Developing Thermo-Responsive Coatings for Enhanced Battery Safety: Assessment and Routes to Sustainable Solutions

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INTRODUCTION AND MOTIVATION

A multifunctional coating was designed as a safety solution for batteries, providing an early warning system for overheating events. To achieve longer lifespans and sustainability, a covalent adaptive network (CAN) was introduced and a recycling method was evaluated.

i. **Thermo-responsiveness**: A tracer gas (TG) is incorporated into a polymer matrix using covalent bonds forming thiourethane bonds. When triggered, the coating releases the TG which can be detected by metal oxide (MOx) sensors.

ii. **Recyclability**: The coating composition is controlled to achieve a low crosslink-density, allowing it to be dissolved in a polar solvent after releasing gas. This enables the reintegration of additional TG and increases the cycle life of the coating.

iii. **Reprocessability**: Disulfide bonds, known for their dynamic properties, are added to the coating to form the CAN, allowing the polymer architecture to be rearranged under external stimuli.

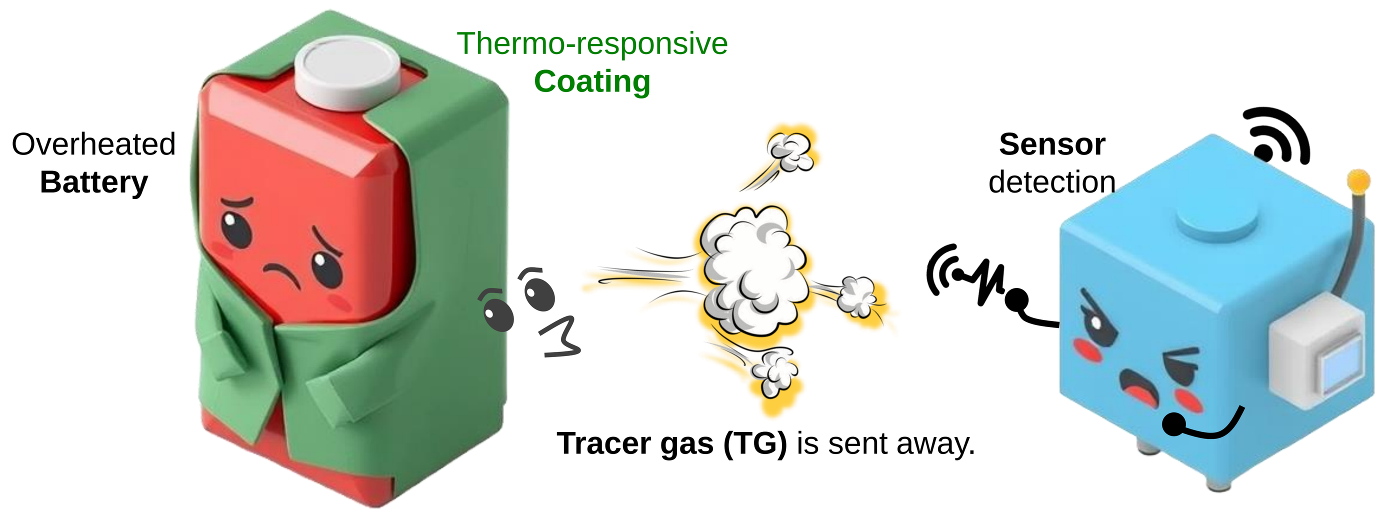
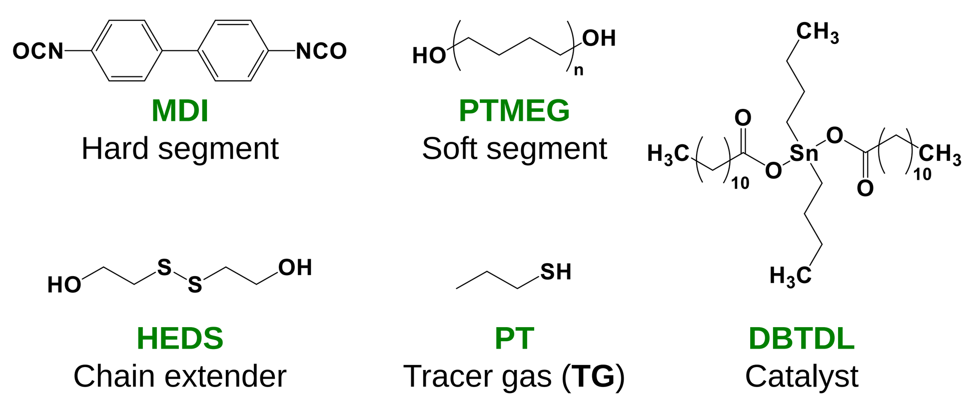


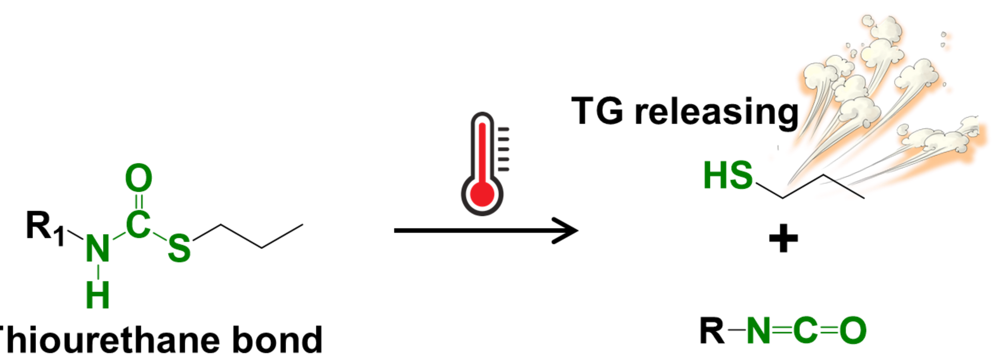
Figure 1: The thermo-responsive property of the coating and working mechanism of safety process. [1]

RESULTS AND DISCUSSION

I. Polyurethane / Polythiourethane coating chemistry and working mechanism



Scheme 1: Coating components



Scheme 2: TG releasing mechanism

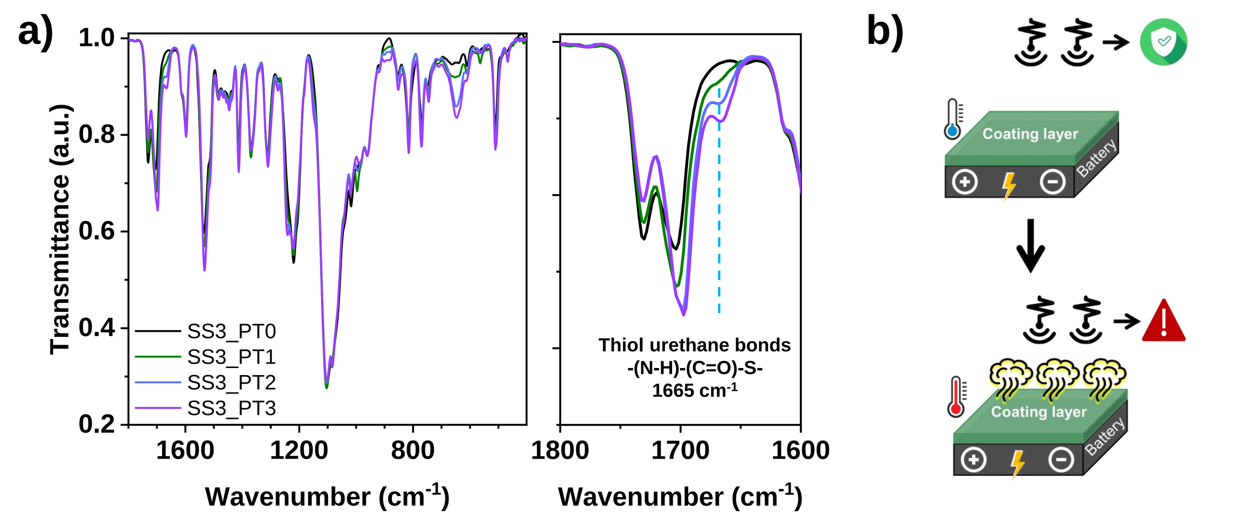


Figure 1: a. FTIR curves for coatings with different TG content; **b.** Working mechanism of thermoresponsive coatings

II. Gas releasing behaviour

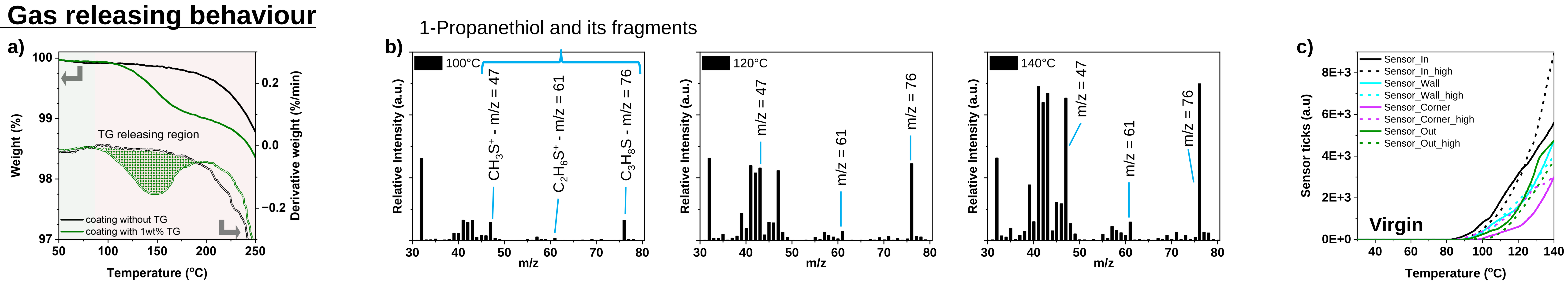
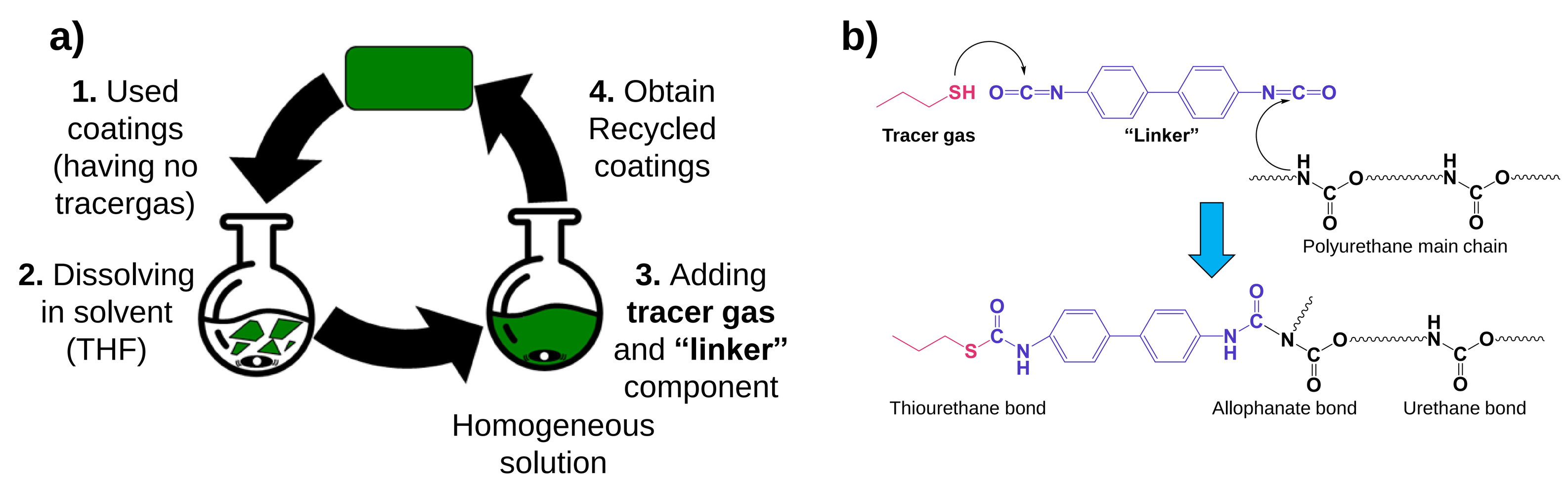


Figure 2: a. TGA and DTG curves of coating with and without TG; **b.** Evolved gas analysis – Mass spectrometer (EGA-MS) mass spectra of outgassed components from SS3_PT1 coating (containing 1wt% of TG); **c.** Sensor test results for virgin coating.

III. Recyclability of the coating after releasing gas



Scheme 3: a. Recycling process for the coating after releasing TG; **b.** Recycling chemistry, the formation of new thiourethane and allophanate bonds.

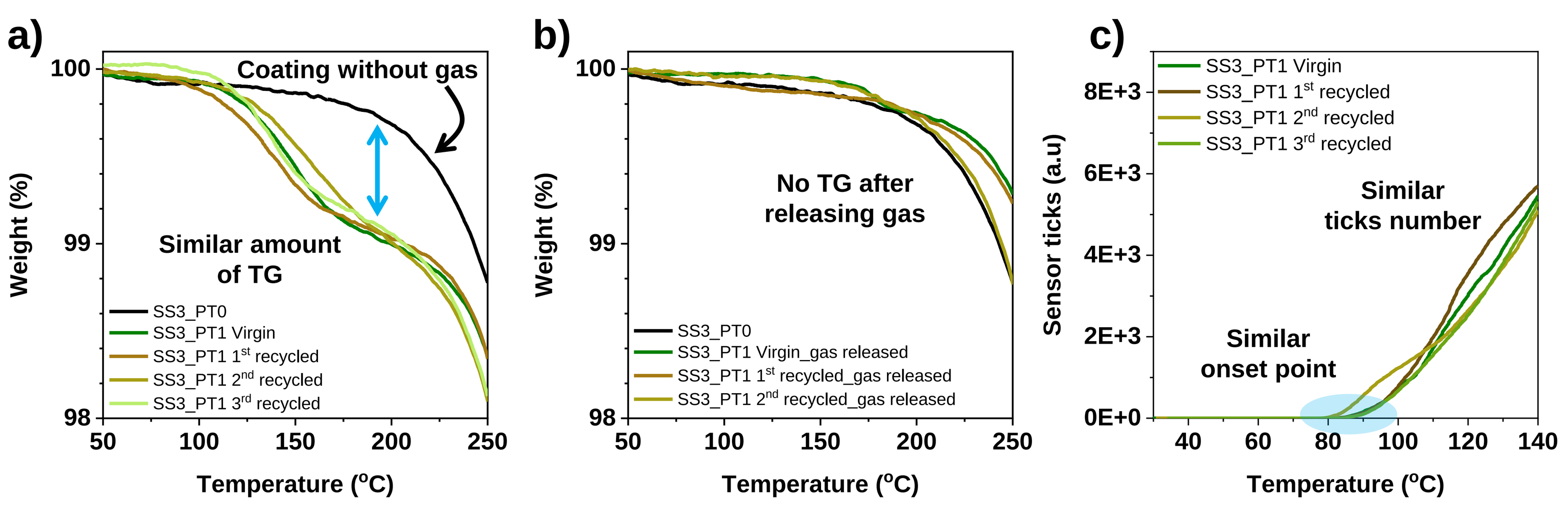
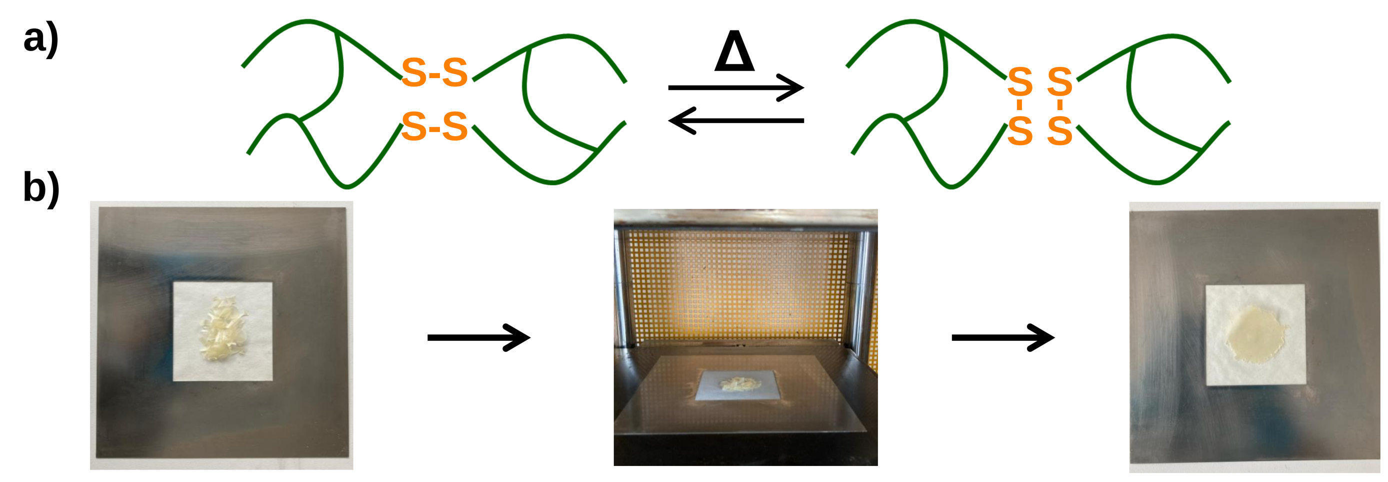
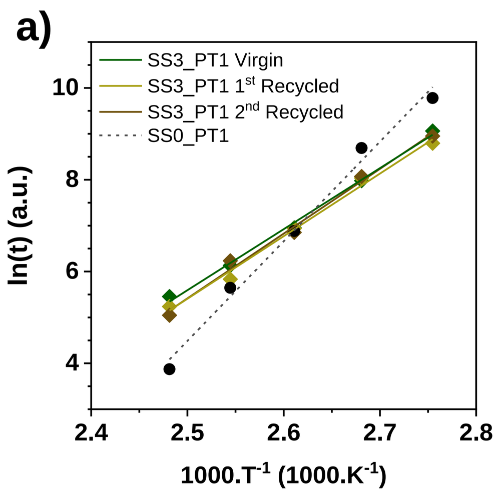


Figure 3: a,b. TGA and DTG curves for virgin and recycled coatings; **c.** Sensor test results from Sensor_In for virgin and recycled coatings.

IV. Reprocessability of the coating after releasing gas



Scheme 4: a,b. Disulfide metathesis and reprocessing process for the coating after releasing TG.



b)

Sample	R^2	E_a (kJ/mol)
SS3_PT1 Virgin	99.58	110.52
SS3_PT1 1st recycling cycle	99.16	113.34
SS3_PT1 2nd recycling cycle	99.16	117.23
SS0_PT1	99.03	180.42

- Disulfide bonds, as switchable dynamic bonds, are benifitial for lowering activation energy.

Figure 4: a. Arrhenius plotting based on stress relaxation behaviour of SS3_PT1 virgin and recycled coatings compared with SS0_PT1, coating without S-S bonds; **b.** Summary table.

CONCLUSIONS

In this work, a novel coating for battery safety is reported, based on its thermoresponsive properties. A tracer gas (TG) can be released from the coating and detected by sensors, enabling an early warning by battery users. Qualitative and quantitative analyses were performed to confirm the presence and amount of TG in the coating, as well as its releasing behavior, using ATR-FTIR, TGA, and EGA-MS.To enhance sustainability and reduce environmental impact, the recycling process of the coating was investigated. Its effectiveness was evaluated using TGA and sensor tests, demonstrating that a comparable amount of TG can be reintroduced into gas-depleted coatings, and that recycled coatings perform similarly to virgin ones. Furthermore, the reprocessability of the coating after releasing gas and the role of disulfide bonds were supported by stress relaxation studies and practical tests.

Reference: [1] https://deepai.org/

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