Electronic supporting information (ESI)

A new Li-rich layered cathode with low lattice-strain for Lithium-ion

batteries

Bingyu Ke, ^{ab} Shiyong Chu, ^{ab} Jing-Chang Li, ^{ab} Xiangqun Xu, ^{ab} Huan Yao, ^{ab} Shaohua Guo ^{*abc} and Haoshen Zhou^b

a. Shenzhen Research Institute of Nanjing University, Shenzhen 51800, China. E-mail: shguo@nju.edu.cn.

b. College of Engineering and Applied Sciences, and Jiangsu Key Laboratory of Artificial Functional Materials, National Laboratory of Solid State Microstructures, Collaborative Innovation Center of Advanced Microstructures, Nanjing University, Nanjing 210093, China.

c. Frontiers Science Center for Critical Earth Material Cycling, Nanjing University, Nanjing, 210023, China.

Correspondence and request for materials should be addressed to S.G. (shguo@nju.edu.cn & guo.shaohua@outlook.com)

Experiments

Material synthesis

 $Li_2Ni_{0.2}Mn_{0.4}Ru_{0.4}O_3$ and Li_2MnO_3 were synthesized by solid state methods. To get $Li_2Ni_{0.2}Mn_{0.4}Ru_{0.4}O_3(LNMR)$, the reagent grade Li_2CO_3 (10% excess), NiO, Mn_2O_3 and RuO_2 were added to the ball milling tank according to the stoichiometric ratio grinding at 300 rpm for 600 min. The powder obtained after drying was pressed into discs under the pressure of 12 MPa, which subsequently was calcined in air at 750 °C for 10 h. While the contrast sample LMO was calcined in air at 500 °C for 20 h. The sample was cooled to room temperature after calcination and then ground into powder. The powder was pressed to discs were grounded into powder to get the LNMR.

Material characterization

The crystal structure characterization of LNMR and LMO were collected on a Bruker D8-Advanced with Cu Kα radiation. Rietveld refinement was obtained using GSAS software. The particle morphology and size were observed by scanning electron microscopy (SEM, Hitachi SU8010) and Transmission electron microscope (TEM, FEI-TF20). Elements distribution was studied using electron diffraction spectroscopy (EDS).

Electrochemical measurements

The active material, acetylene black and the PVDF binder were fully mixed in a weight ratio of8:1:1 and then coated on the Al foil. The electrode was dried in a vacuum oven at 120°C for 5 h, after that the dried electrode sheet was cut into a disc with a diameter of 12 mm. 1 M LiDFOB in

EC:DMC:EMC = 1:1:1 served as the electrolyte, and a glass fiber membrane was used as the separator. Using Li metal as anode and the prepared electrode as cathode, assembled into a CR2032 coin-type cells in a glove box filled with argon. Electrochemical impedance spectroscopy (EIS) measurements were detected by solartron 1260-1287.

Sample		LNMR
Space Group	C2/m	
Cell Parameters	a(Å)	5.017992
	b(Å)	8.326029
	c(Å)	5.061442
	α(°)	90.000
	β(°)	109.364
	γ(°)	90.000
	volume(Å ³)	199.504
Agreement Factors	R _{wp} (%)	9.18
	R _p (%)	7.91
	CHI ²	3.458

Tab. S1. Refinement of lattice parameters of LNMR by Rietveld method.

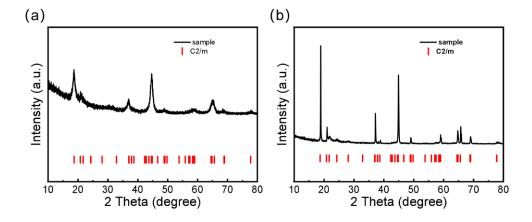


Fig. S1 X-ray diffraction pattern of contrast sample LMO sintering at (a) 500 °C and (b) 900 °C

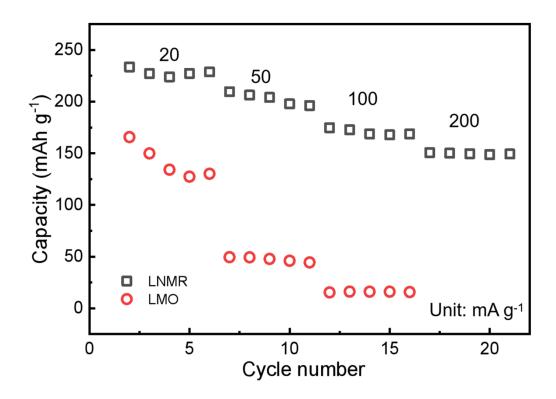


Fig. S2 The comparison of rate performance for LNMR and LMO.

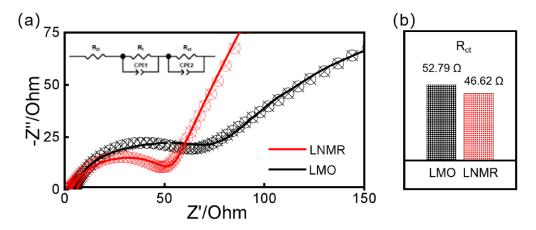


Fig. S3 (a) Nyquist plots of EIS and the fit for LNMR and LMO electrodes. (b) The R_{ct} of LNMR and LMO electrodes.