

Supporting Information

**The synergistic effect between $\text{LiNi}_{0.5}\text{Co}_{0.2}\text{Mn}_{0.3}\text{O}_2$ and $\text{LiFe}_{0.15}\text{Mn}_{0.85}\text{PO}_4/\text{C}$ on
rate and thermal performance for lithium ion battery**

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Simulation section

In this work, we have developed an electrochemical model based on the Newman's pseudo two-dimensional (P2D) electrochemical model¹ for battery discharge processes to predict the cell rate performance of different blend ratios. For blend cathode containing two active materials, the model comprises assumption that both active materials are distributed homogeneously with uniform particle radius in the electrode area. During the discharge process, the lithium ions are extracted from the anode and migrate to the cathode surface, then insert into the cathode through electrochemical reaction, and vice versa in the charging process. The model describes the mass balance and the charge conservation in both solid and liquid phases. The Butler-Volmer equation is used to describe the dynamic lithiation/delithiation reactions between the active electrode particles and the electrolytes during battery operation. Related equations can be searched by relevant literature², which will not be repeated here.

To simulate the electrochemical performance of the blended cathodes, it is essential to test the parameters of two pure materials. Equilibrium potentials of two pure materials are obtained by very low rate discharge test of the half-cell made of single pure material. The Figure S1 demonstrates the equilibrium potential profiles of two single material electrode.

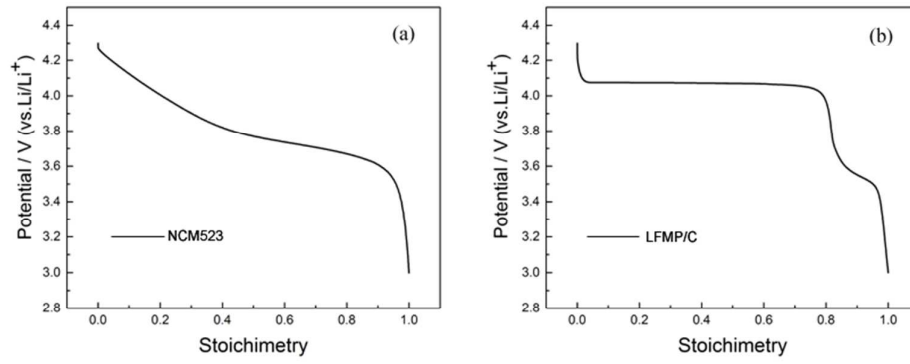


Figure S1. Equilibrium potential of pure (a)NCM523 (b)LFMP/C electrodes by C/25 discharge experiments.

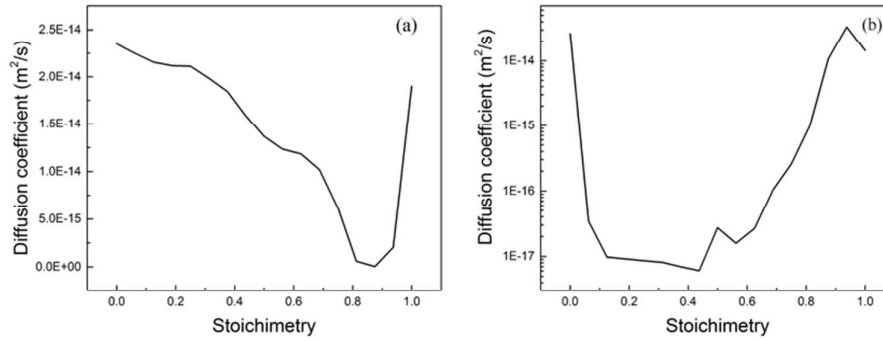


Figure S2. Dynamic diffusion coefficient of (a)NCM523 (b)LFMP/C by GITT experiments

The design of the electrode is directly related to the battery performance, especially the rate performance. A thicker electrode can provide a higher capacity.³ In contrast, a thinner electrode can show a better performance under high rate conditions because of their smaller mass transfer limitations. The lithium ions will travel a shorter distance in a liquid phase, relative to a thick electrode. The diffusion process limitations are considered the main factors affecting the battery rate performance. Therefore, we employ the galvanostatic intermittent titration technique (GITT) experiments to

quantify the dynamic diffusion coefficient of the two active cathode materials.⁴ The

diffusion coefficient is calculated by the simplified formula, $D_s = \frac{4}{\pi\tau} \left(\frac{mV_M}{MS} \right)^2 \left(\frac{\Delta E_s}{\Delta E_t} \right)^2$. The

Figure S2 demonstrates the diffusion coefficient profiles of two single material electrode.

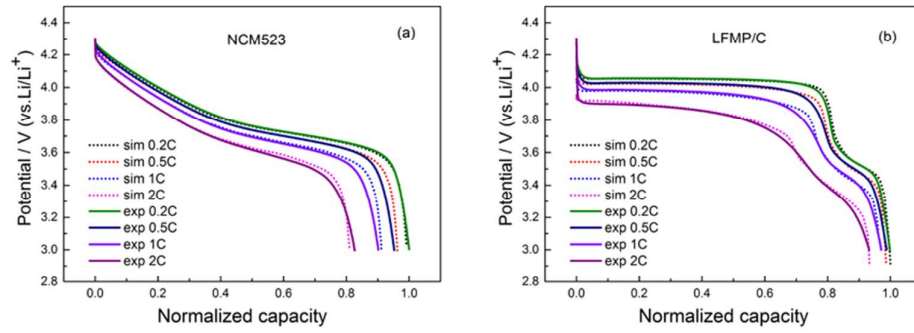


Figure S3. Experimental discharge profile and simulated discharge profile of (a) NCM523

(b) LFMP/C at C/5, C/2, 1C, 2C

In order to verify the correctness of the model, the developed model has been validated with the experimental data. The Figure S3 demonstrates the validation of half cells with two single electrodes. The simulative rate performance of single material electrode shows a good agreement with the experimental data.

Experiment section

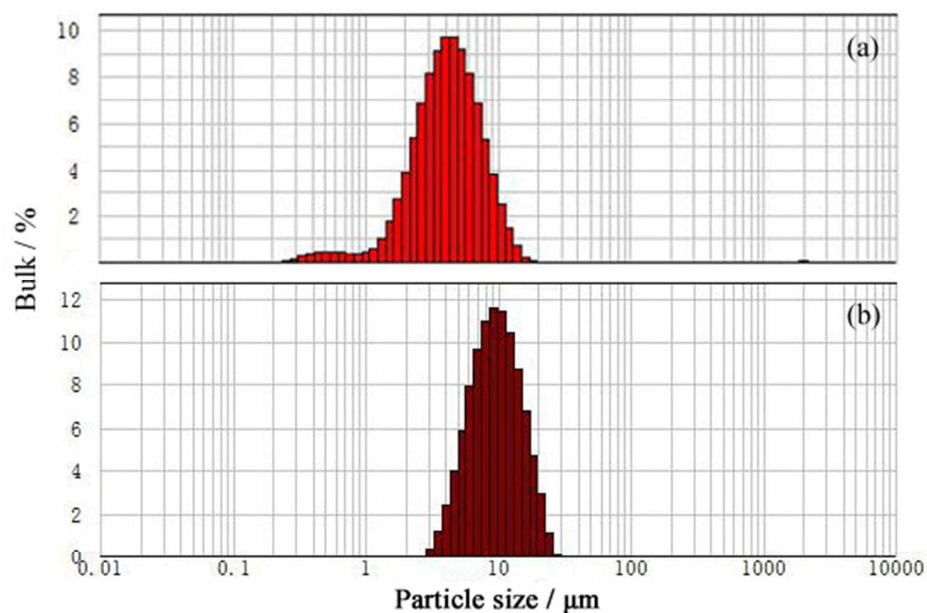


Figure S4. Particle size of two single cathode materials (a) NCM523, (b) LFMP/C

The particles of NCM523 and LFMP/C are demonstrated in the Figure S4. It is obviously the particle size of each single material is homogeneous as we observed in the SEM images with NCM523 of 4.3 μm and LFMP/C of 9.8 μm in average, respectively.

References

1. Doyle, M.; Fuller, T. F.; Newman, J. S., Modeling of Galvanostatic Charge and Discharge of the Lithium/Polymer/Insertion Cell. *Journal of the Electrochemical Society* 1993, 140, 1526-1533.
2. Cai, L.; White, R. E., Mathematical Modeling of a Lithium Ion Battery With Thermal Effects in COMSOL Inc. Multiphysics (MP) Software. *Journal of Power Sources* 2011, 196, 5985-5989.

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4. Rashid, M.; Gupta, A., Experimental Assessment and Model Development of Cycling Behavior in Li-Ion Coin Cells. *Electrochimica Acta* 2017, 21, 1498-1499.