

Supporting Information

Achieving High Specific Capacity of Lithium-ion Battery Cathode by Modification with “N-O·” Radicals Oxygen-containing Functional Groups

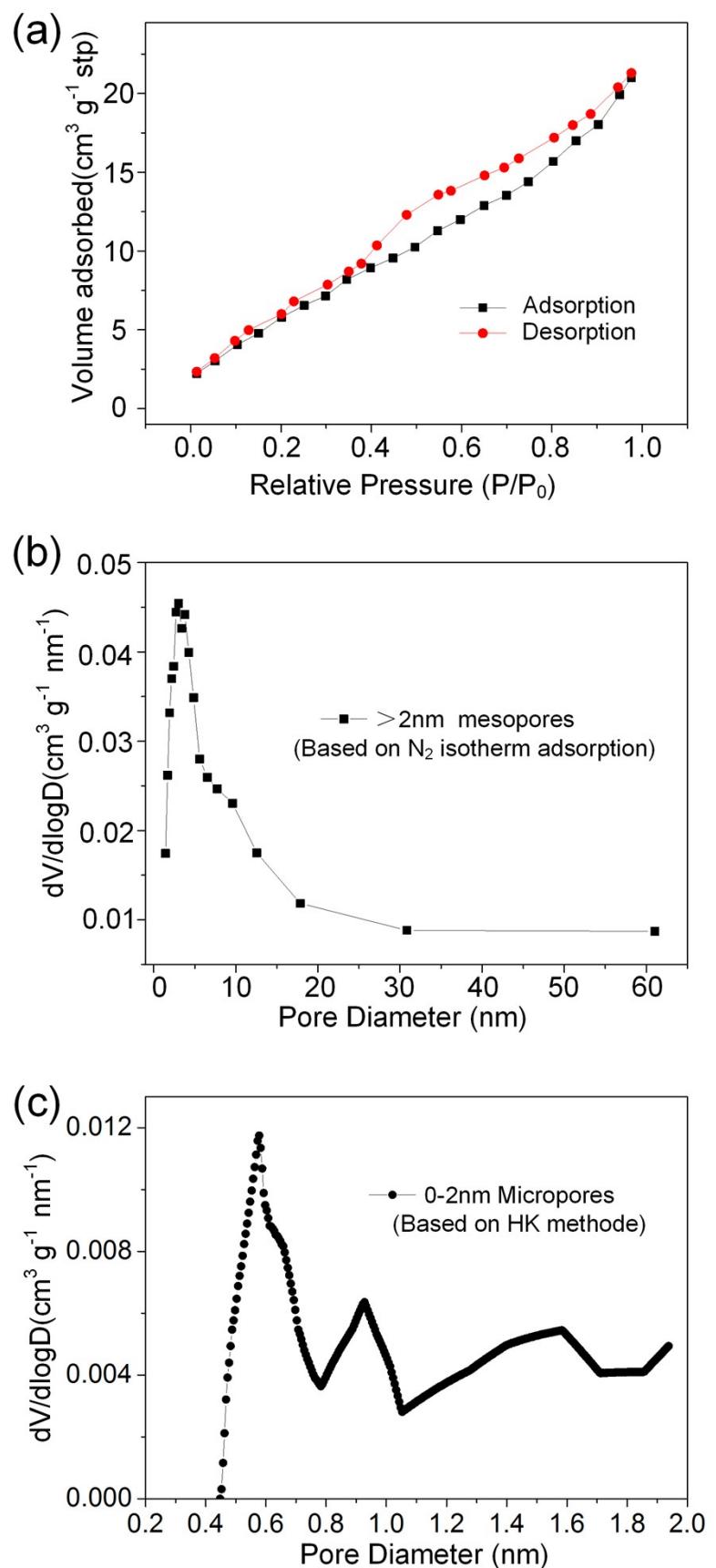
Chengyi Lu,^a David W. Rooney,^b Xiong Jiang,^a Wang Sun,^a Zhenhua Wang,^{*ac} Jiajun Wan^d and Kening Sun^{*ac}

^aSchool of Chemistry and Chemical Engineering, Beijing Key Laboratory for Chemical Power Source and Green Catalysis, BIT-QUB Joint Center on Novel Energy and Materials Research, Beijing Institute of Technology, Beijing, 100081, China.

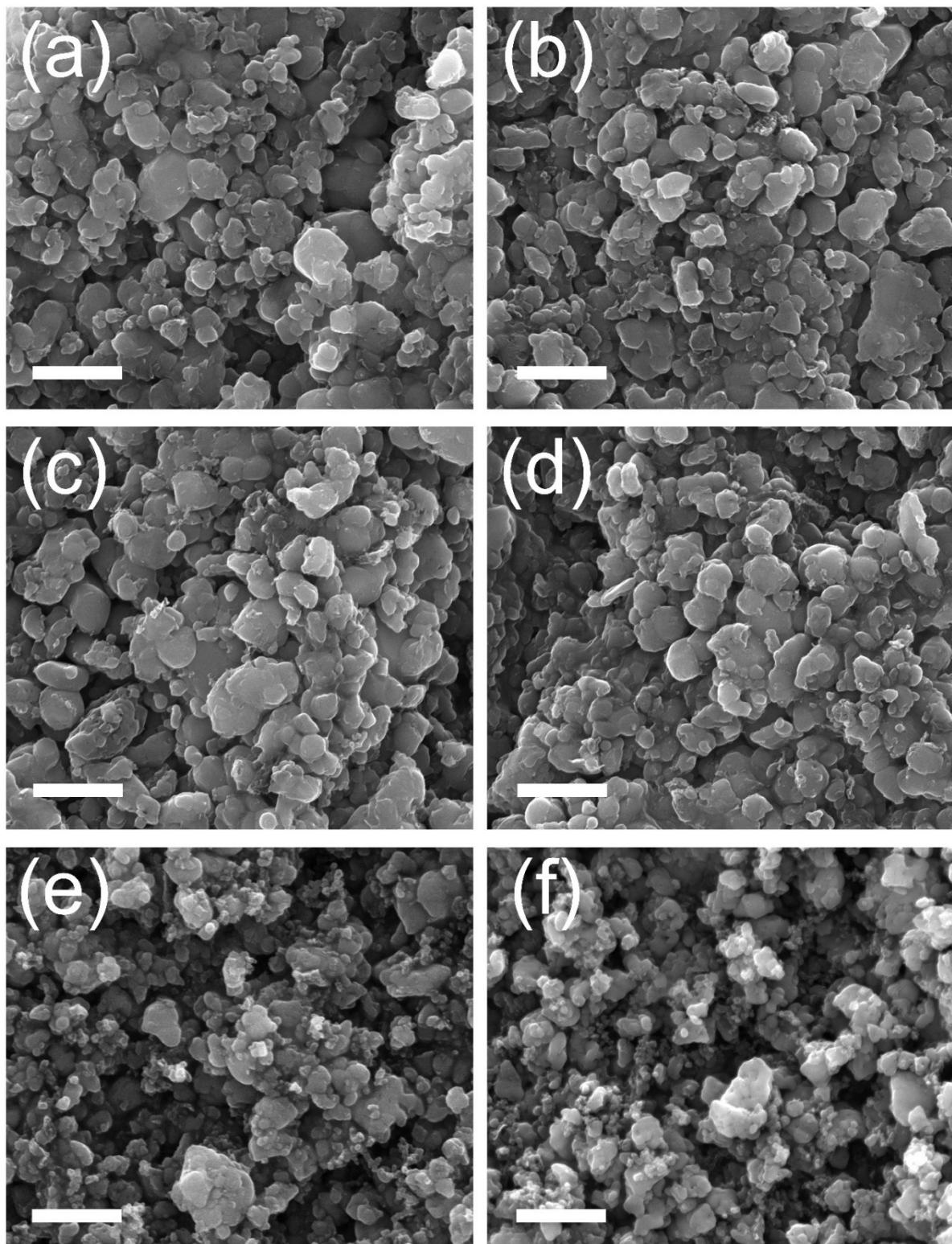
^bSchool of Chemistry and Chemical Engineering, Queen's University Belfast, Belfast BT9 5AG, Northern Ireland.

^cCollaborative Innovation Center of Electric Vehicles, No.5 Zhongguancun South Avenue, Beijing, 100081, China.

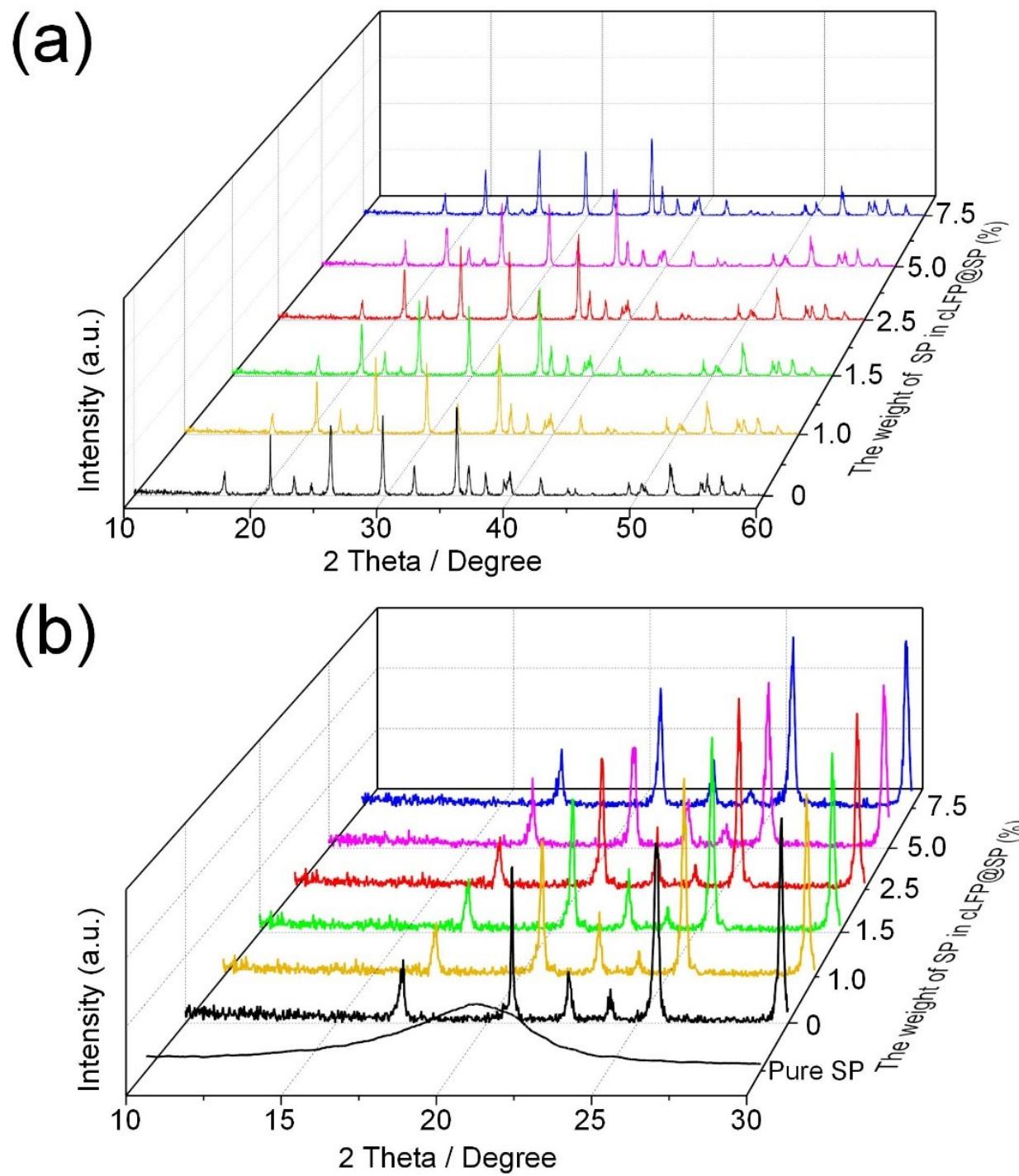
^dPhoton Sciences Directorate, Brookhaven National Laboratory Building 744 Ring Road, Upton, New York 11973, USA.



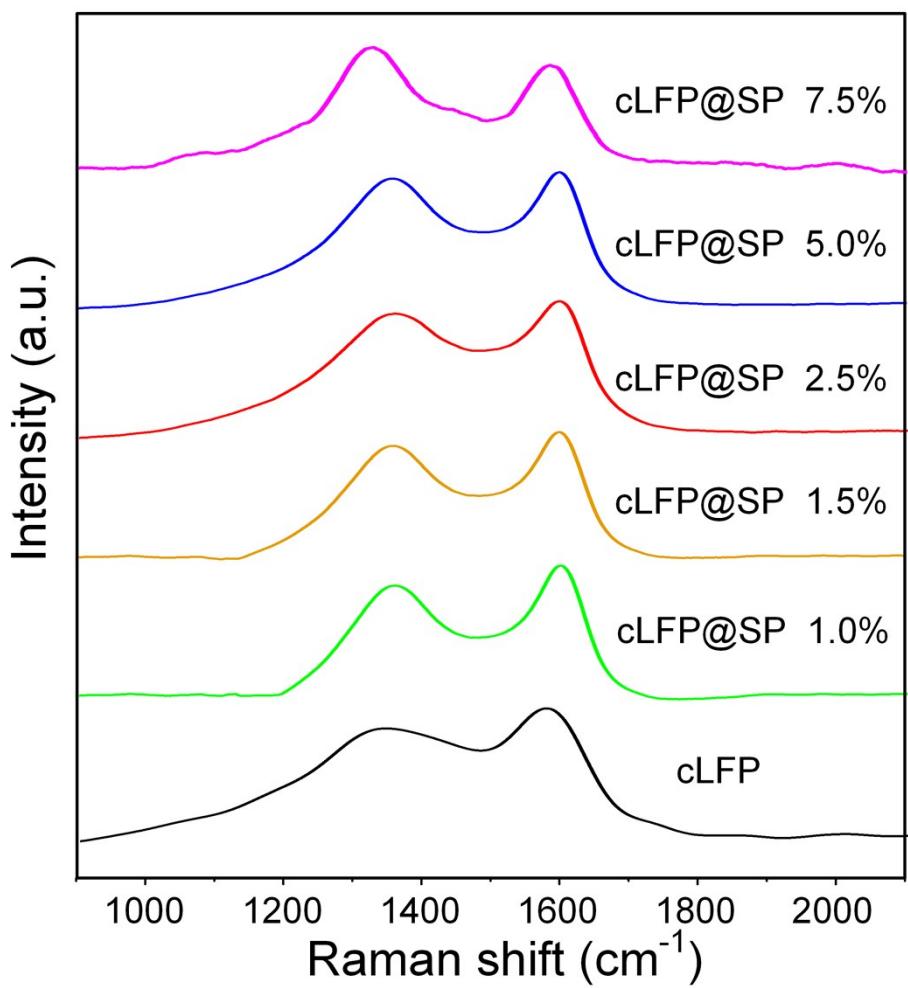
Supplementary Fig S1. Nitrogen adsorption–desorption isotherms and pore size distribution



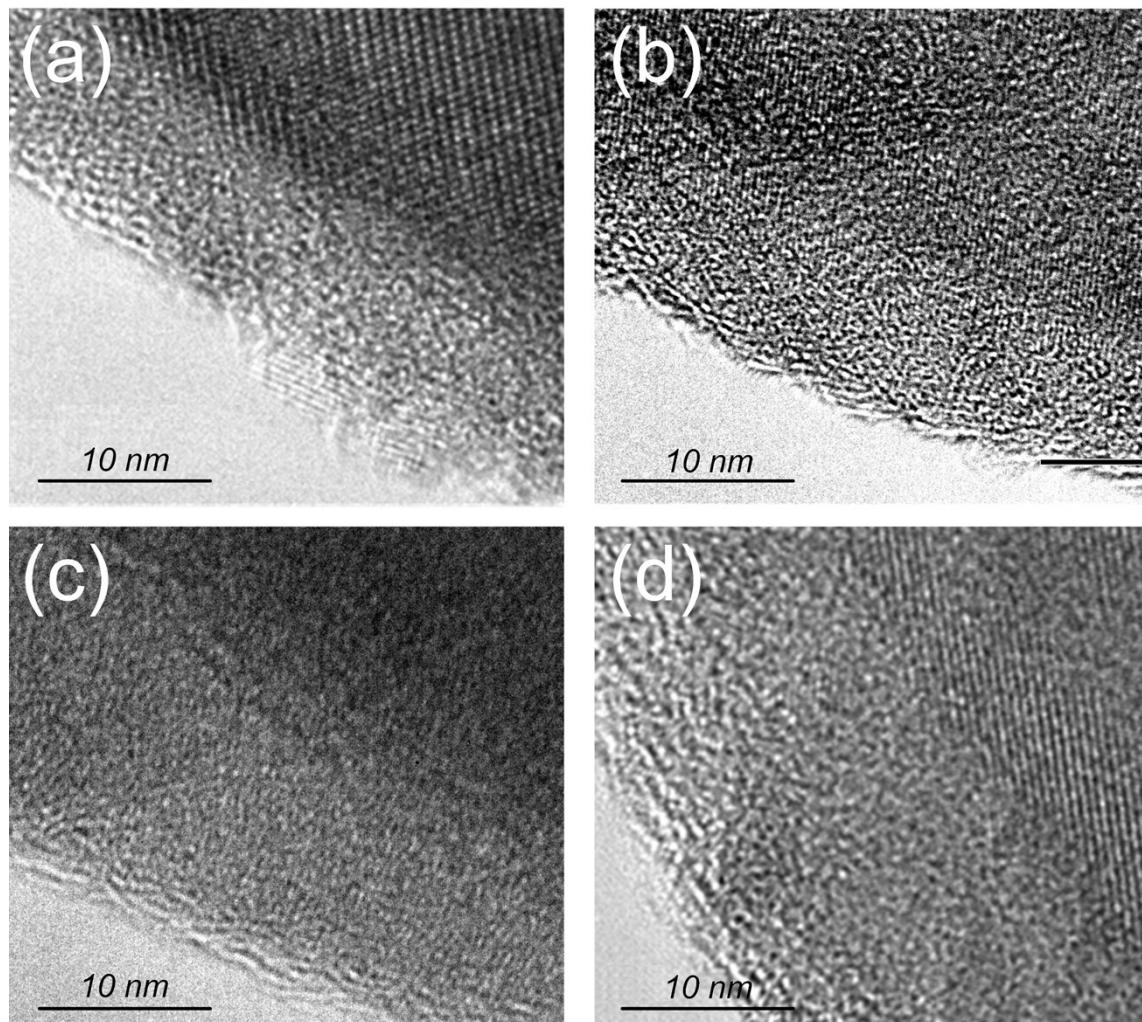
Supplementary Fig S2. The SEM of cLFP@SP with different weight of SP: (a) cLFP with 0% SP, (b) cLFP with 1.0% SP, (c) cLFP with 1.5% SP, (d) cLFP with 2.5% SP, (e) cLFP with 5.0% SP, (f) cLFP with 7.5% SP. Scale bar 1 μ m.



Supplementary Fig S3. The XRD of cLFP@SP with different weight of SP 0, 1.0%, 1.5%, 2.5%, 5% and 7.5%: (a) the scope of 10 degree to 60 degree, (b) the scope of 10 degree to 30 degree.

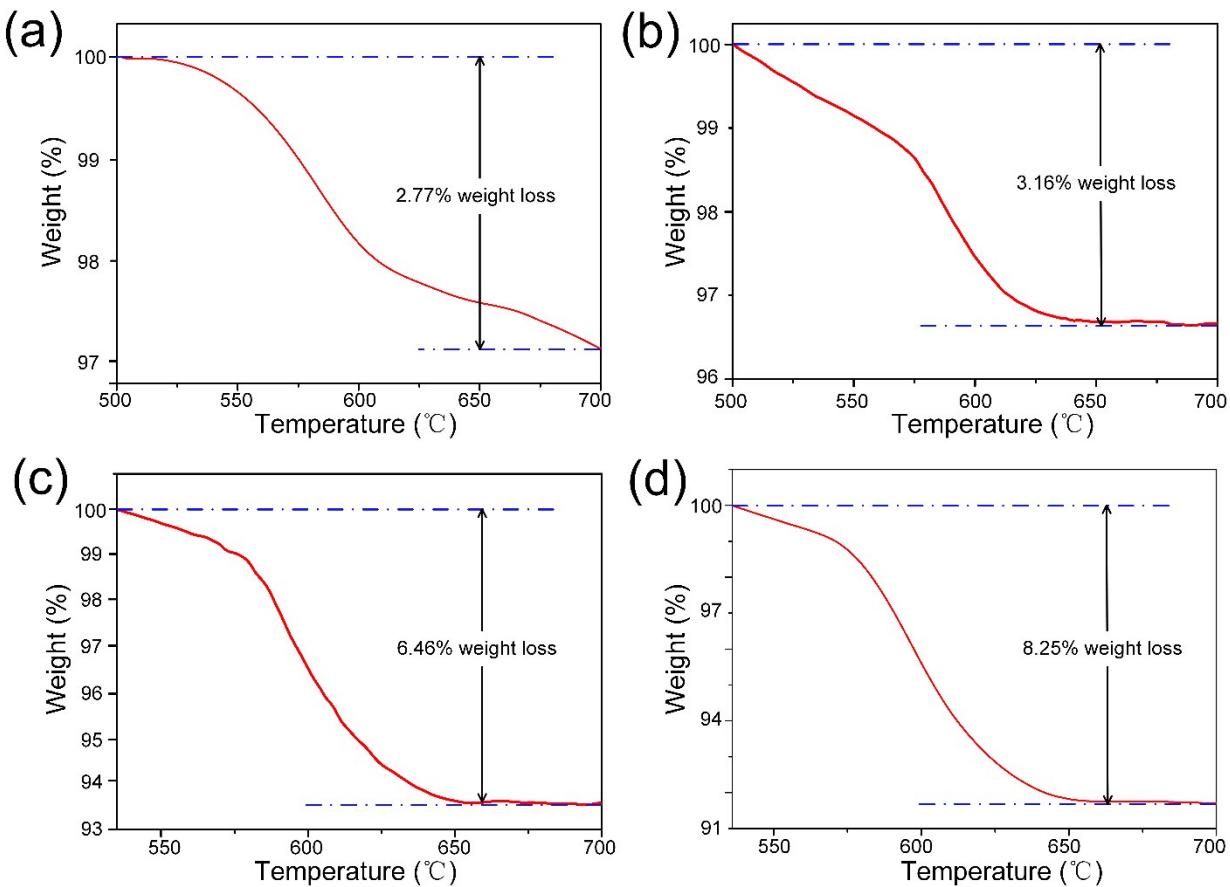


Supplementary Fig S4. The Raman spectra of cLFP@SP with different weight of SP 0, 1.0%, 1.5%, 2.5%, 5.0% and 7.5% at 900~2100 cm⁻¹.

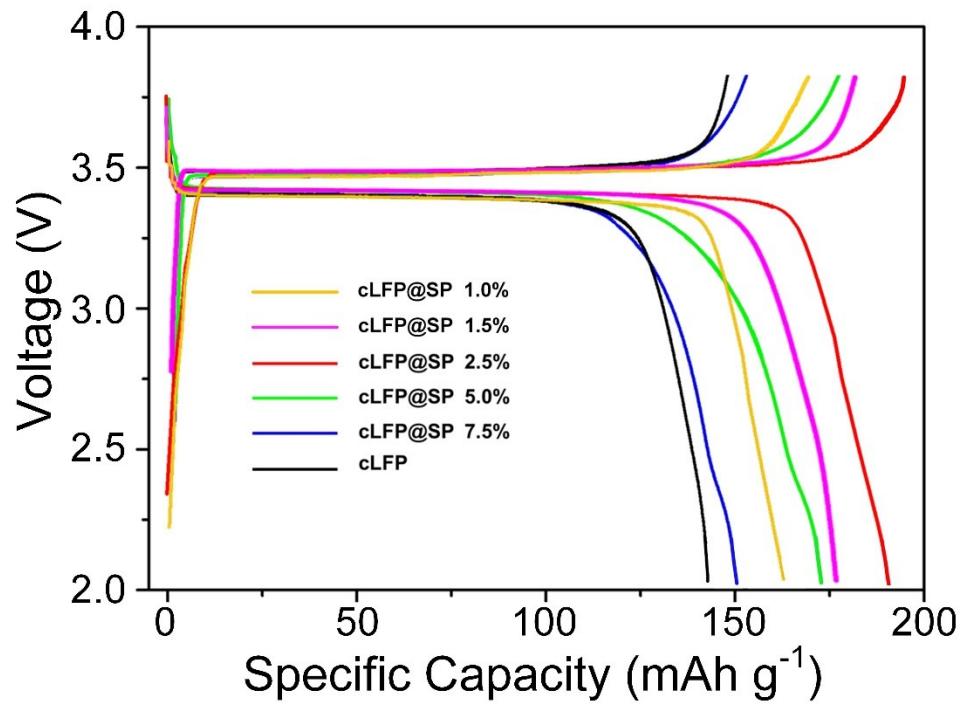


Supplementary Fig S5. The HRTEM of cLFP@SP with different weight of SP 1.0%, 1.5%, 5.0% and 7.5%:

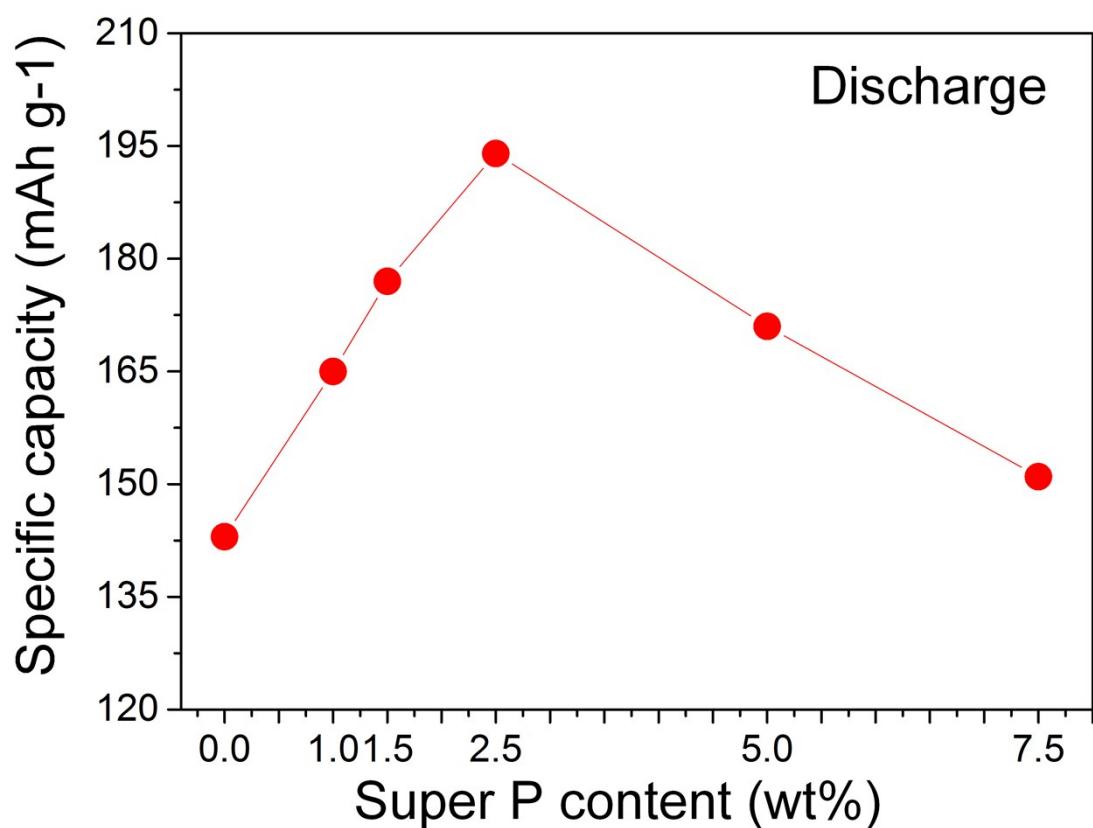
(a) cLFP with 1.0% SP, (b) cLFP with 1.5% SP, (c) cLFP with 5.0% SP, (d) cLFP with 7.5% SP.



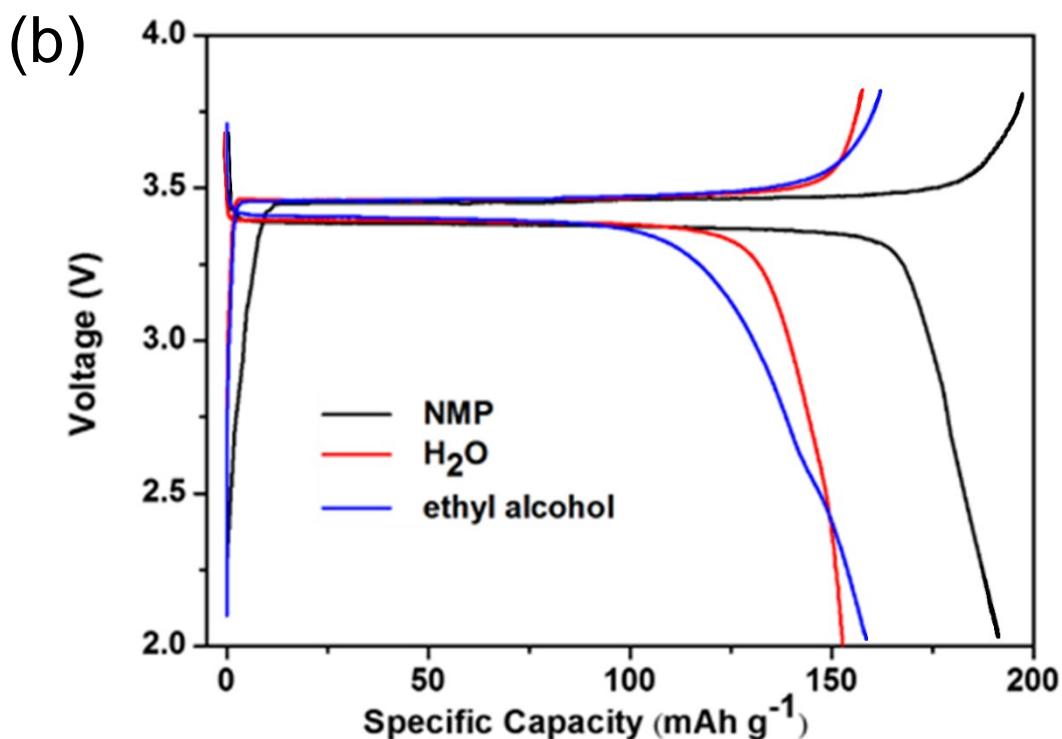
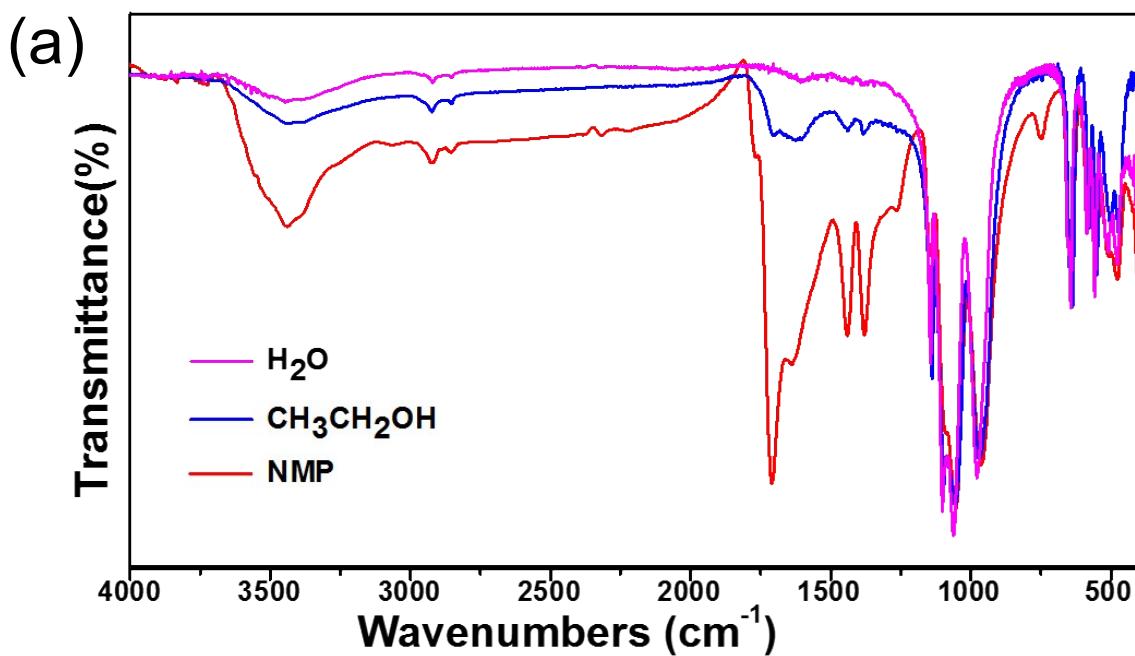
Supplementary Fig S6. The TG of cLFP@SP with different weight of SP 1.0%, 1.5%, 5% and 7.5%, the heating rate:10.0 (K/min): (a) cLFP with 1.0% SP, (b) cLFP with 1.5% SP, (c) cLFP with 5% SP, (d) cLFP with 7.5% SP.



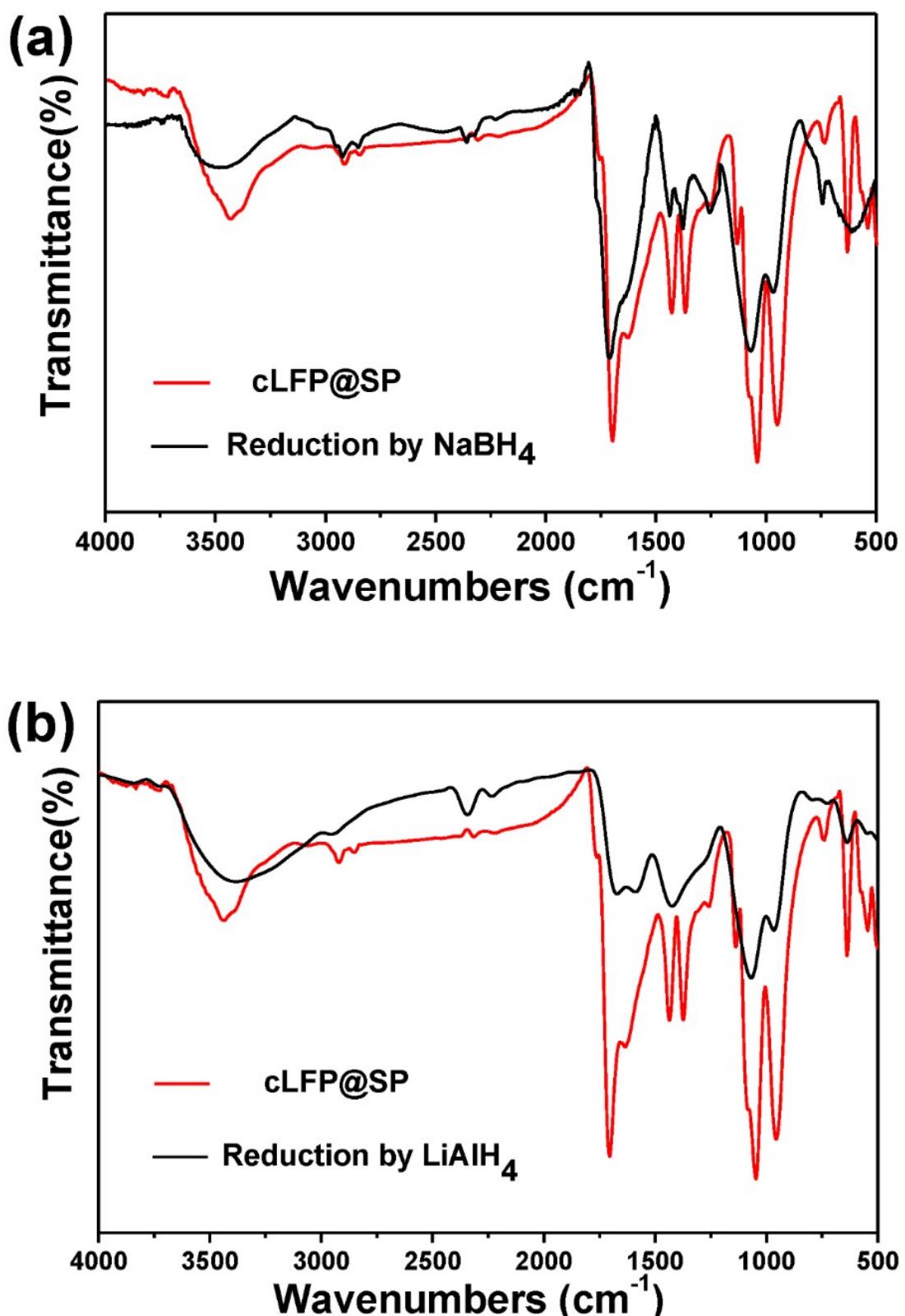
Supplementary Fig S7. The Initial charge and discharge curves of cLFP@SP with different weight of SP 0, 1.0%, 1.5%, 2.5%, 5.0% and 7.5% at 0.1C.



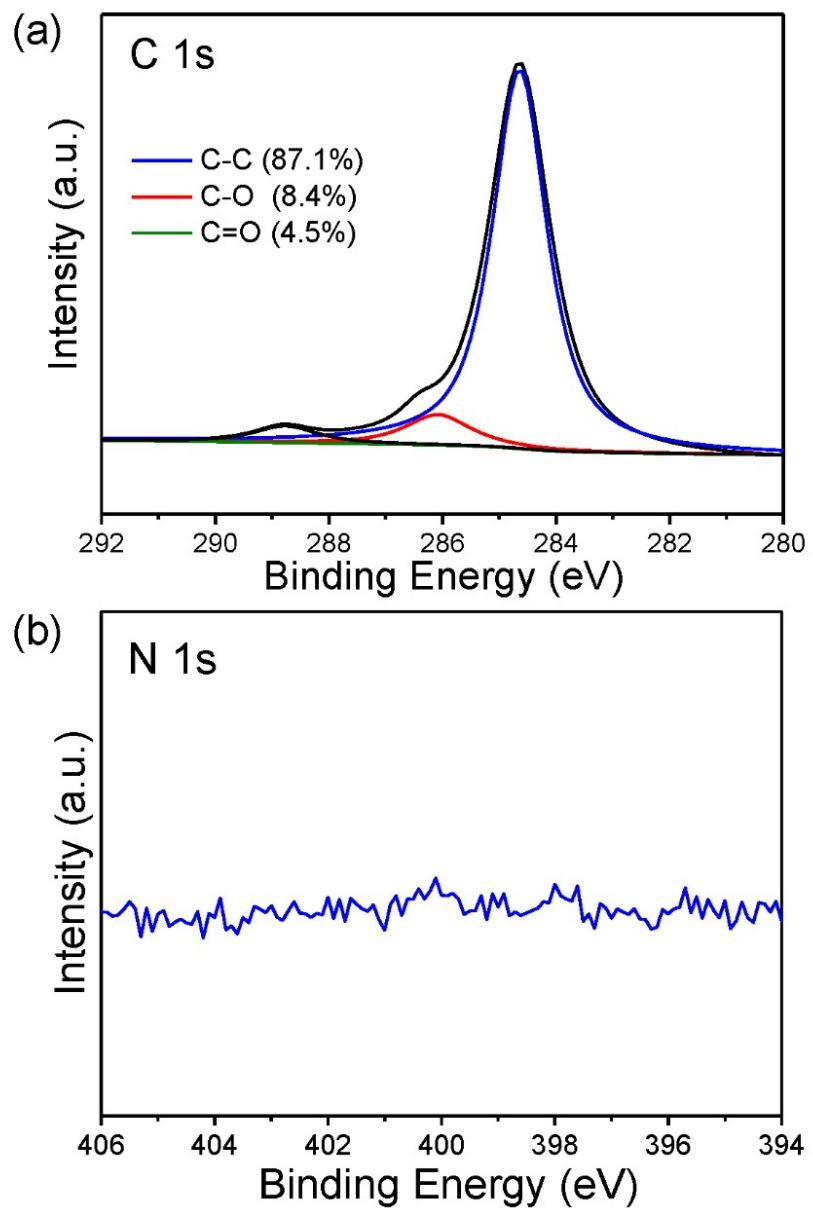
Supplementary Fig S8. The specific capacity as a function of Super P content. The SP weight of cLFP@SP is 0%, 1%, 1.5%, 2.5%, 5% and 7.5%, respectively.



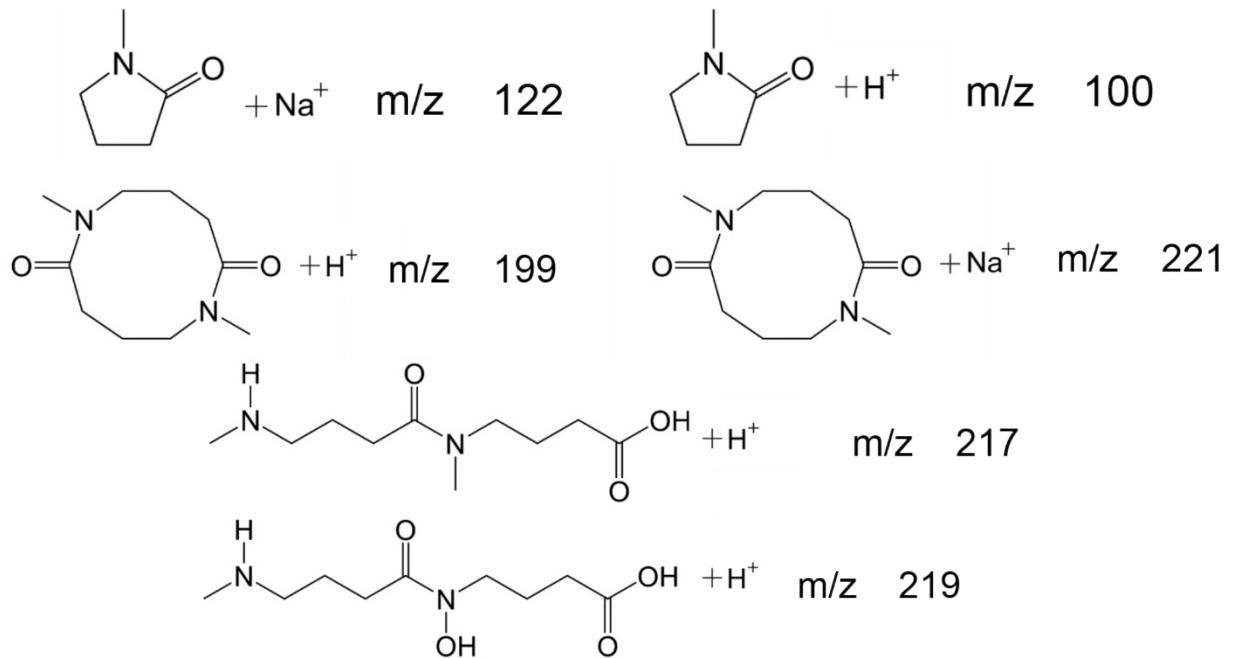
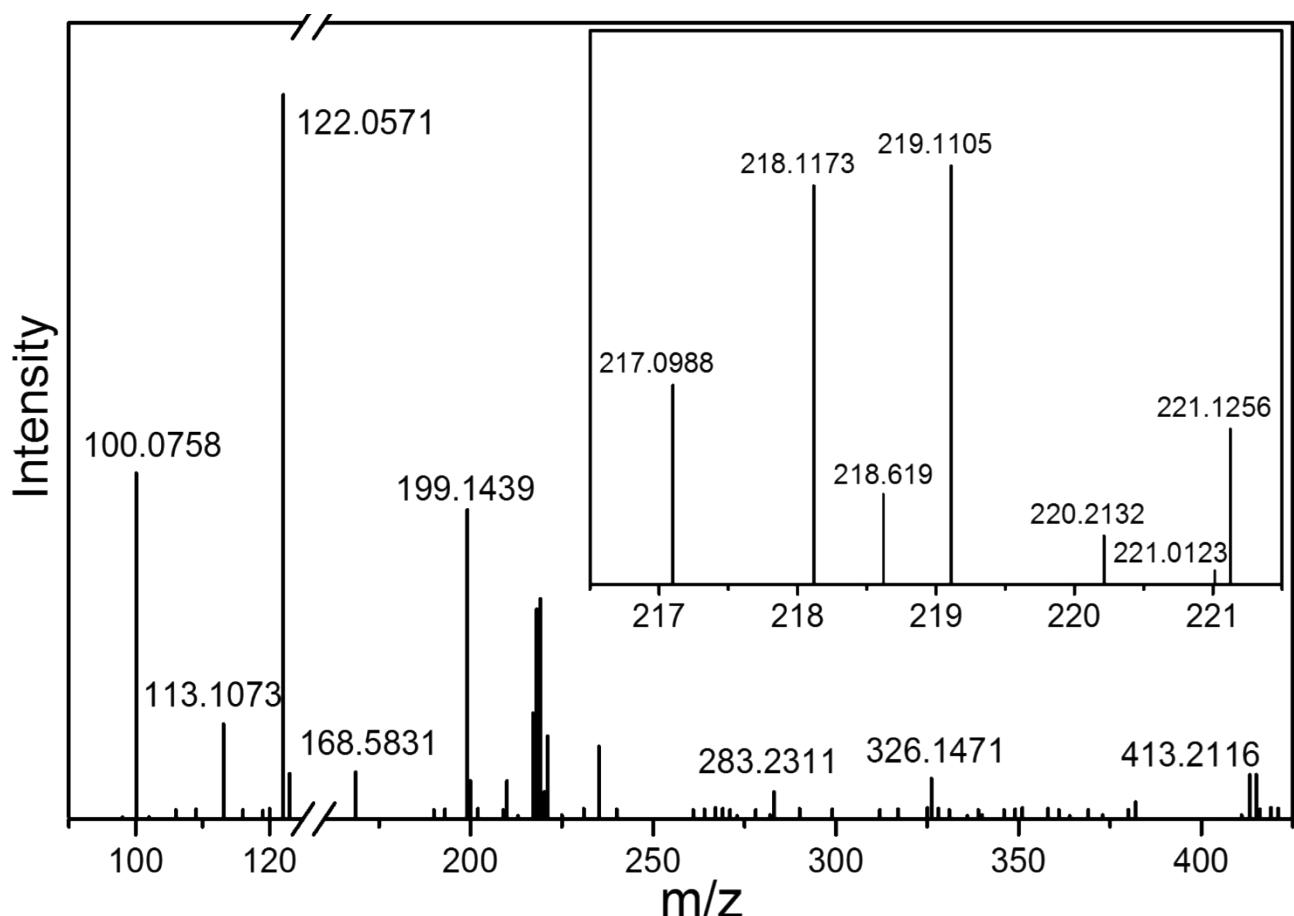
Supplementary Fig S9. The structure characterization and electrochemistry performance with different solvent: (a) The structure characterization of cLFP@SP with different solvent H₂O, Ethyl alcohol and NMP: Infrared spectrum of cLFP@SP (with H₂O, ethyl alcohol and NMP); (b) the Initial charge and discharge curves of cLFP@SP (with ethyl alcohol, H₂O and NMP) at 0.1C.



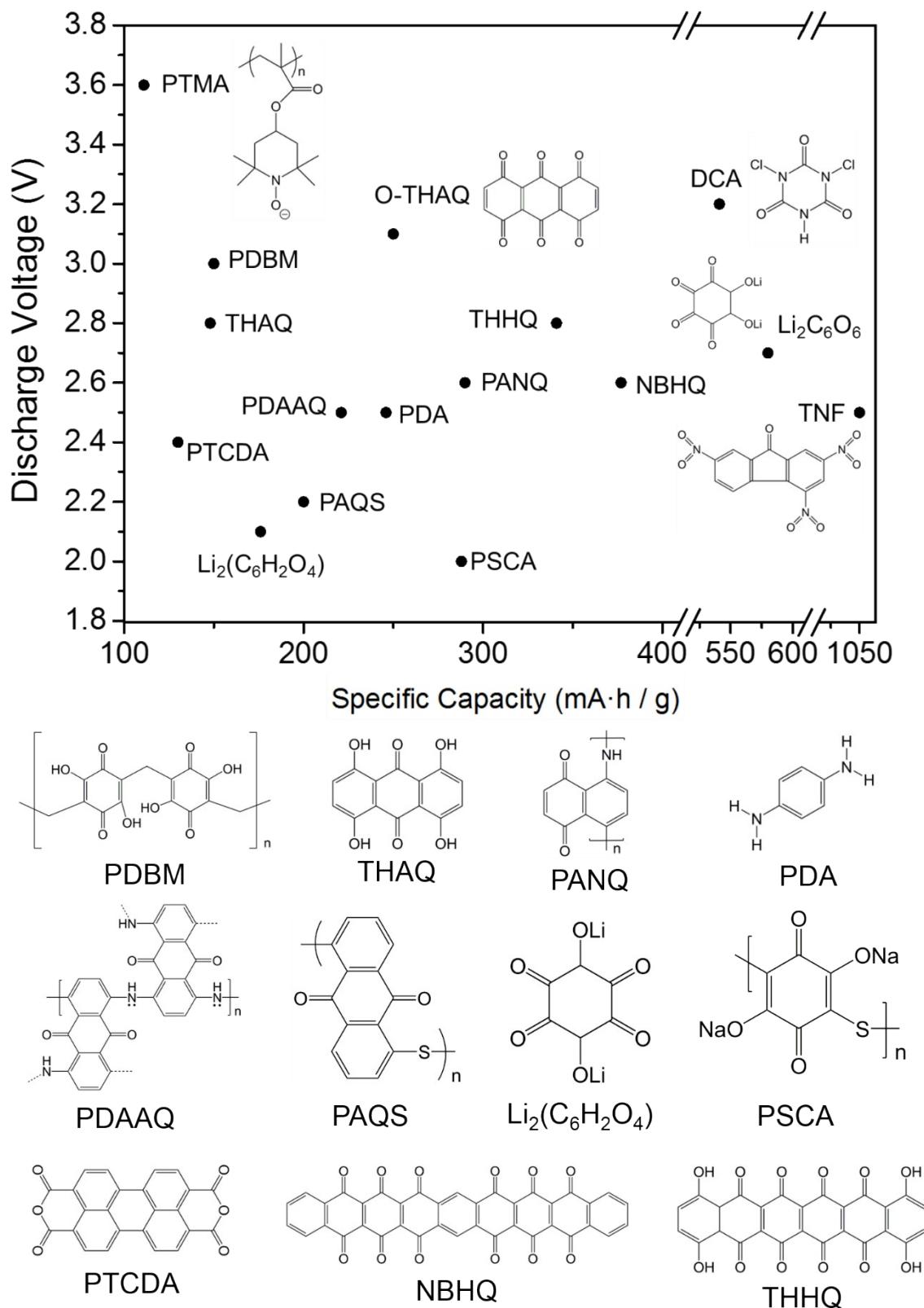
Supplementary Fig S10. The structure characterization of cLFP@SP: (a)Infrared spectrum of cLFP@SP before and after reduction by NaBH_4 ; (a)Infrared spectrum of cLFP@SP before and reduction by LiAlH_4 .



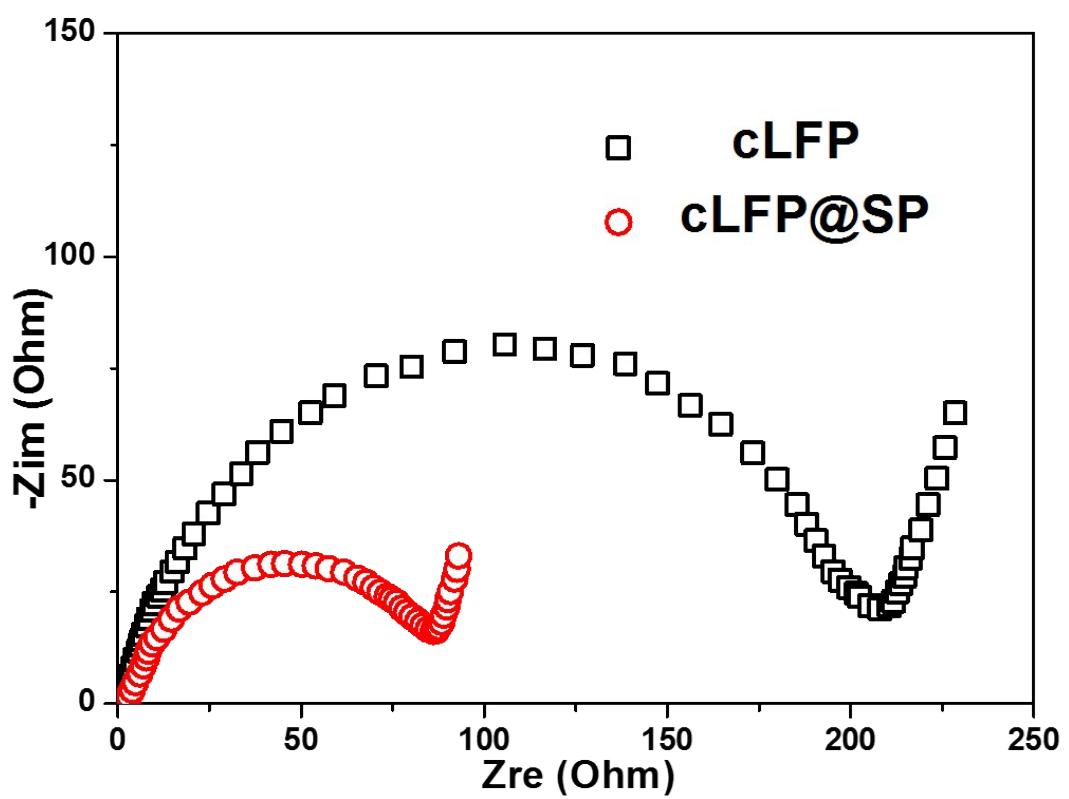
Supplementary Fig S11. Summary of atomic ratios on the basis of the intensities of N 1s peaks and C 1s peaks of cLFP (the SP weight of cLFP@SP is 0%, which is used in the same process with cLFP@SP).



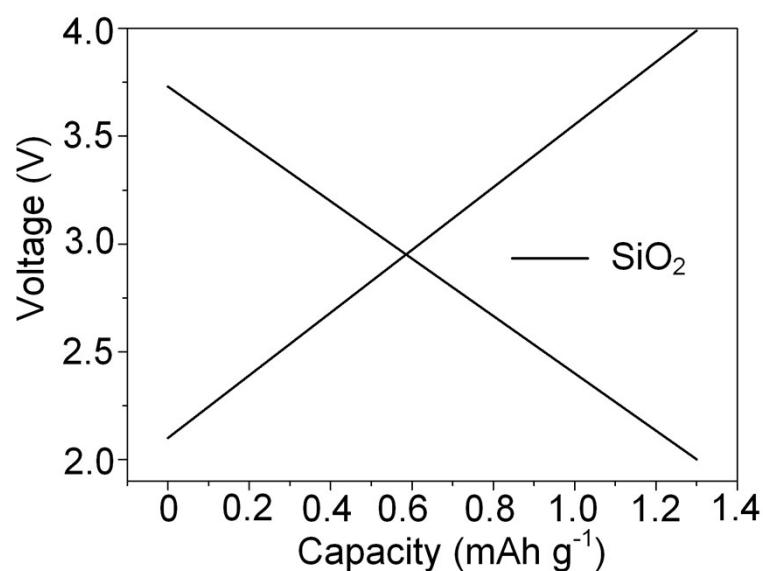
Supplementary Fig S12. The mass spectrometric analysis of NMP after Pyrolysis. The NMP reacts with moisture in the air at high temperatures, leading to breakage of the carbon-nitrogen bonds in the five membered pyrrole ring and the possible structures are inferred from the obtained fragmentation ions.



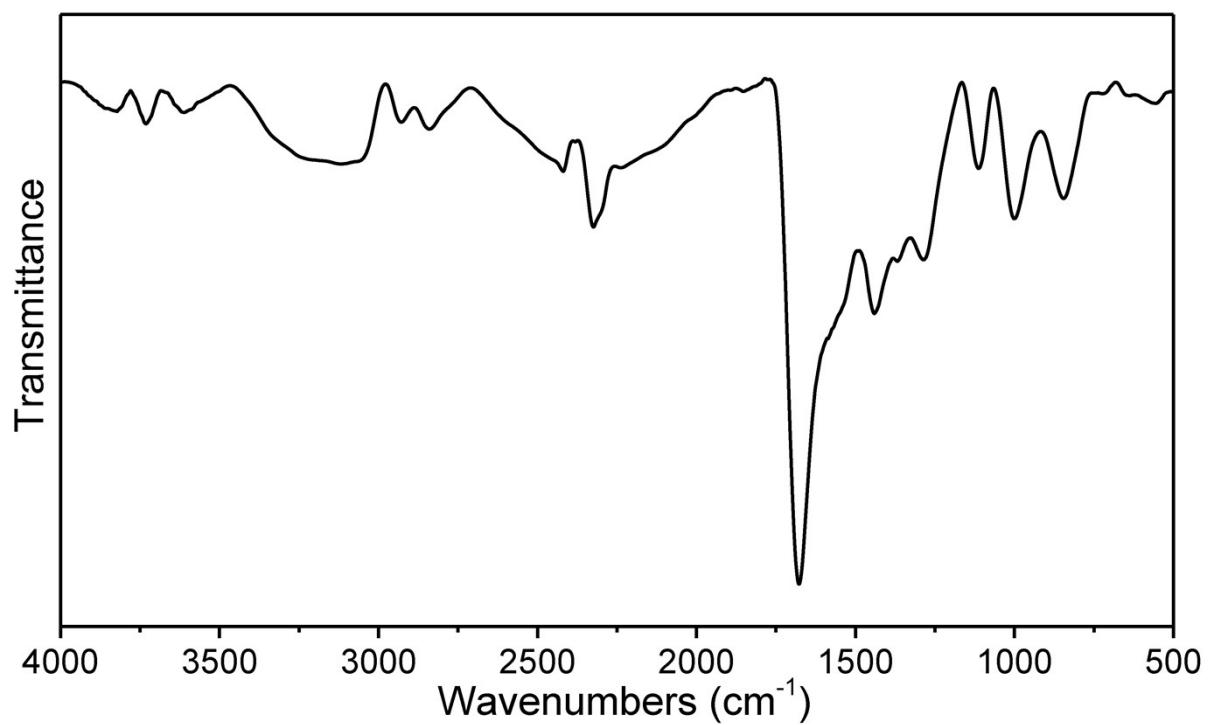
Supplementary Fig S13. The specific capacity and voltage plateau of different structure organic cathodes.¹⁻



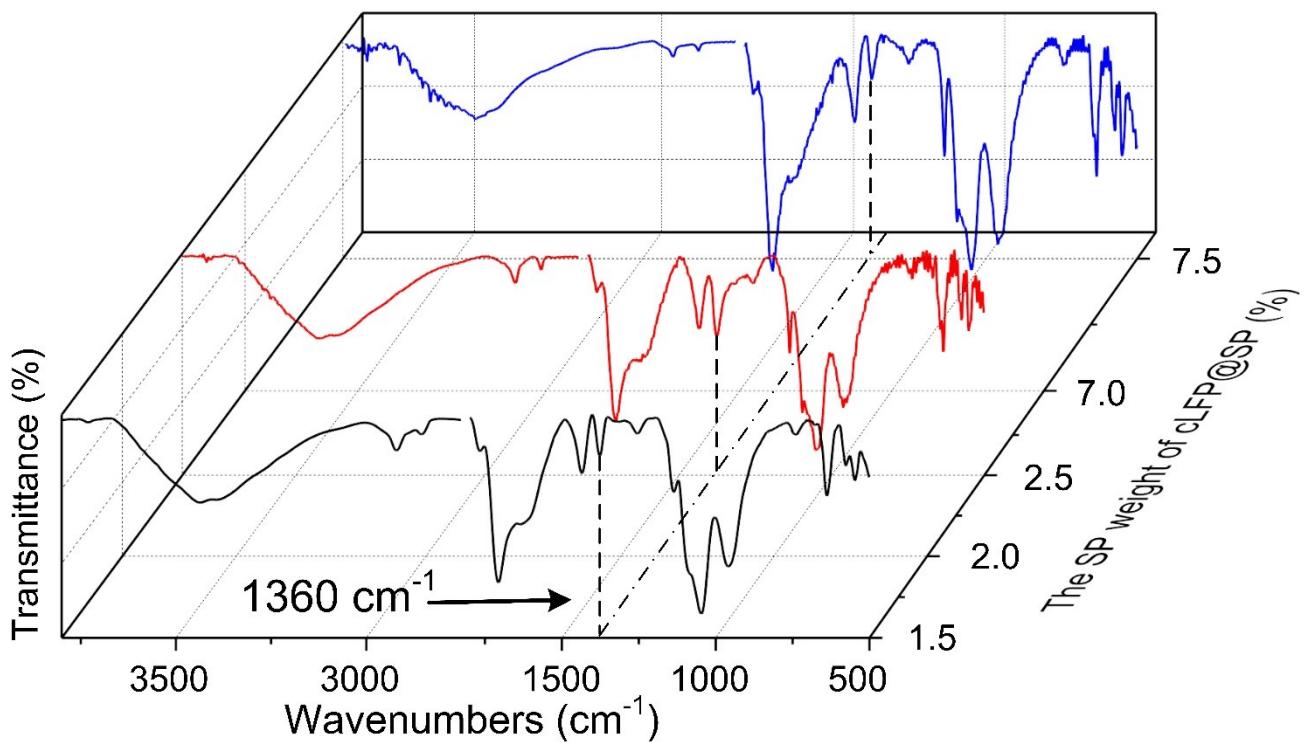
Supplementary Fig S14. Electrochemical impedance spectroscopy (EIS) results of cLFP and cLFP@SP (at a state of no any measurement of charge and discharge).



Supplementary Fig S15. The Initial charge and discharge curves of SiO_2



Supplementary Fig S16. The Infrared spectra of SP which is used in the same process with cLFP@SP.



Supplementary Fig S17. Infrared spectrum of cLFP@SP with different SP weight

References

- 1 H. Kim, D. H. Seo, G. Yoon, W. A. Goddard, Y. S. Lee, W. S. Yoon, K. Kang, *J. Phys. Chem. Lett.*, 2014, **5**, 3086-3092.
- 2 H. Chen, M. Armand, G. Demainly, F. Dolhem, P. Poizot, J. M. Tarascon, *Chemsuschem*, 2008, **1**, 348-355.
- 3 D. H. Seo, H. Kim, H. Kim, W. A. Goddard, K. Kang, *Energy Environ Sci*, 2011, **4**, 4938-4931.
- 4 H. Chen, M. Armand, M. County, M. Jiang, C. P. Grey, F. Dolhem, J. M. Tarascon, P. Poizot, *J. Am. Chem. Soc.*, 2009, **131**, 8984-8988.
- 5 T. Boschi, R. Pappa, G. Pistoia, M. Tocci, *J. Electroanal. Chem.*, 1984, **176**, 235-242.
- 6 M. Pasquali, G. Pistoia, T. Boschi, P. Tagliatesta, *Solid State Ionics*, 1987, **23**, 261-266.
- 7 W. K. Wang, Y. Y. Zhang, A. B. Wang, Z. B. Yu, M. F. Han, Y. S. Yang, *Acta Phys.-Chim. Sin.*, 2010, **26**, 47-50.
- 8 T. L. Gall, K. H. Reiman, M. C. Grossel, J. R. Owen, *J. Power Sources*, 2003, **119**, 316-320.
- 9 M. C. Pham, B. Piro, E. A. Bazaaroui, M. Hedayatullah, J. C. Lacroix, P. Novák, O. Haas, *Synthetic Metals*, 1998, **92**, 197-205.
- 10 D. Haringer, P. Novak, O. Haas, B. Piro, M. C. Pham, *J. Electrochem. Soc.*, 1999, **146**, 2393-2396.
- 11 Z. Tang, G. X. Xu, *Acta Phys.-Chim. Sin.*, 2003, **19**, 307-310.
- 12 Z. Song, H. Zhan, Y. Zhou, *Chem. Commun.*, 2008, **5**, 448-450.
- 13 T. Ohzuku, Z. Takehara, S. Yoshizawa, *Electrochim. Acta*, 1979, **24**, 219-222.
- 14 D. L. Williams, J. J. Byrne, J. S. Driscoll, *J. Electrochem. Soc.*, 1969, **116**, 2-4.
- 15 S. I. Tobishima, J. I. Yamaki, A. Yamaji, *J. Electrochem. Soc.*, 1984, **131**, 57-63.
- 16 X. Han, C. Chang, L. Yuan, T. Sun, J. Sun, *Adv. Mater.*, 2007, **19**, 1616-1621.
- 17 Q. Huang, E. D. Walter, L. Cosimescu, D. Choi, J. P. Lemmon, *J. Power Sources*, 2016, **306**, 812-816.
- 18 J. K. Kim, J. H. Ahn, G. Cheruvally, G. S. Chauhan, J. W. Choi, D. S. Kim, H. J. Ahn, S. H. Lee, C. E. Song, *Met. Mater. Int.*, 2009, **15**, 77-82.
- 19 K. Nakahara, J. Iriyama, S. Iwasa, M. Suguro, M. Satoh, E. J. Cairns, *J. Power Sources*, 2007, **163**, 1110-1113.
- 20 H. Nishide, S. Iwasa, Y.-J. Pu, T. Suga, K. Nakahara, M. Satoh, *Electrochim. Acta*, 2004, **50**, 827-831.