharge capacities at the 100th cycles are 158.3, 159.9, 158.9 mAh g^{-1} with capacity retentions of 95.1 %, 96.1 %, and 95.6 %, respectively. This result indicates that an appropriate amount of NH_4VO_3 treatment (0.5 wt%) is most effective for improving the cycling performance of NCM622. Therefore, the 0.5 wt% NH_4VO_3 treatment amount is subsequently used to study the effect of calcination temperature on electrochemical performance of NCM622.

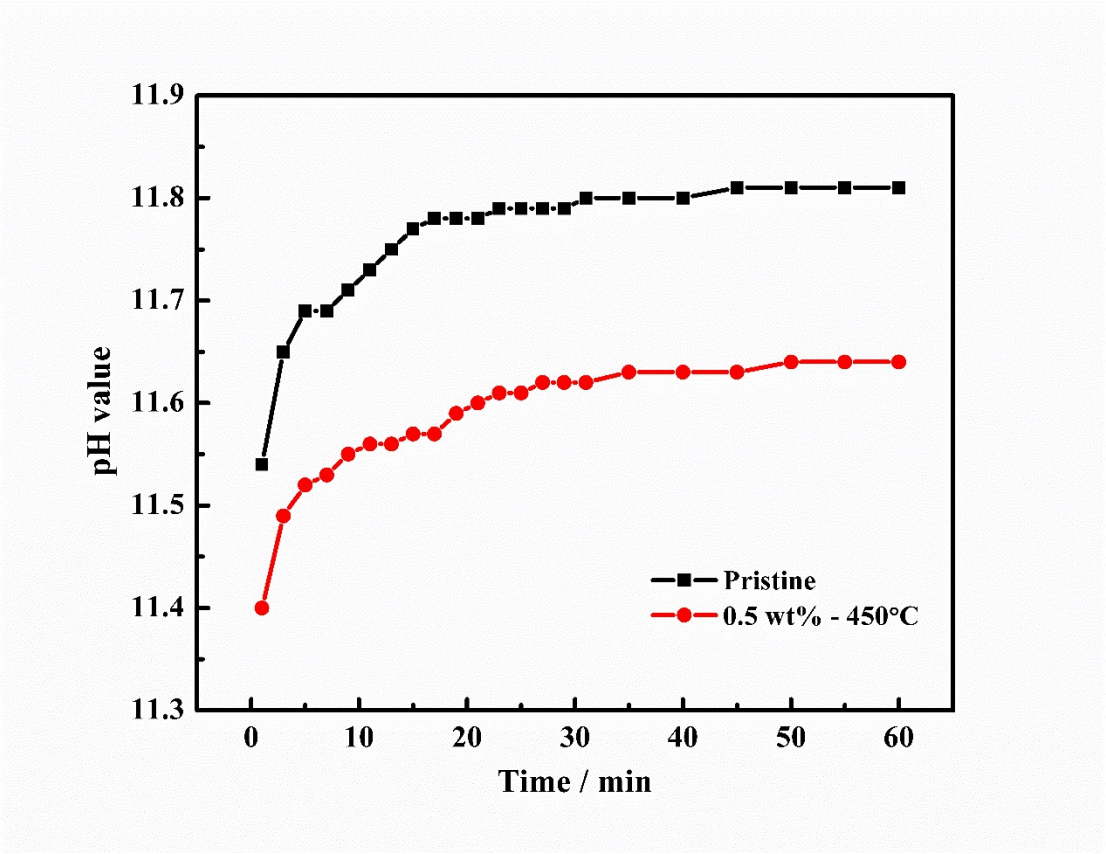

Fig. S3 pH value changes as a function as time for the pristine and 0.5 wt%–450 ºC samples.

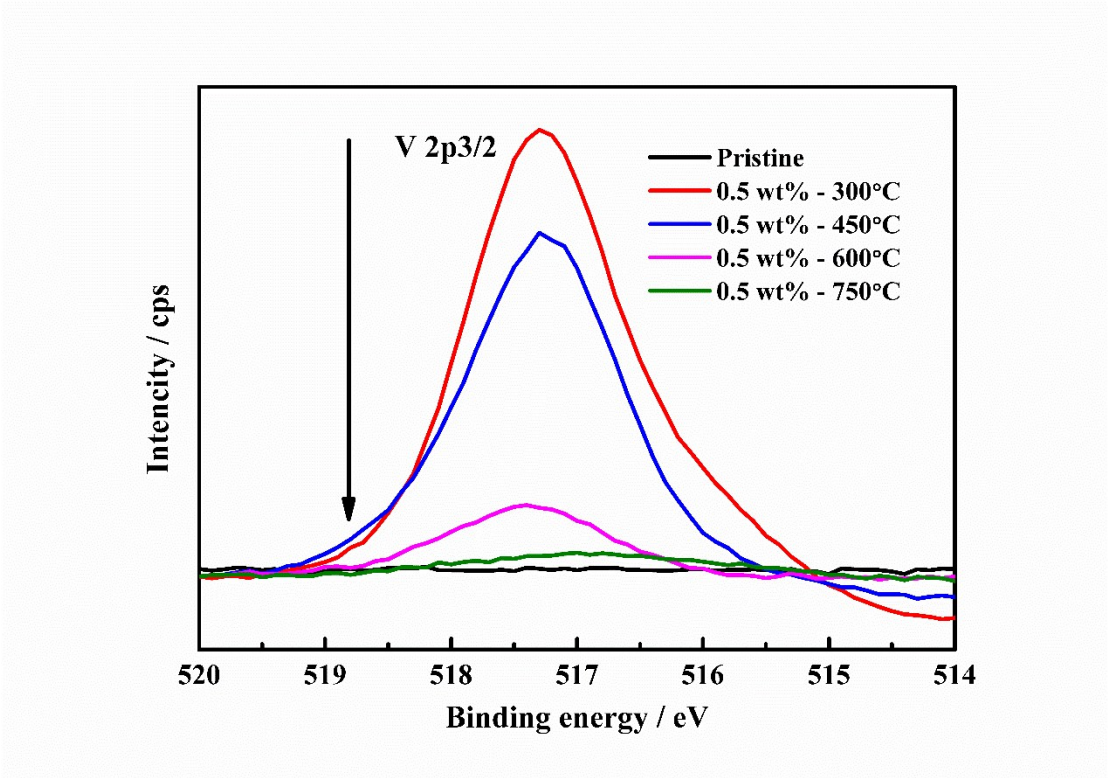

Fig. S4 XPS spectra of V $2p_{3/2}$ for the pristine and 0.5 wt% NH_4VO_3 treated samples at different annealing temperature.

Table S2 Detailed values of discharge capacity and capacity retention for the pristine and 0.5 wt% NH_4VO_3 treated NCM622 sintered at different temperature

Samples	Discharge capacity (mAh g^{-1})			Capacity retention (%)
	1st	6th	100th	
Pristine	174.7	166.1	154.1	92.8
0.5wt%–300ºC	174.3	165.7	154.3	93.1
0.5wt%–450ºC	172.5	166.4	159.9	96.1
0.5wt%–600ºC	173.1	162.9	153.9	94.5
0.5wt%–750ºC	168.1	160.3	148.3	92.5

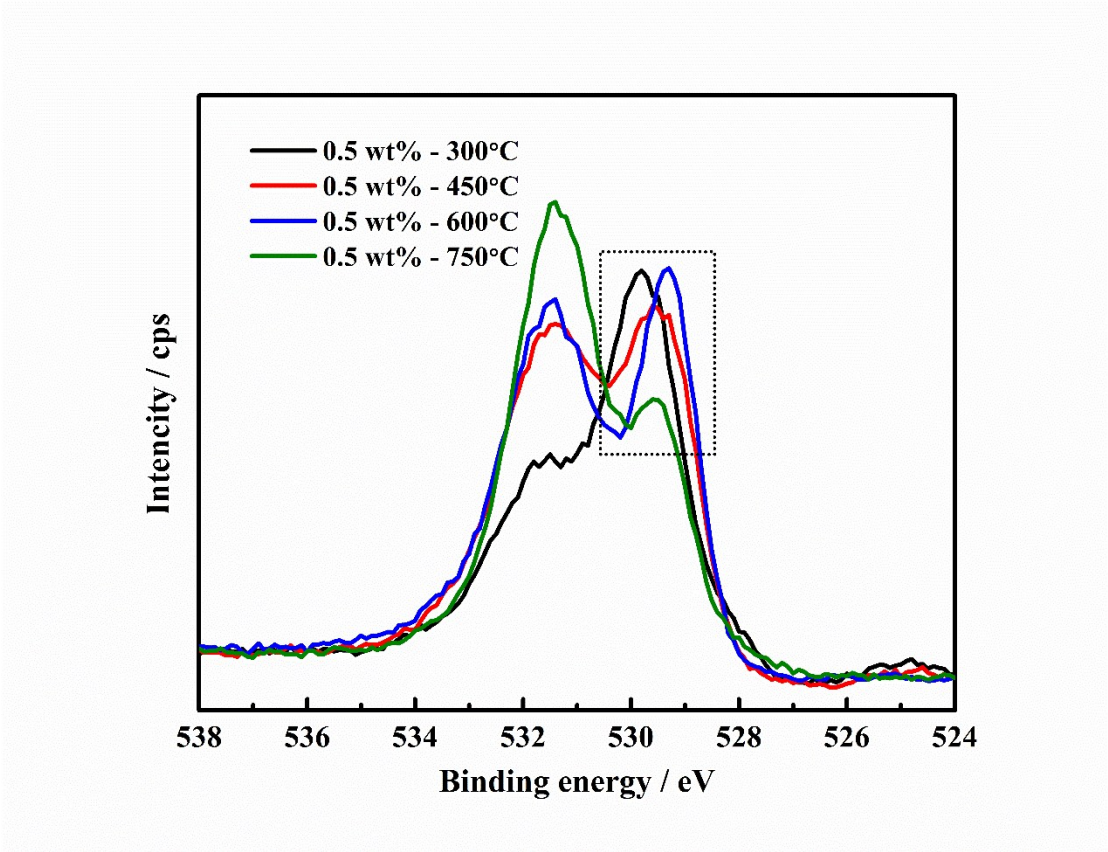

Fig. S5 XPS spectra of O1s for the pristine and 0.5 wt% NH_4VO_3 treated NCM622 sintered at different temperature.

Table S3 The refined XPS binding energies and peak percent for the pristine and 0.5 wt%–450 ºC samples

	Samples	Pristine		0.5wt%–450ºC	
		Bind energy (eV)	Peak percent (%)	Bind energy (eV)	Peak percent (%)
C 1s	C-C	284.8	27.8	284.9	37.0
	C-H	286.3	35.0	286.4	35.8
	C-O	287.5	8.5	288.2	4.7
	C=O	289.1	3.7	289.4	1.9
	C-F/CO_3	290.8	25.0	290.9	20.7
O 1s	M-O	530.1	5.0	530.2	7.5
	C=O	533.3	45.6	532.5	46.6
	C-O	533.8	49.4	533.9	45.9
F 1s	LiF	684.5	40.5	685.0	11.8
	$Li_xPO_yF_z$/Li_xPF_y	685.1	32.0	/	/
	C-F	687.6	27.5	687.9	88.2