

## Project Overview

- Project Goal:** Development of larger area temperature monitoring system for ESS safety.
- Current Practice:** ESS uses thermocouples to monitor battery temperature, but it is challenging to monitor the temperature of every single cell in a bank of thousands of batteries for overheating.
- Why ORNL:** ORNL has expertise in synthesizing materials, slurry development, and 20 years of thermal runaway battery testing experiences.
- Innovation:** Developing temperature sensitive paint that provides early detection of thermal runaway by releasing a detectable gas at lower temperatures. Using chemical specific sensors, an early warning signal can be generated and can offer extensive signal coverage.
- Impact:** The paint can be utilized in ESS, electric vehicles, basically every place that Li-batteries are used. This paint offers an additional safety layer for users/consumers, alerting possible thermal runaway events before a failure occurs, thereby allowing sufficient time to implement a mitigation plan.
- Alignment:** Safety and reliability are the most concerning issues in any ESS. This effort aligns OE and DOE's mission to maintain a reliable power grid.

## Existing issue

- Thermal runaway is the most reported safety issue of Li-ion batteries in ESS.<sup>1</sup>
- It is challenging to monitor the temperature of every single cell in a bank of hundreds and thousands of batteries.
- Battery failure usually starts from a hot spot in a single cell, which presents an impossible task to use temperature sensors effectively.<sup>2</sup>
- The batteries may continue to overheat without flames, leading to a thermal runaway event slowly over time.
- ESS needs a large-area temperature monitoring system.

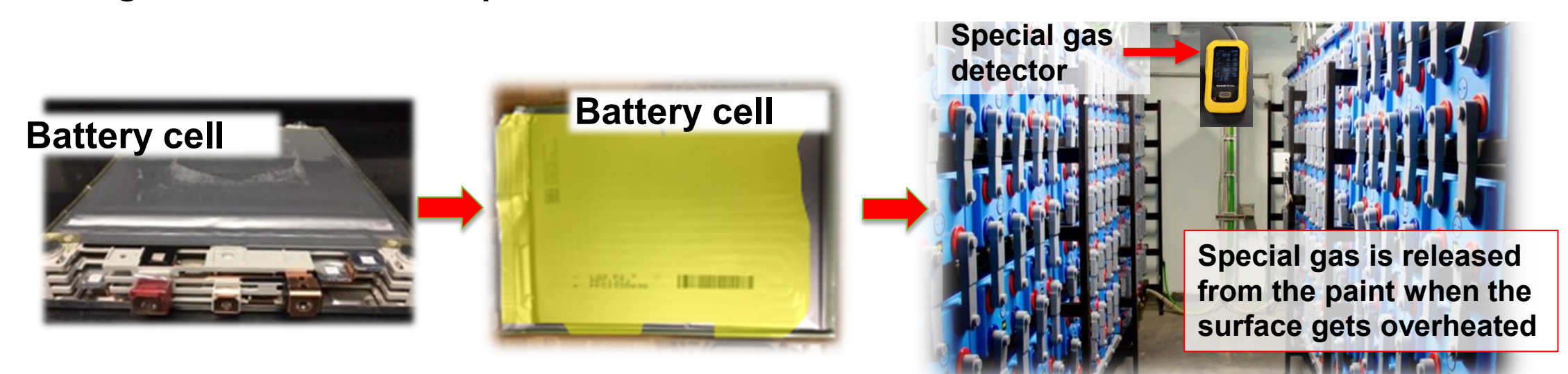


## Potential solution

- A temperature-sensitive paint: The low-cost paint can be applied to every cell and cover all surfaces for an ESS.

## Our approach

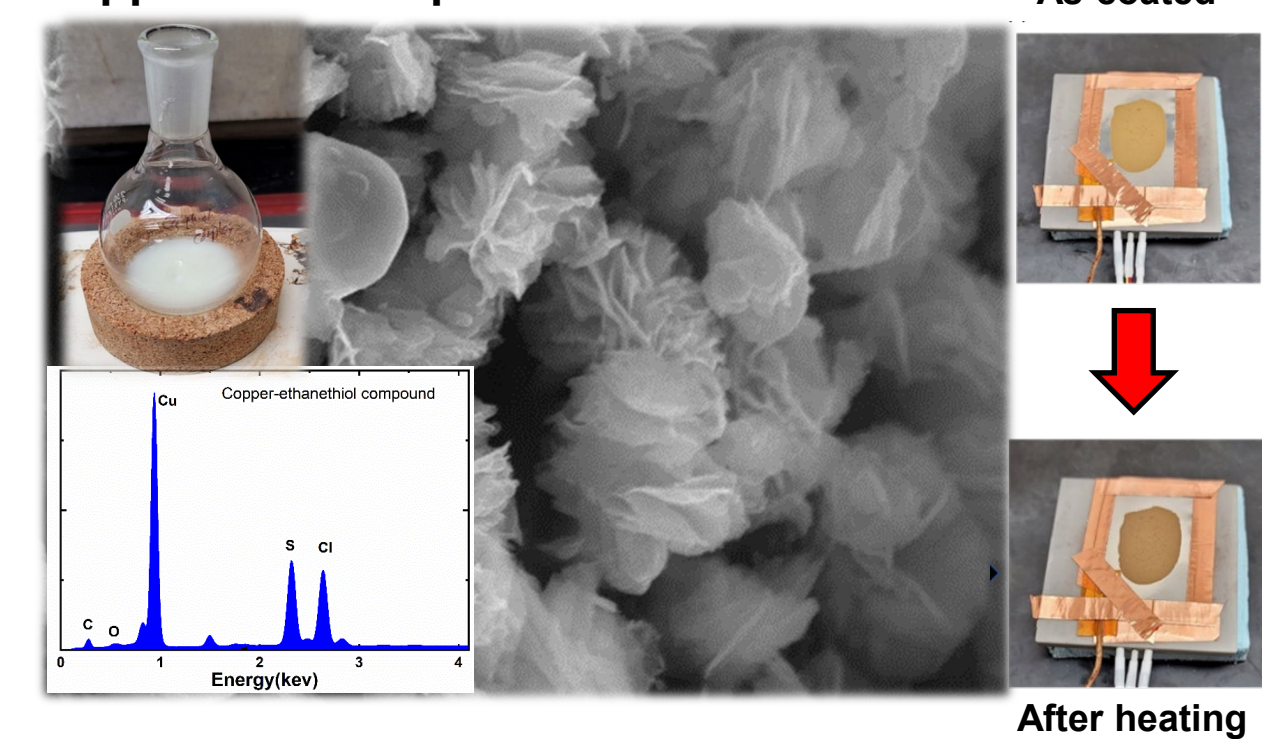
- Entrap/attach molecules (e.g., thiols) in larger molecules designed to release the gas when a specific threshold temperature is reached.<sup>3</sup>
- A special gas detector placed to sense and alarm if the designated molecule is detected.
- Fundamental understanding and identifying the gas species released by thermal sensitive compounds to determine the right gas sensor for specific compounds.
- Understanding of metal, sulfur and hydrocarbon reactivity and thermal decomposition pathways to tune the compounds onset gas release temperatures.



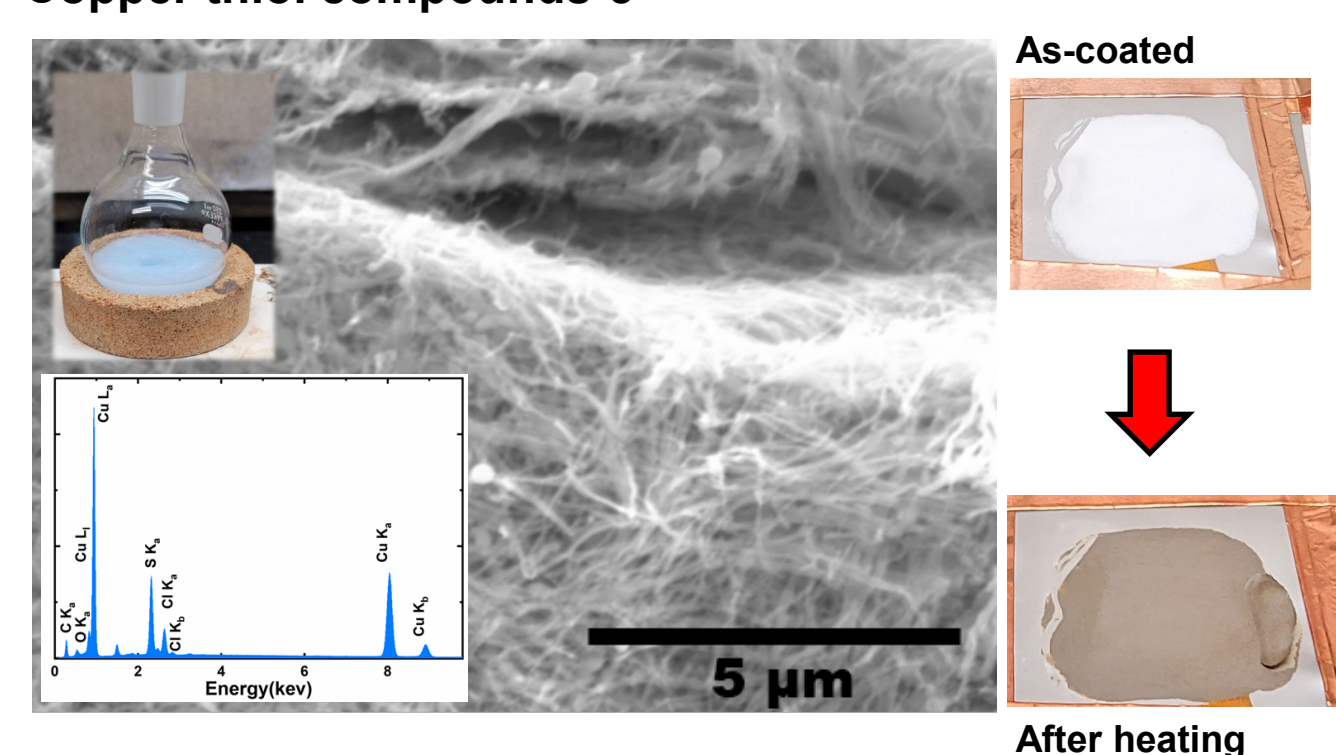
## Methods

### Thermal-sensitive compounds synthesis and characterization

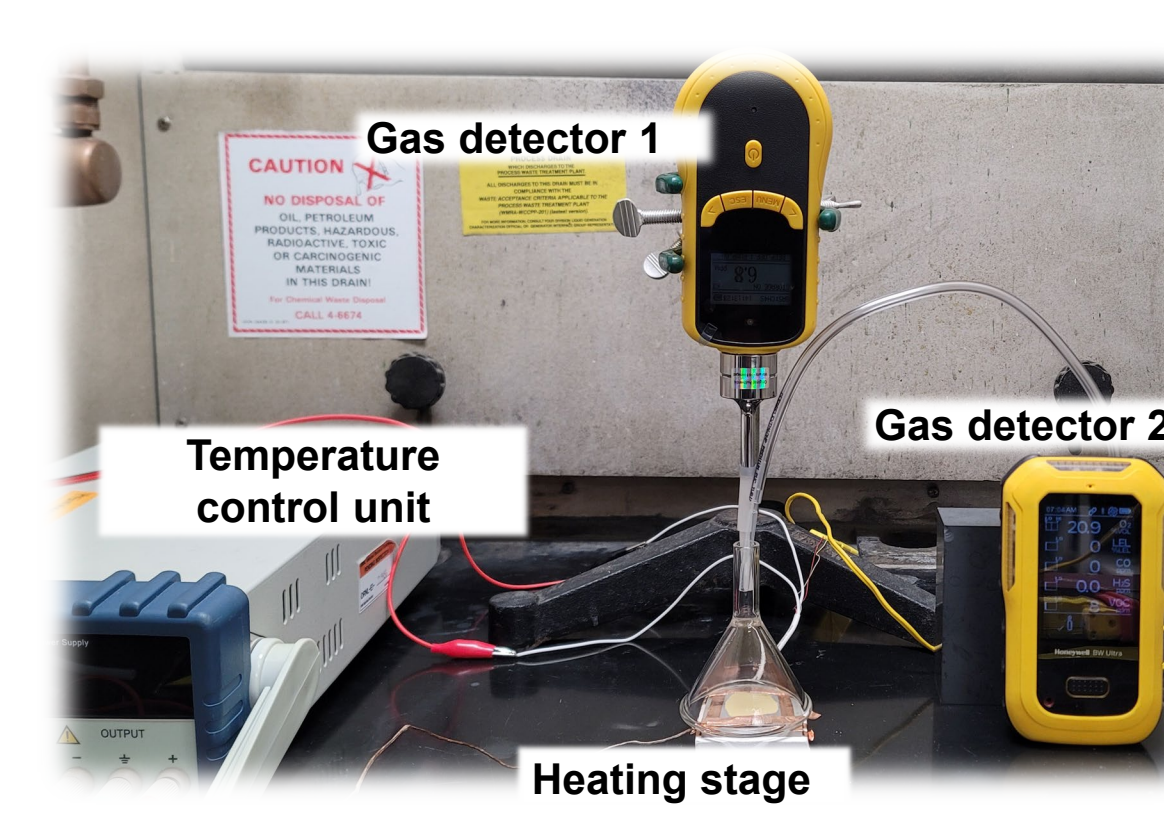
#### Copper thiol compounds-1



#### Copper thiol compounds-3



### Thermal runaway simulation setup



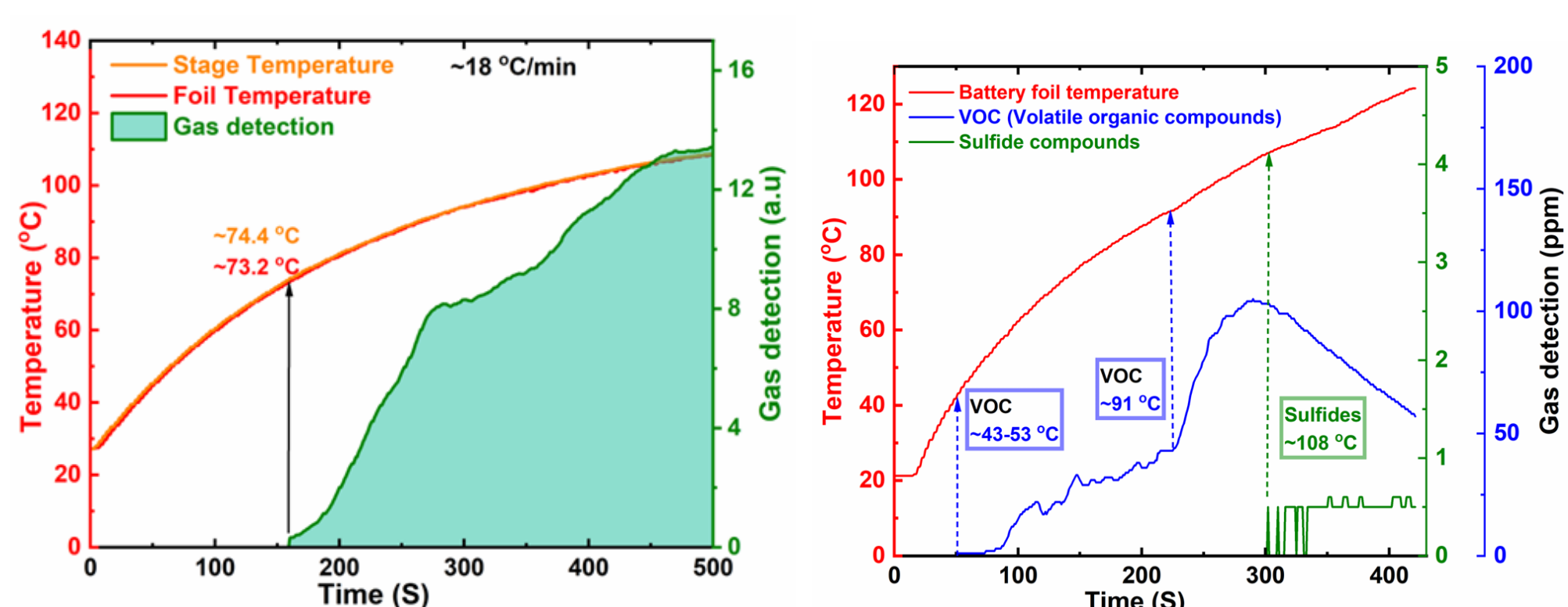
### The onset of gas release temperature can be tuned

Copper-thiol compound	Onset gas released temperature (°C)
Compound - 1	72-75
Compound - 2	84-96
Compound - 3	120-127
Compound - 4	152-163
Compound - 5	172-174



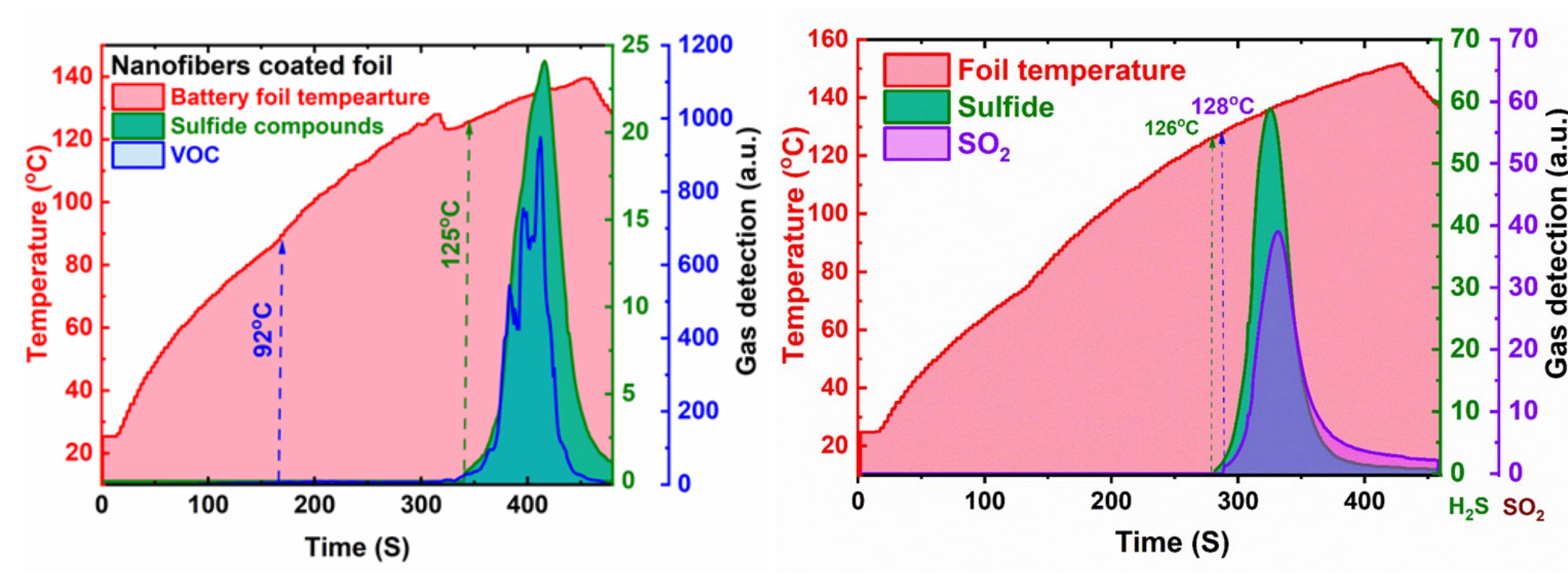
## Results

### Copper-thiolate compound-1



Onset gas release temperature  
Mercaptan: 73-78 °C / VOC: 53 °C / Sulfide: 115-120 °C

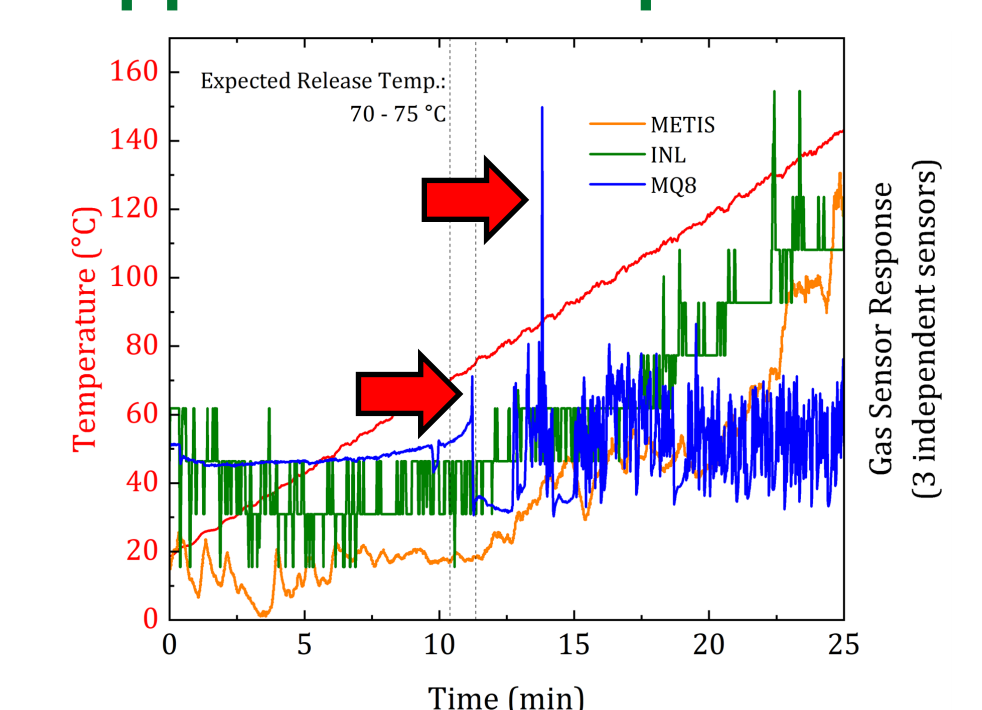
### Copper-thiolate compound-3



Onset gas release temperature :  
Mercaptan : 120-125 °C / VOC: 117 °C / Sulfide: 125-127 °C / SO<sub>2</sub> : 128 °C

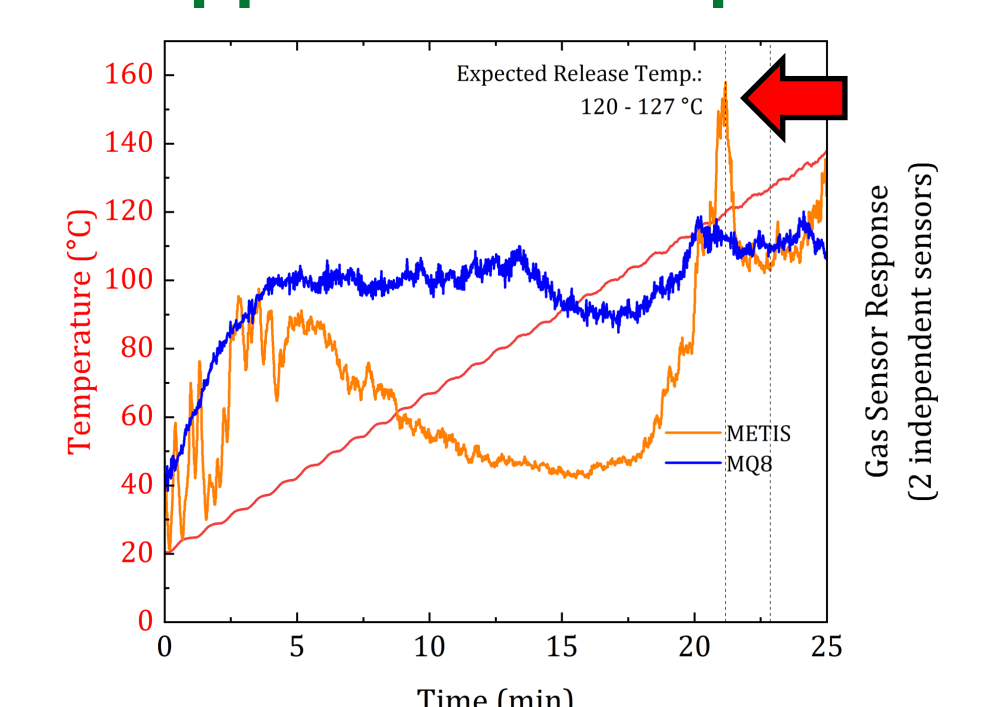
### Collaboration with SANDIA National Laboratory: Alex Bates and Loraine Torres-Castro

#### Copper-thiol compound-1



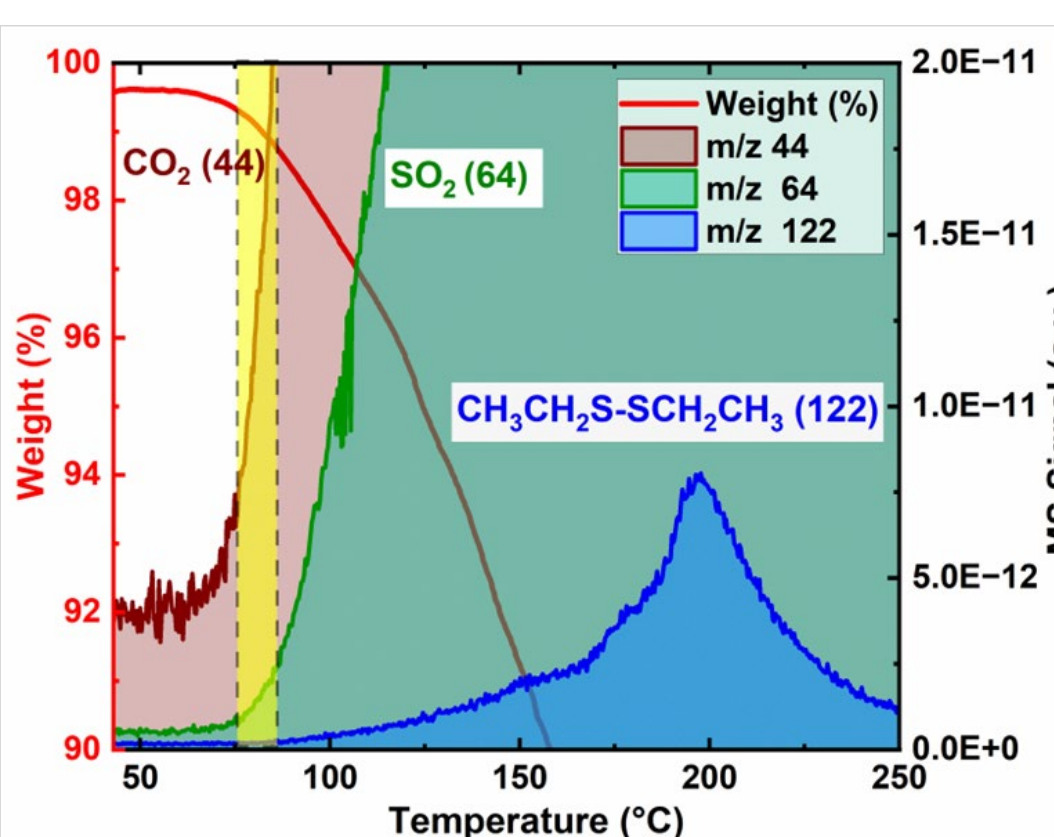
MQ8 sensor: 75 °C and 102 °C

#### Copper-thiol compound-3

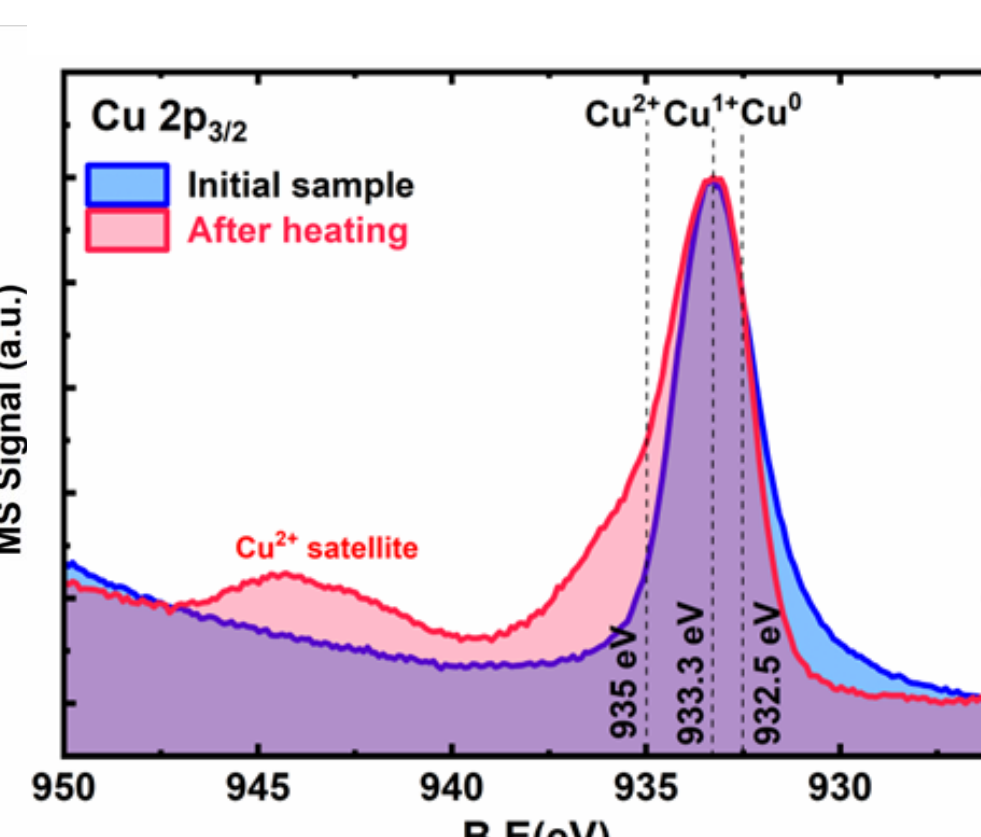


METIS sensor: 115 °C

### TGA-MS:

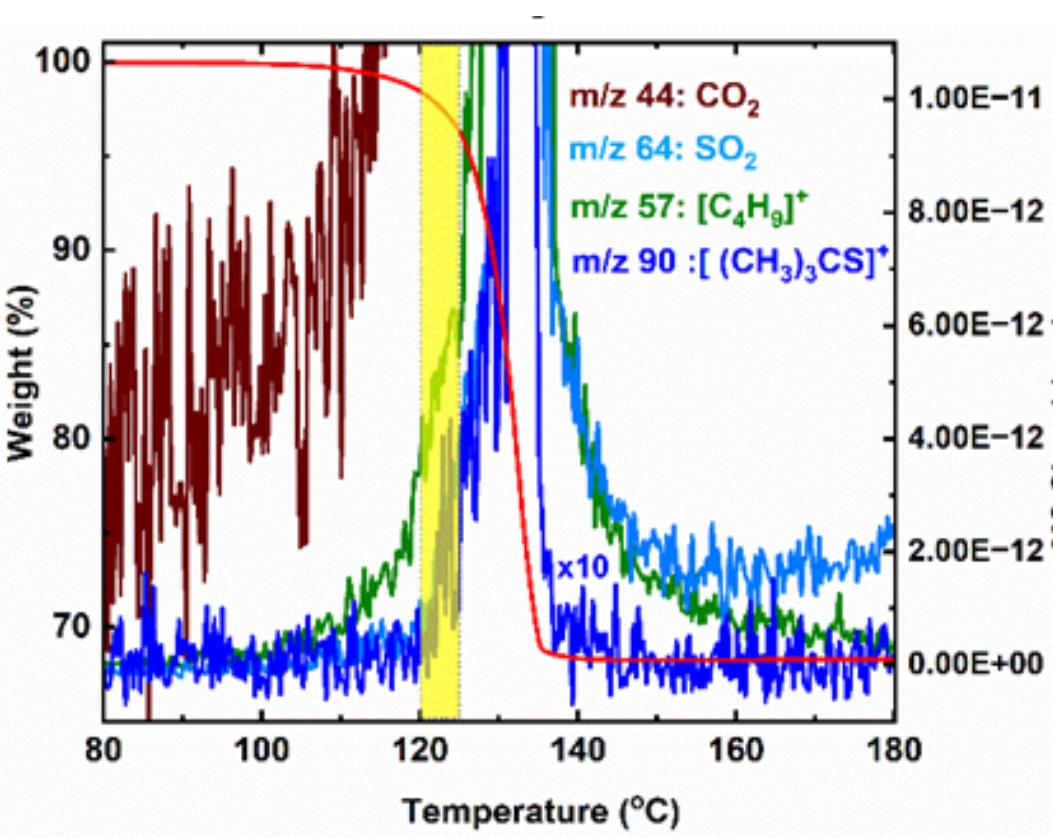


### XPS



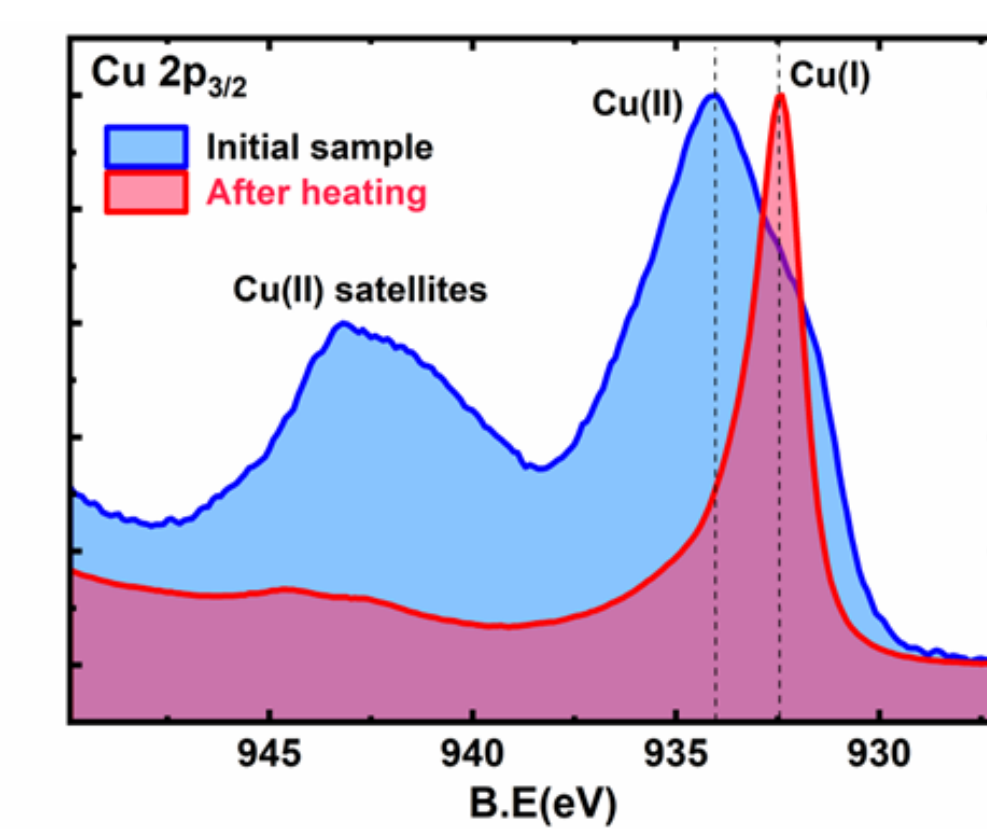
Oxidize Cu(I) to Cu(II)

### TGA-MS



Consistent with SO<sub>2</sub> and sulfides gas

### XPS



Reduce Cu(II) to Cu(I)

## Conclusions

- Copper-thiolate compounds thermally decompose and release volatile compounds (VOC, sulfur dioxide, sulfide) when the critical temperature is reached.
- Onset gas release temperature is tuned by changing the chemistry of the thiol groups.
- TGA-MS data aligned well with the gas sensor response.
- The thermal process and gas releases induced an oxidation state change of Cu.
- Gas detection depends on the gas species and the particular detector/ sensor utilized.
- Independent tests at ORNL and SANDIA agreed on the onset gas release temperatures.

## Acknowledgements

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- SANDIA National Laboratory.