Electronic Supplementary Material (ESI) for ChemComm

Improving the Cycling Stability of LiNi0.8Co0.1Mn0.1O2 by Boron doping to inhibit Li/Ni Mixing

Ziru Hu[a], Donghong Duan[a],Haorui Wang[a],Shoudong Xu[a],Liang Chen[a] and Ding Zhang*[b]

College of Chenmical Engineering and Technology,Taiyuan University of Technology

School of Chemical Engineering & Pharmacy,Wuhan Institute of Technology

* Corresponding authors.

E-mail addresses: zhangding@wit.edu.cn

Experimental section

1. Material preparation

For the synthesis of NCM811 and B-doped NMC811, the cathode material was prepared using the $Ni_{0.8}Co_{0.1}Mn_{0.1}(OH)_2$ hydroxide precursor (ternary positive electrode network), LiOH-H_2O (Aladdin Chemical),and H_3BO_3.The pristine NCM811 material was synthesized by sintering a mixture of the precursor and LiOH-H_2O.To synthesize the 0.5, 1, and 1.5 mol% boron doped materials(named, 0.5B-NCM811,1.0B-NCM811,1.5B-NCM811,respecti-vely), the $Ni_{0.8}Co_{0.1}Mn_{0.1}(OH)_2$ precursor was mixed with H_3BO_3 and LiOH-H_2O [transition metal (TM)/Li/B=1:1.03,0.5/1.0/1.5 %].The $Ni_{0.8}Co_{0.1}Mn_{0.1}(OH)_2$ precursor,H_3BO_3,LiOH-H_2O were homogeneously mixed and ground, and then, the mixture was sintered. The pristine material and the comparison materials were sintered under the same conditions. First, the mixture was calcined at 600 °C for 6 h. Then, the prepared material was calcined at 780 °C for 12 h again in an oxygen atmosphere.

2. Materials characterization

Powder X-ray diffraction (XRD) was used to study the structural features of samples,with a scan rate of 4°/min and a 2θ measurement range of 10–90° in Rigaku Ultima IV. Rietveld analysis of the XRD patterns was performed using the general structural analysis system (GSAS). X-ray photoelectron spectroscopy (XPS) was performed using an X-ray photoelectron spectrometer (Thermo ESCALAB 250XI). Scanning electron microscopy (SEM) was performed using a scanning electron microscope (JEOL JSM-7001F) to determine the surface morphology of the samples.

3. Electrochemical measurements

A CR2025 half-coin cell was assembled using the synthesized cathode material. The prepared powder cathode material was mixed with a polyvinylidene fluoride (PVDF) and conductive additive (Super P) in a weight ratio of 8:1:1 in N-methyl pyrrolidone (NMP). The mixed slurry was stirred and coated onto an aluminum foil, which was then baked in a vacuum oven at 100 °C for 12 h. After drying, the aluminum foil was rolled and sliced. A 1 mol/L $LiPF_6$/EC+EMC+DMC (1:1:1 by volume) electrolyte, a lithium metal anode, and a polypropylene (PP) diaphragm were used to assemble a half-cell in an argon glove box. The charge–discharge tests were performed using a Blue Electric charge–discharge tester, in which a current density of 0.1 C was used for the first 3 cycles and then the current density of 1 C was maintained for cycling in a voltage range of 2.75–4.3 V. The high- and low-temperature tests were performed using a high- and low-temperature chamber (MJS-E42). Electrochemical impedance spectroscopy (EIS) was performed using Coster (CS3104), and cyclic voltammetry (CV) was performed using the Blue Battery test system.

Table S1

Table S1 The structural parameters of different materials obtained by Rietveld

Sample	a	b	V	$R_{wp}(\%)$
NCM811	2.8623	14.152	100.409	11.2
1.0B-NCM811	2.8717	14.193	101.361	12.2

Figure S1

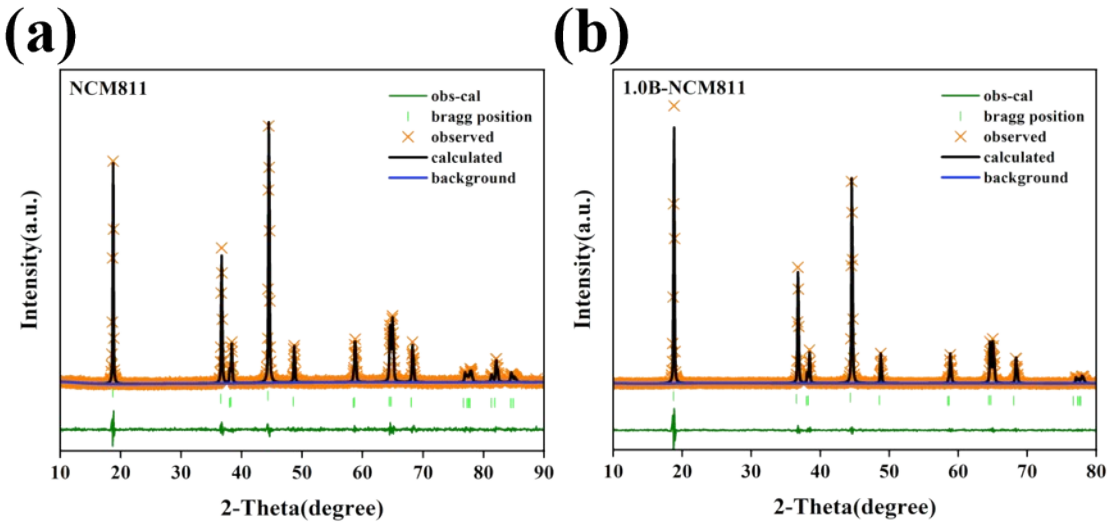

Figure S1 XRD refinement results of (a) NCM811 and (b) 1.0B-NCM811.

Figure S2

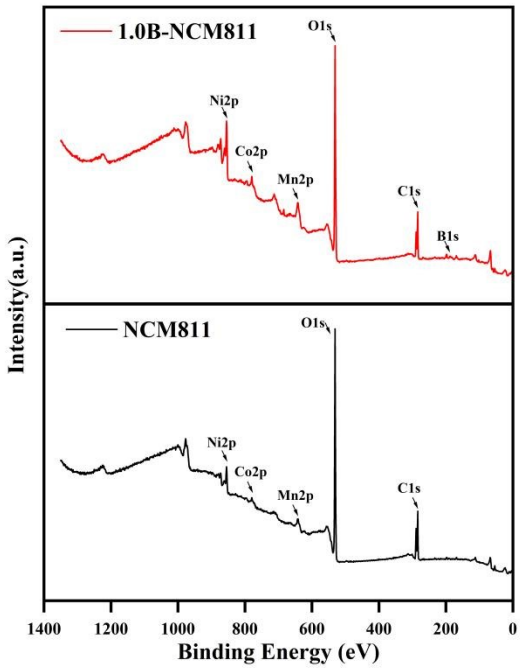

Figure S2 XPS spectra of NCM811 and 1.0B-NCM811.

Figure S3

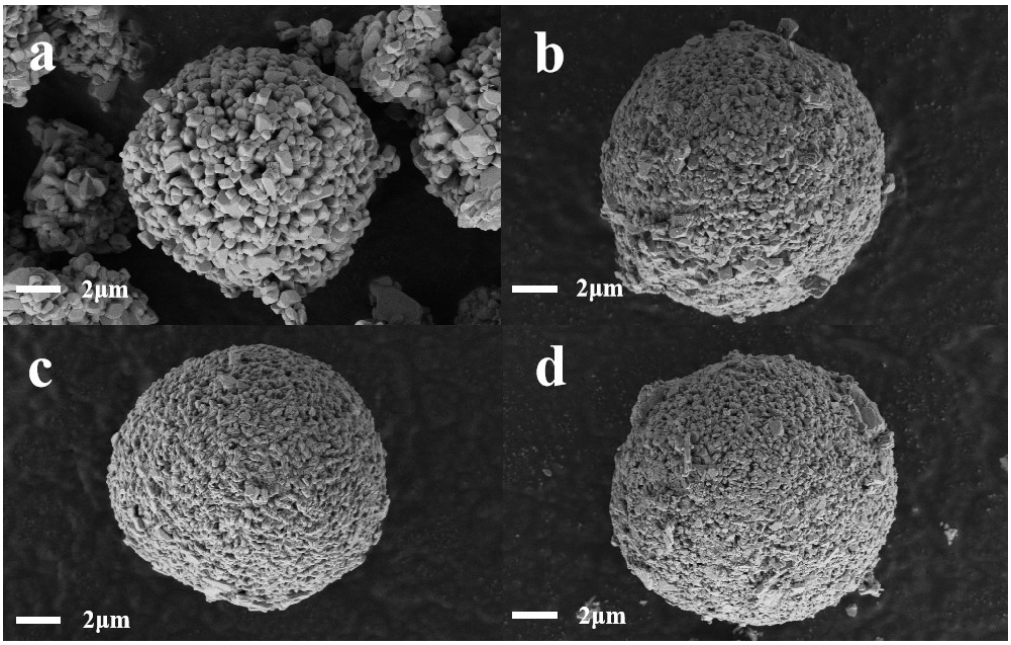

Figure S3 SEM images of (a) NCM811; (b)0.5B-NCM811;(c) 1.0B-NCM811, and (d)1.5B-NCM811.

Figure S4

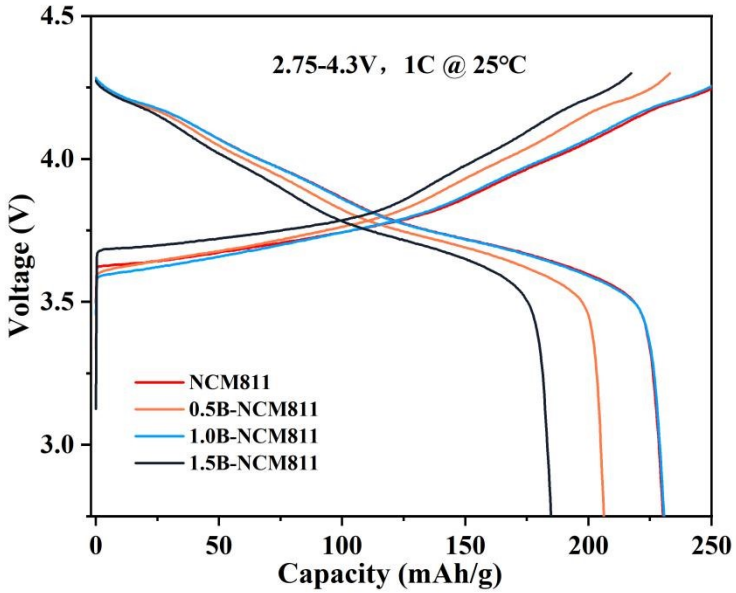

Figure S4 Initial charge–discharge curves of NCM811, 0.5B-NCM811, 1.0B-NCM811, and 1.5B-NCM811 at 0.1 C and 2.7–4.3