Toward a Better Understanding of the Surface Effect through the Design of Binders in Lithium Sulfur Batteries

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Abstract

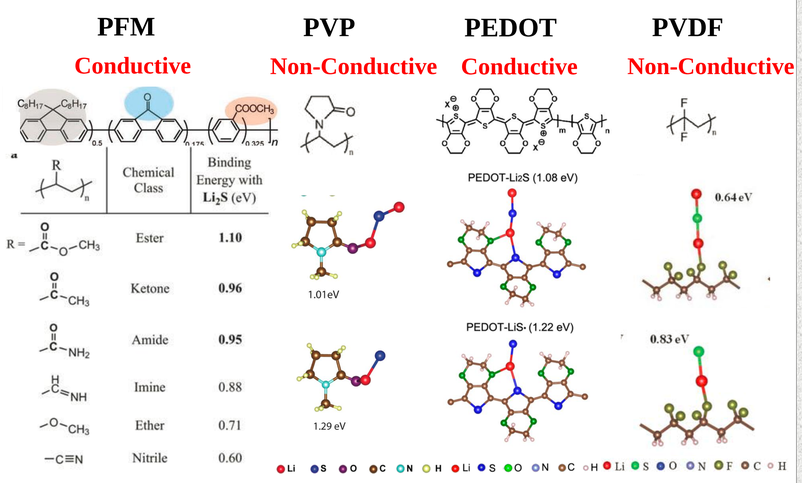
Sulfur species dissolution and phase transformation during the charge and discharge process strongly affect the performance of lithium sulfur (Li-S) batteries. Interface properties play an important role in these batteries. In this work, four kinds of binders with different chemical and electrical properties were employed to study how the interface properties affected the battery reaction mechanism. The phase transformation of sulfur species was studied in detail. Remarkable differences were observed among cathodes with different binders. More solid-phase sulfur precipitation was observed with binders that have carbonyl functional groups, like poly(9, 9-dioctylfluorene-co-fluorenone-co-methylbenzoic ester) (PFM) and poly(vinylpyrrolidone) (PVP), in both fully charged and discharged states. Also, the improved conductivity from introducing conductive binders greatly promoted sulfur species precipitation. These findings suggest that the contributions from functional group affinity and binder conductivity lead to more sulfur transformation into the solid phase, so the shuttle effect can be greatly reduced, and a better cell performance can be obtained.

Experimental

- ❑Electrode composition: sulfur: binder: AB=50:10:40 (wt.%)
- ❑Sulfur loading: 0.3 mg/cm^2
- ❑Electrolyte: PEGDME+1M LiTFSI+1 wt.% $LiNO_3$
- ❑Cell type: 2325 coin cell
- ❑Electrochemical test instrument: Maccor series 4000

Results and Discussion

1. Different affinity between Li_xS and Binder

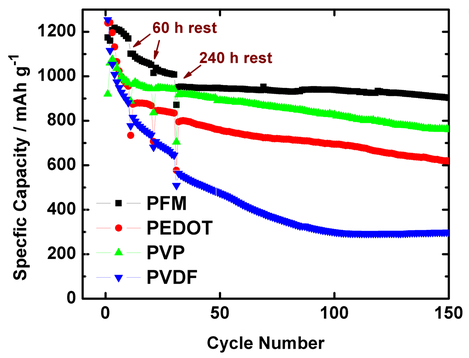


Calculation data source: Li et al., Nano Letters, 2013; Zheng et al., Nano Letters, 2013

- ➢Comparison between the performance of PFM-S and PVP-S can show the surface modification effect of conductive binder, when they both has carbonyl group.
- ➢Comparison between the performance of PFM-S and PEDOT-S can provide information about the effect of function group and their binding affinity with Li_xS ($0<x\leq2$).

2. Cycling and self-discharge performance of cathodes with different binders

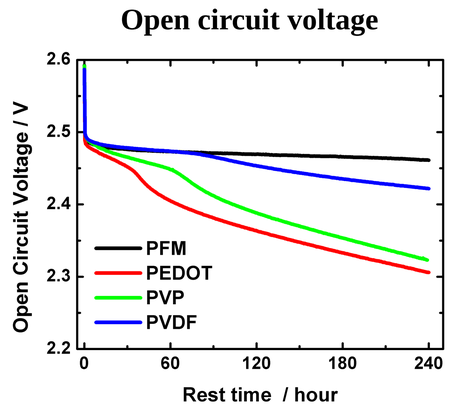
2.1 Cycling and self-discharge performance



Test Procedure:
10 cycle C/10
+ self-discharge 60h
+ 10 cycle C/10
+ self-discharge 60h
+ 10 cycle C/10
+ self-discharge 240h

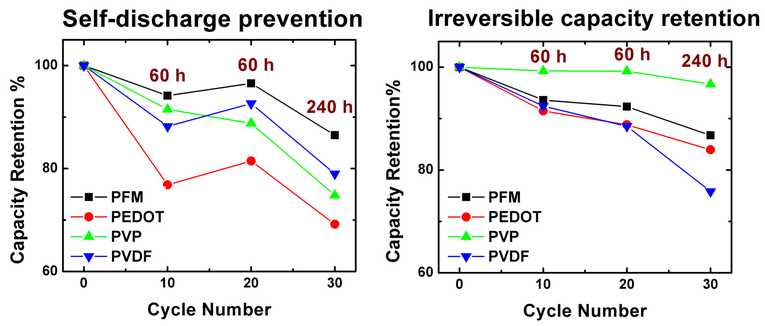
Self-discharge are done at fully charge state.

2.2 Open circuit voltage change during self-discharge test

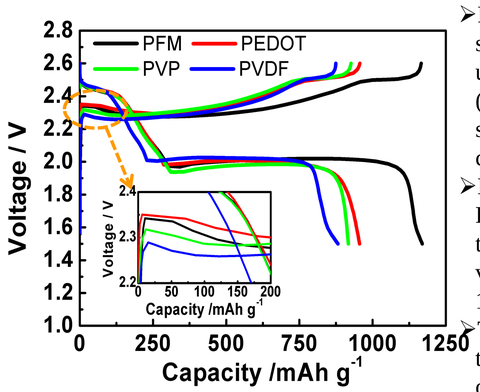


- ➢ The open circuit voltage was closely related to the sulfur species in fully charged state and their reaction activity.
- ➢ The voltage drop indicated that some chemical reactions occurred spontaneously during the rest in fully charged state.
- ➢ PFM has positive effect in eliminating this effect.

2.3 Self-discharge data analysis



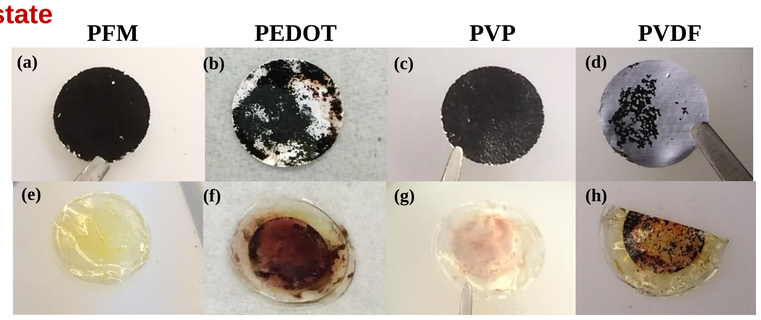
2.4 Voltage profile of electrode with different binder



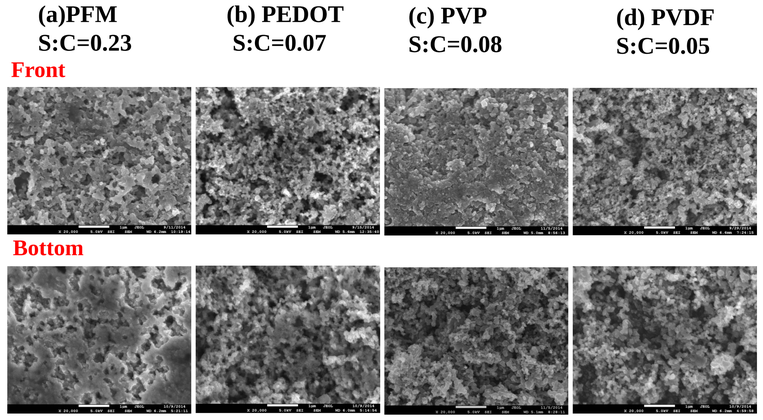
- ➢PFM-S and PVP-S showed the same discharge capacity in the upper voltage plateau region (2.6 V- 1.95 V) indicating the same amount of S_8/Li_2S_8 changed into dissolved state.
- ➢More capacity was obtained by Li_2S precipitation in PFM-S than in PVP-S in the lower voltage plateau region (1.95 V-1.5 V).
- ➢This can provide evidence of the surface modification effect of conductive binder.

3. Post-test analysis of the Li-S batteries

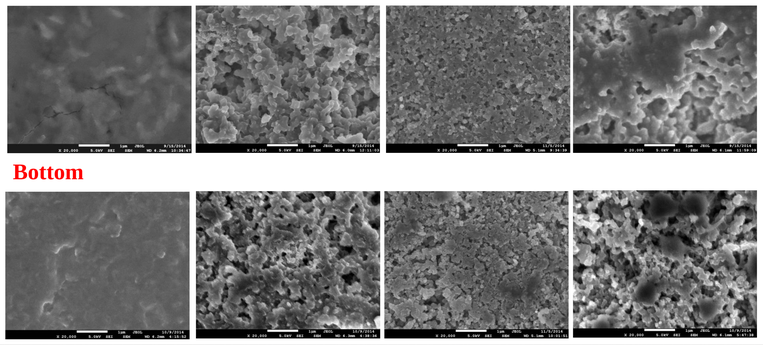
3.1 Photo images of electrode and separator in fully charged state



3.2 Electrode morphology and EDX in fully charged state



3.3 Electrode morphology and EDX in fully discharged state



CONCLISION

- **Binders with carbonyl groups (PFM and PVP) can provide preferred surface for sulfur species precipitation.**
- **The conductive binders can provide the largest surface area for reactions to take place.**

REFRENCES

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ACKNOWLEDGMENTS

Funding support: Exploratory Battery Materials Research (BMR) program

LBL colleagues: Ying Bai, Wen Yuan, Zhe Jia, Jinglei Lei, Na Lin. Guo Ai is supported by the China Scholarship Council Fellowship.