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Supplementary Information for

"Application of Sulfur-doped Carbon Coating on the Surface of

Li₃V₂(PO₄)₃ Composite Facilitate Li-ion Storage as Cathode

Materials" by

Cong Wang, Ziyang Guo, Wei Shen, Aili Zhang, Qunjie Xu, Haimei Liu*, Yonggang

Wang*

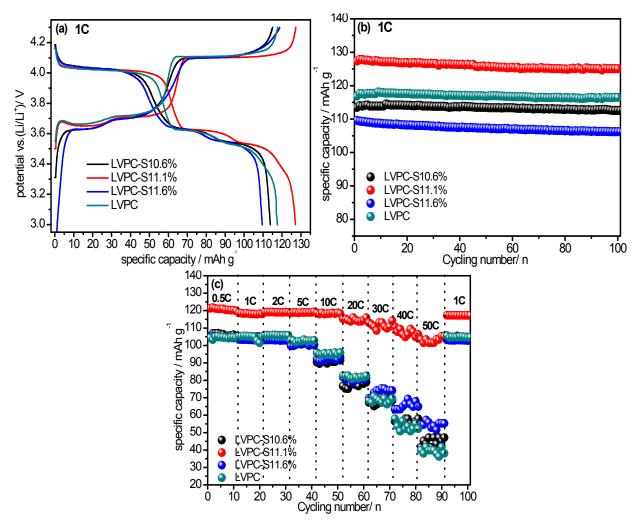


Fig. S1 (a) Initial charge-discharge curves and (b) cycling performances of LVPC and various LVPC-S samples which with various S contents at 1C; (c) rate performances of LVPC and various LVPC-S samples which with various S contents; all the tests were employed in the potential window of 3.0 - 4.3 V (vs. Li/Li⁺).

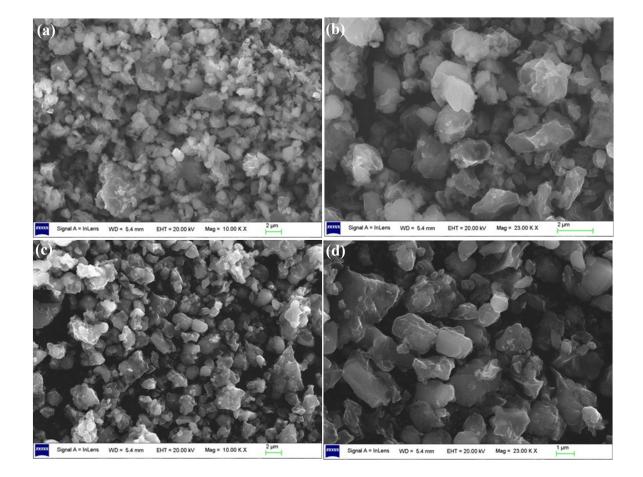


Fig. S2 SEM images of (a) and (b) LVPC-S11.1% and (c) and (d) LVPC.

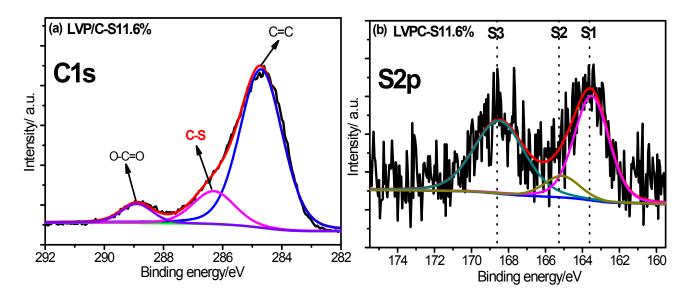


Fig. S3 High-resolution (a) C1s and (b) S2p spectrums of LVPC-S11.6%.

In order to further confirm the effects of S doping amount on the variation of chemical bonding between carbon and sulfur in carbon coated layer, X-ray photoemission spectroscopy (XPS) studies of LVPC-S11.6% were also carried out. **Fig. S3a** displays the high-resolution C1s spectrum of LVPC-S11.6%, the C1s peak of sp² carbon is also appeared at 284.6 eV; however, compared with LVPC (Fig. 3c), a fitted peak of C-S bond is also appeared at 268.5 eV on C1s spectrum of LVPC-S11.6%, which further proves the successful S-doping in carbon coated layer.^{S1,S2} Furthermore, compared with LVPC, because of the introduction of C-S bond, the C1s peak of LVPC-S11.6% also broadens obviously. **Fig. S3b** exhibits the high-resolution S2p spectrum of LVPC-S11.6%, there are three main peaks existed in that of LVPC-S11.6% at the binding energies of 163.6, 165.2 and 168.5 eV. Two fitted peaks at 163.6 (S1) and 165.2 eV (S2), respectively, are in agreement with the S2p_{3/2} and

 $S2p_{1/2}$ of the - S - C - S - covalent bond of the thiophene-S owing to their spin-orbit

couplings.^{S3,S4} The fitted peak at 268.5 eV (S3) should be assigned to the sulfate (-

C - SO₄ - C -) or sulfonate (- C - SO₃ - C -)^{S5-S7}. When carefully compared with S2p spectrums of LVPC-S11.1% and LVPC-S11.6% in Fig. 3b and Fig. S3b, respectively; the peak area of the fitted peak at 168.5 eV of LVPC-S11.6% is obviously larger than that of LVPC-S11.1%, which means with the increase of S doping amount in LVPC-S, the doping proportion of the sulfate (- C - SO₄ - C -) or

sulfonate (- C - SO₃ - C -) increased apparently. The existence of sulfate (-C-SO₄-

C–) and sulfonate (–C–SO₃–C–) will induce numerous O elements in carbon coated layer which make negative effects on the conductivity and electrochemical activity of carbon coated layer. As a result, the improvement of electrochemical properties will be limited. As a consequence, if S doping amount in the carbon coated layer is inadequate, the doping proportion of thiophene-S will insufficient, therefore, the modification effects of S-doped carbon coating on the electrochemical activity and conductivity of carbon layer will unobvious; On the other hand, if S doping amount in the carbon coated layer is excessive, lots of sulfate (–C–SO₄–C–) or sulfonate (–C–SO₃–C–) will existed in carbon layer, which will make negative effects on the electrochemical properties of LVPC-S samples. In other word, if the S doping amount in the carbon coated layer of Li₃V₂(PO₄)₃ is moderate, S-doped carbon coating approach can make the most positive effects on the electrochemical properties of Li₃V₂(PO₄)₃ cathode materials.

References

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