A full battery system of prelithiated phosphorus/sulfurized pyrolyzed poly(acrylonitrile) with safety and effective electrolyte

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Calculation of energy density

The Capacity is calculated based on the mass of the S in the S@PAN cathode in the Li_3P-S full cell. The average voltage in the full cell is selected as Voltage. So, the calculation of Energy density is based on the following equation:

Energy density = Capacity × Voltage = 720 mA h g^{-1}× 0.9 V = 648 Wh/kg

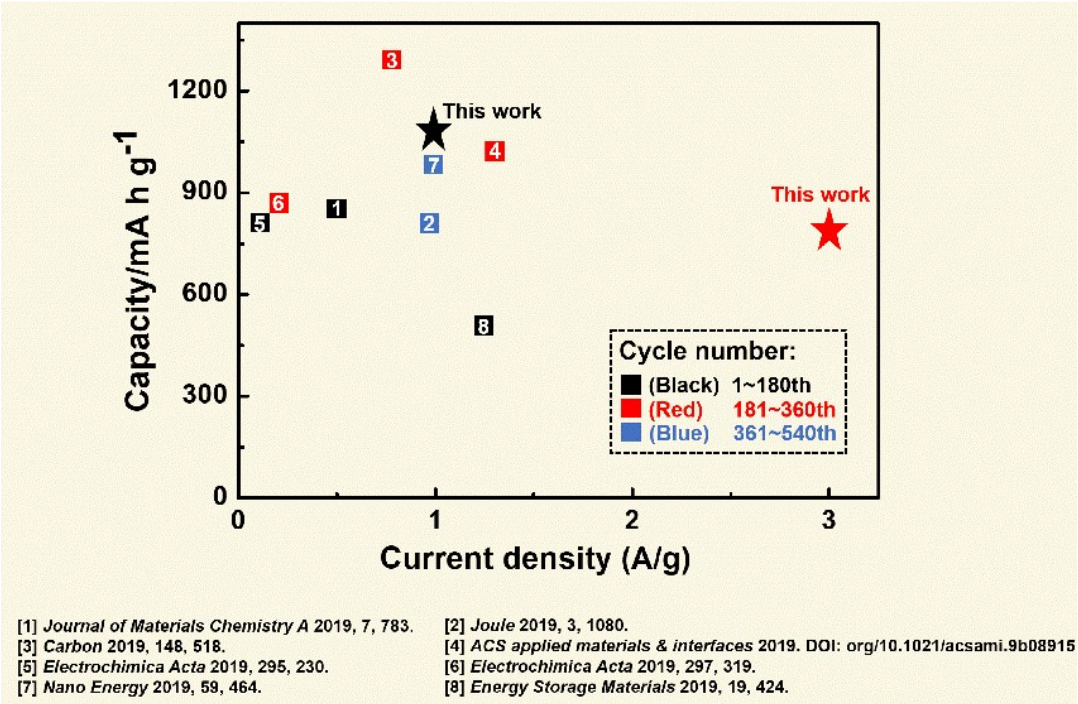

Figure S1 Cycling performance of this study was comparable with those of previous studies on P-based composite anodes.

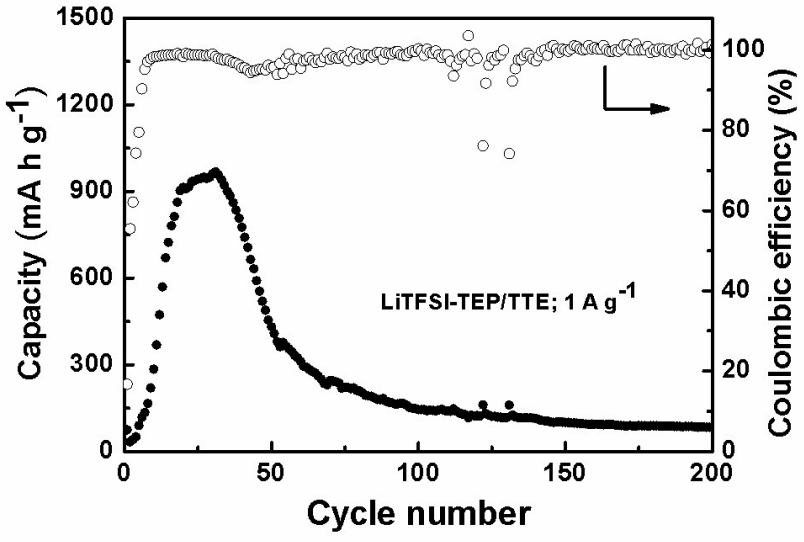

Figure S2 Cycle performance of RP/CNT composites in LiTFSI-TEP/TTE electrolyte at 1 A g^{-1}.

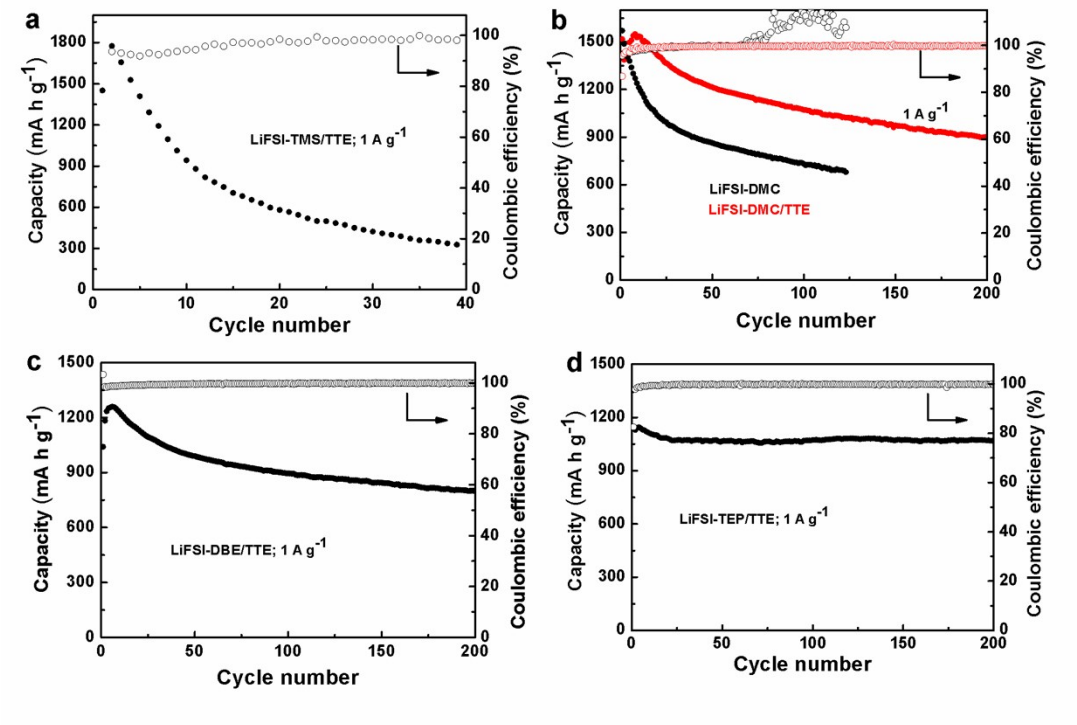

Figure S3 Cycle performance of RP/CNT composites in LIFSI-TMS/TTE, LIFSI-DMC/TTE, LIFSI-DBE/TTE and LIFSI-TEP/TTE at 1 A g^{-1}.

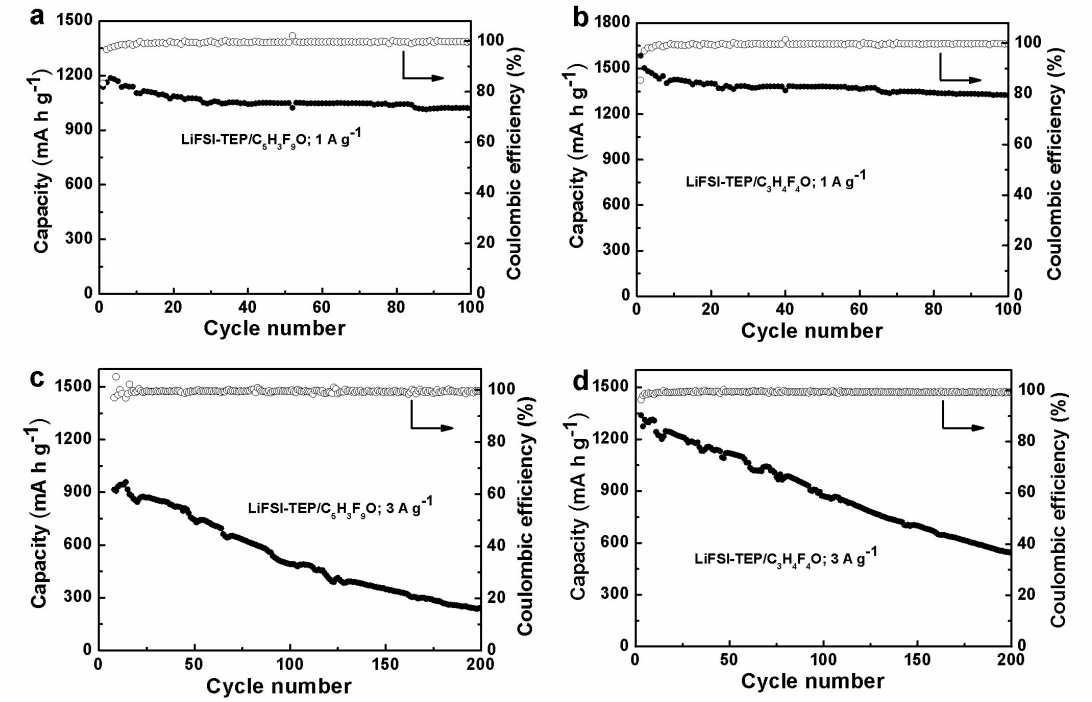

Figure S4 a) Cycle performance of RP/CNT anode in LiFSI-TEP/$C_5H_3F_9O$ electrolyte at 1 A g^{-1}. b) Cycle performance of RP/CNT anode in LiFSI-TEP/$C_3H_4F_4O$ electrolyte at 1 A g^{-1}. c) Cycle performance of RP/CNT anode in LiFSI-TEP/$C_5H_3F_9O$ electrolyte at 3 A g^{-1}. d) Cycle performance of RP/CNT anode in LiFSI-TEP/$C_3H_4F_4O$ electrolyte at 3 A g^{-1}.

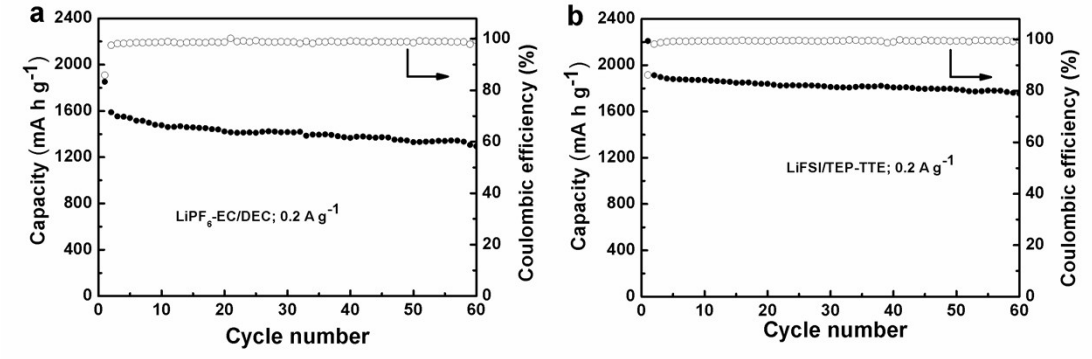

Figure S5 Cycle performance of RP/CNT composites in $LIPF_6$-EC/DEC and LIFSI-TEP/TTE electrolytes at 0.2 A g^{-1}.

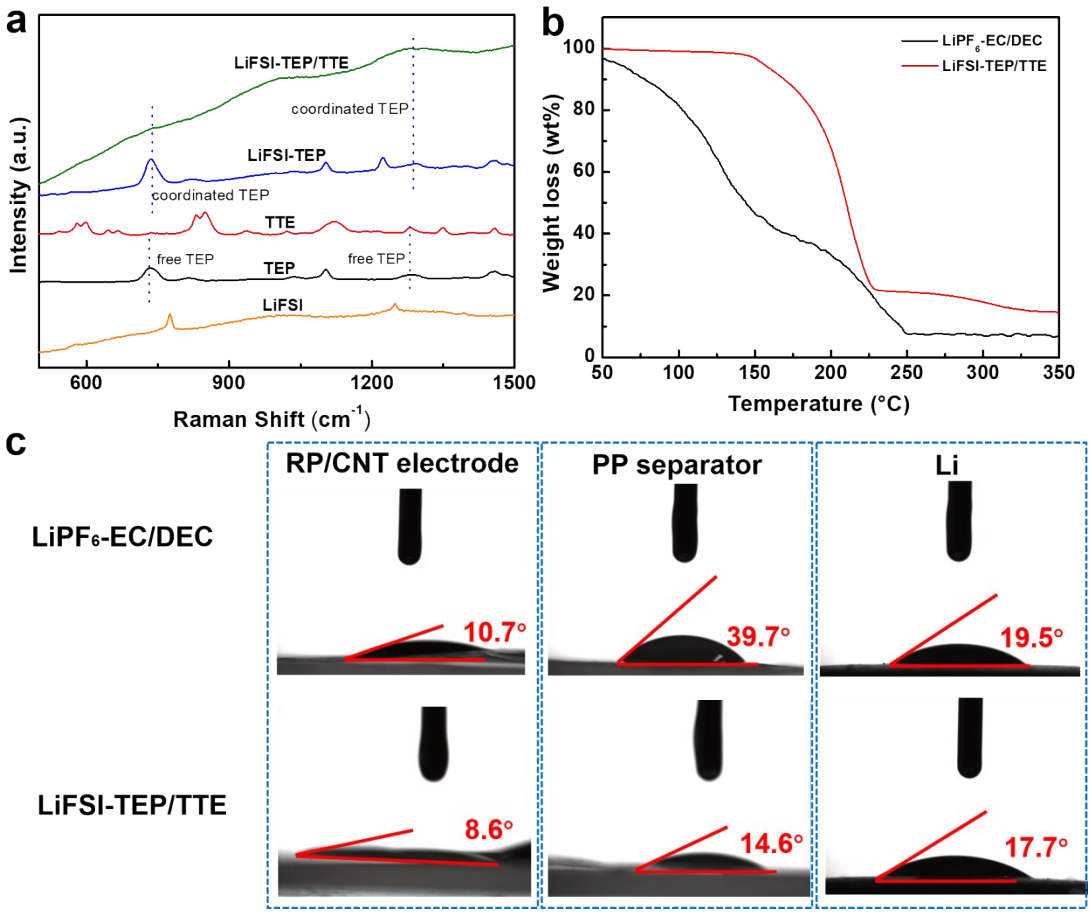

Figure S6 a) Raman spectra of LiFSI, TEP, TTE, LiFSI-TEP and LiFSI-TEP/TTE electrolytes. b) TG analysis of $LiPF_6$-EC/DEC and LiFSI-TEP/TTE electrolytes. c) Contact angles of $LiPF_6$-EC/DEC and LiFSI-TEP/TTE electrolytes.

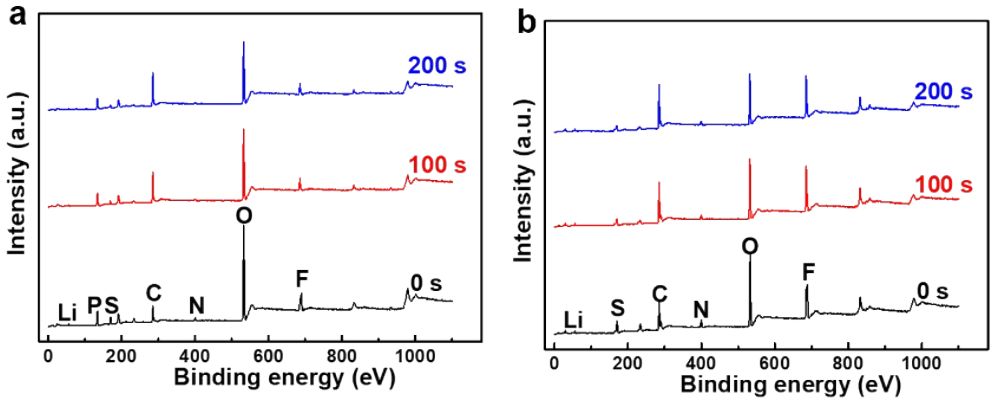

Figure S7 XPS full survey spectra of P anode and S cathode with different etched time.

Table S1 Comparison of the $LiPF_6$-EC/DEC and LiFSI-TEP/TTE electrolytes based on the environmental impacts, physicochemical and electrochemical properties.

Composition of electrolytes	**Melting/boiling point (°C)**	**Flammability**	**Dielectric constant (°C)**	**Wettability**	**Compatibility with P anode and S cathode**
$LiPF_6$-EC/DEC (1:1 volume ratio)	-43/127 for DEC 37/128 for EC	Yes	31.1 for DEC 160 for EC	Good	Bad
LiFSI-TEP/TTE (1:3 volume ratio)	-56/220 for TEP -97/93 for TTE	No	117 for TEP	Good	Good

Table S2 Summary of the contributions of solvation sheath structure and LiFSI salt in LiFSI-TEP/TTE electrolytes.

Composition of electrolytes	**Molar number and LUMO value of $[Li\text{-}4TEP]^+$ solvation structure**	**Molar number and LUMO value of LiFSI salt**
LiFSI-TEP/TTE	$0.72*10^{-3}$ mol	$1.28*10^{-3}$ mol

-2.806 eV	-1.947 eV