

Supporting Information

Inverse Vulcanization of a Natural Monoene with Sulfur as Sustainable

Electrochemically Active Materials for Lithium-Sulfur Batteries

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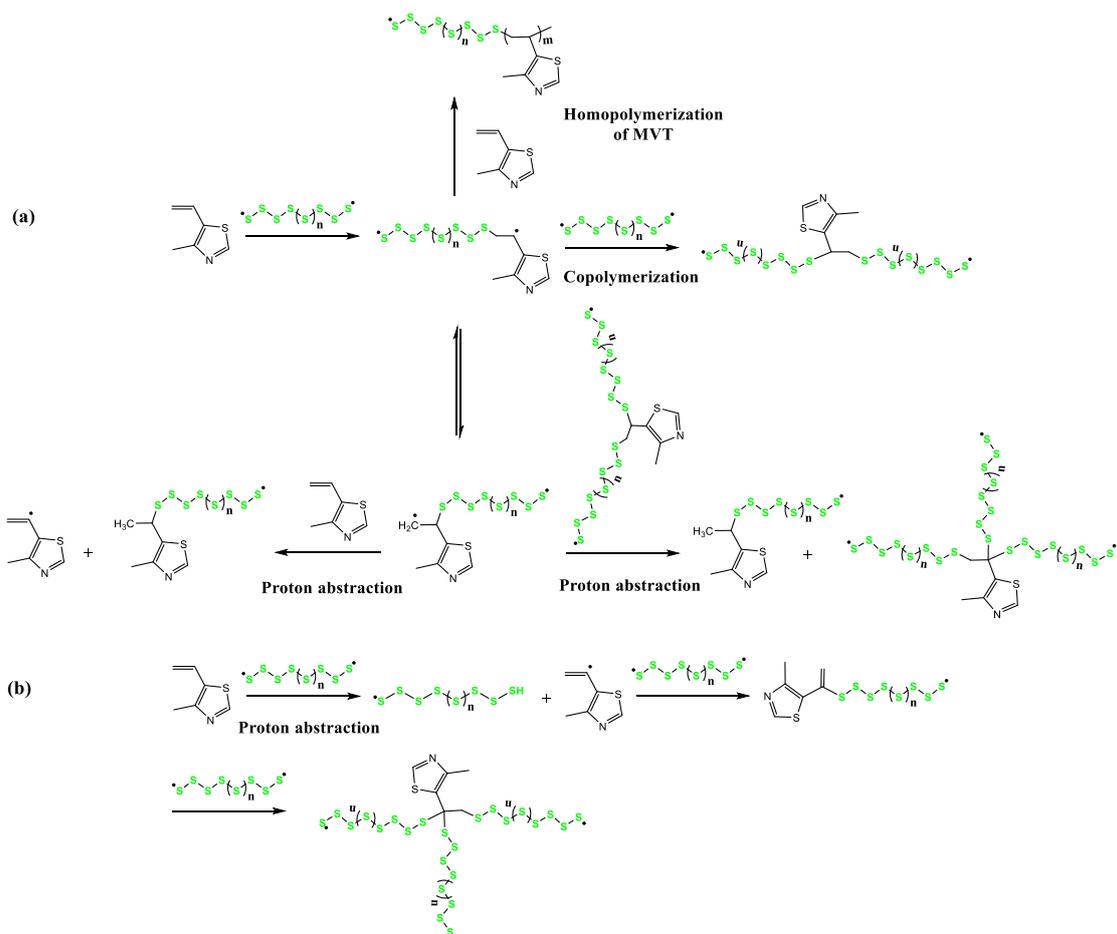


Figure S1 Proposed polymerization mechanism for poly(S-MVT) copolymer.



Figure S2 Photographs of poly(S-MVT) with different MVT content, MVT content stated above.

In order to test the solubility of the copolymer, we selected poly(S-MVT)s with MVT content of 10%, 30%, and 50% for testing. As shown in Figure S2, all the three poly(S-MVT)s have good solubility in THF and chloroform but can only partially dissolve in CS₂.



Figure S3 Photographs of poly(S-MVT)s in CS₂, THF and chloroform, MVT content stated above.

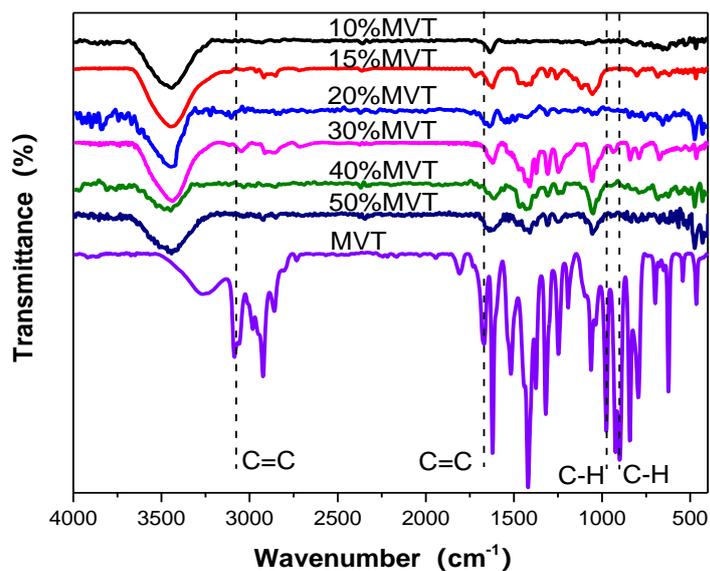


Figure S4 FT-IR spectra for MVT and all poly(S-MVT)s at different MVT content, MVT content stated above.

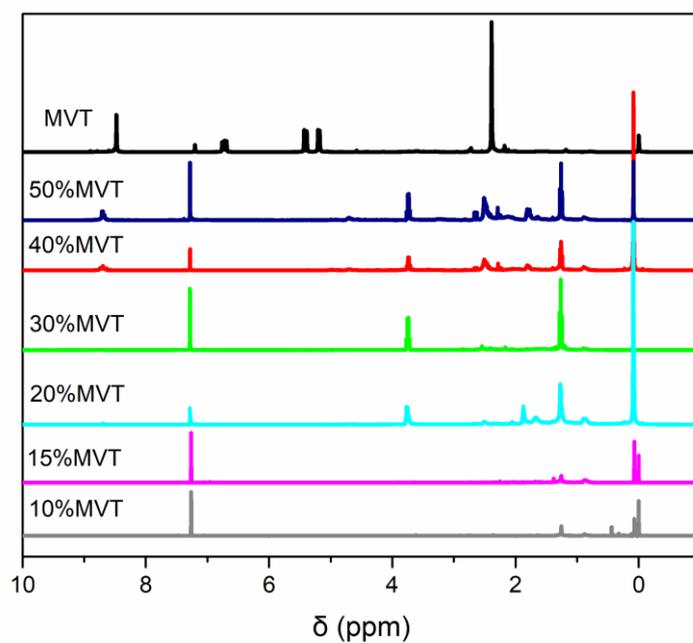


Figure S5 HNMR spectra for MVT and all poly(S-MVT)s at different MVT content, MVT content stated above.

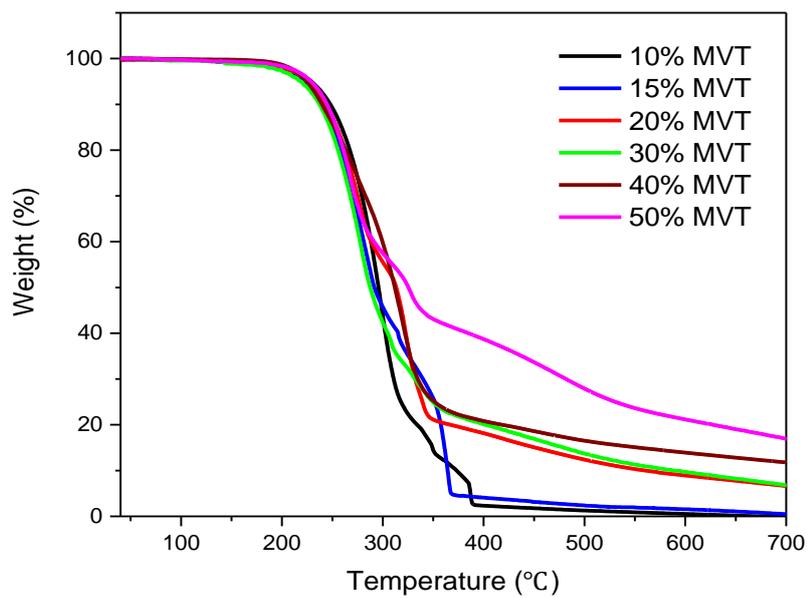


Figure S6 TGA curves of poly(S-MVT)s with different MVT content.

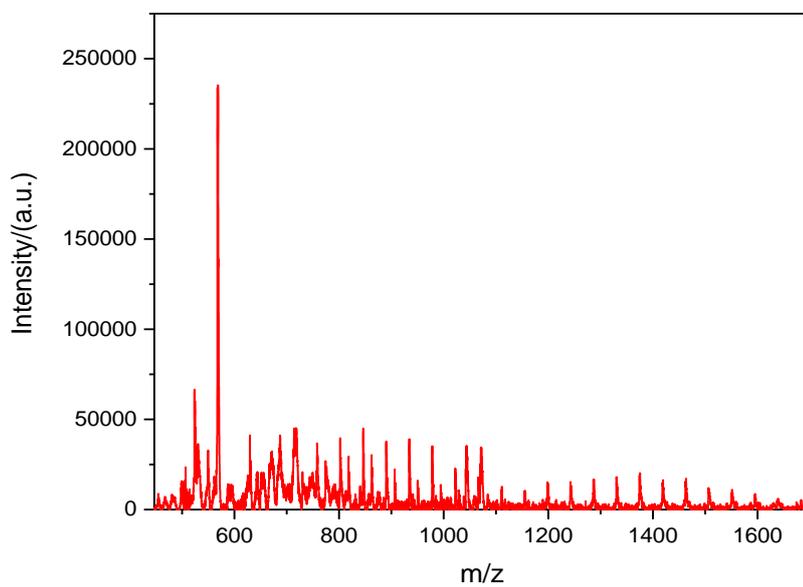


Figure S7 MALDI-TOF MS spectrum of poly(S-MVT) (50% MVT).

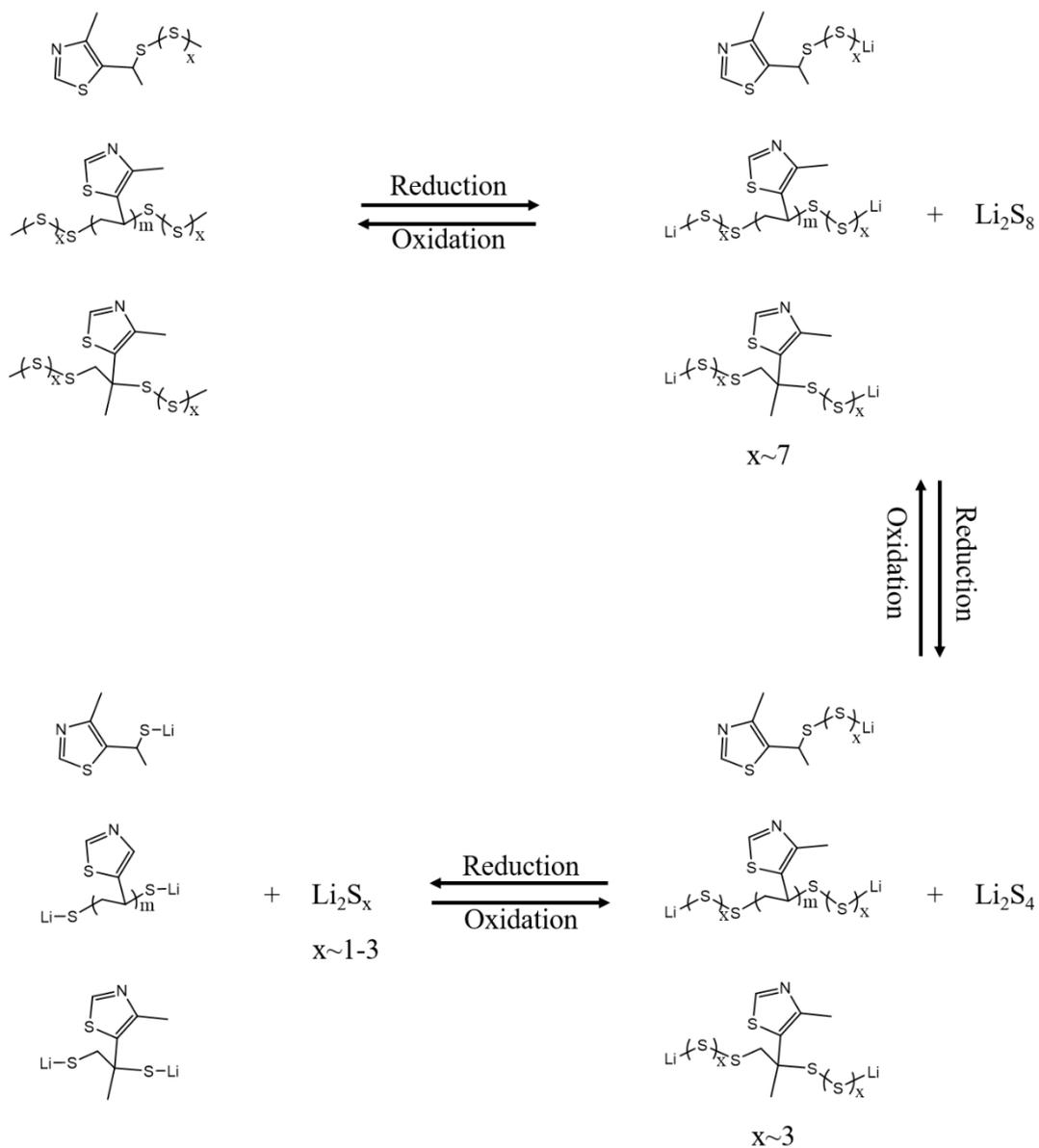


Figure S8 The possible electrochemical reactions of the poly(S-MVT) based cathode.

Table S1 Characteristics and electrode performance comparison of the present work with the recently reported literature.

| Sulfur-containing polymers | Monomer | Renewable/ Sustainable | electrode performance | Reference |
|-------------------------------------------------------------------------------------------------------------------------|-----------------------------------------|---------------------------|----------------------------------------------------------------------------------------------------------|-----------|
| poly(S-co-EAE) | eugenol allyl ether | Yes | 557 mAh g ⁻¹ based on S after 100 cycles at 0.1C | [1] |
| SVOCs | vegetable oil | Yes | 554 mAh g ⁻¹ based on S after 100 cycles at 0.1C | [2] |
| Si-69 (C ₉ H ₂₁ O ₃ SiS ₄ SiO ₃ H ₂₁ C ₉) | None | No | 163 mAh g ⁻¹ even after 200 cycles at 0.2 Ag ⁻¹ | [3] |
| poly(S-Sty-P) | styrene-peanut oil | No | 611 mAh g ⁻¹ based on S after 100 cycles at 0.2C | [4] |
| poly-(S-r-p)p | hexakis(styrene oxy)cyclotriphosphazene | No | 350 mAh g ⁻¹ based on S after 100 cycles at 0.5C | [5] |
| poly(S-MVT) | 4-Methyl-5-vinylthiazole | Yes | 514 mAh g ⁻¹ based on copolymer (605 mAh g ⁻¹ based on S) after 100 cycles at 0.1C | This work |

[1] A. Hoefling, T.N. Dan, Y.J. Lee, S.W. Song, P. Theato. A sulfur–eugenol allyl ether copolymer: a material synthesized via inverse vulcanization from renewable resources and its application in Li–S batteries. *Mater. Chem. Front.* 2017, 1,1818.

[2] Yamabuki, K., Itaoka, K., Shinchi, T., Yoshimoto, N., Ueno, K., Tsutsumi, H.. Soluble sulfur-based copolymers prepared from elemental sulfur and alkenyl alcohol as positive active material for lithium-sulfur batteries. *Polymer* 2017, 117: 225-230.

[3] Xing, C., Xue, P., Gu, X., Lai, C.. Communication—Organic Silane Coupling Agent Si-69: A New Organosulfur Cathode Material for Rechargeable Lithium Batteries. *J. Electrochem. Soc.* 2018, 165(16):A3782-A3784.

[4] Wang, J. and Zhang, S. A Novel Sulfur-Based Terpolymer Cathode Material for Lithium–Sulfur Battery. *Energy Technol.* 2020, 8(5), 2000057.

[5] Serkan Yeşilot, Sedat Küçükköylü, Emrah Demirb, Rezan Demir-Cakan. Phosphazene based star-branched polymeric cathode materials via inverse vulcanization of sulfur for lithium–sulfur batteries. *Polym. Chem.* 2020, 11, 4124-4132.