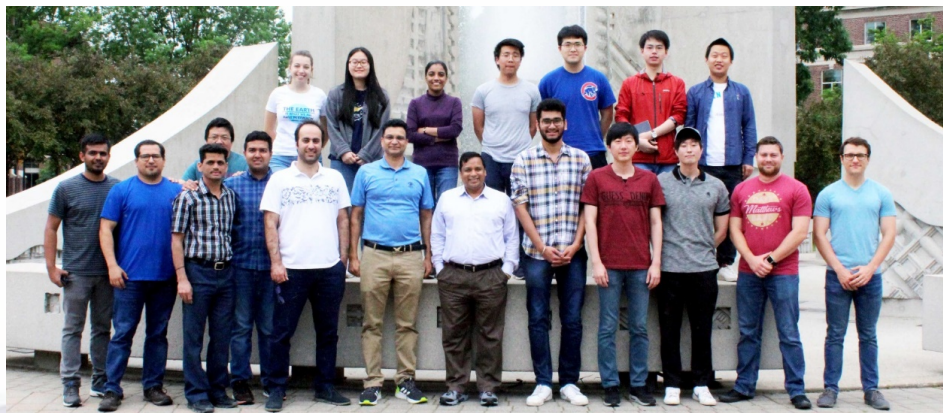


# Impedimetric Chemo-sensing of Volatile Organic Compounds Released from Li-ion Batteries

**Vilas G. Pol**

*Professor of Chemical Engineering*



**Presented By:**  
**Palwinder Kaur**  
**Visiting Scholar (OVD Fellow)**

# Purdue's Research on Battery Technologies

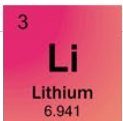
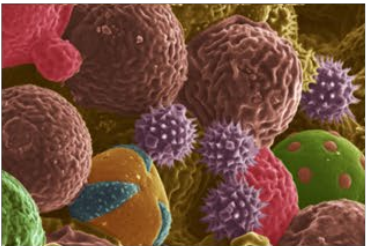
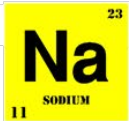
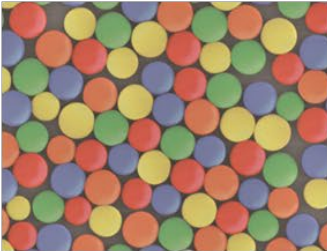
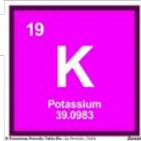
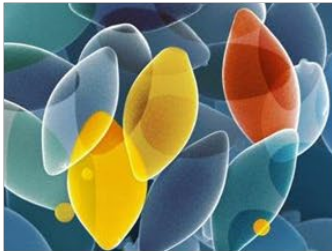
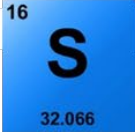
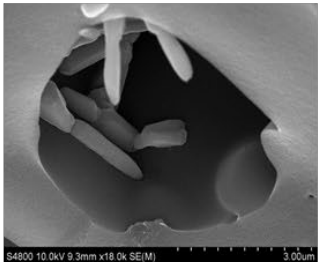


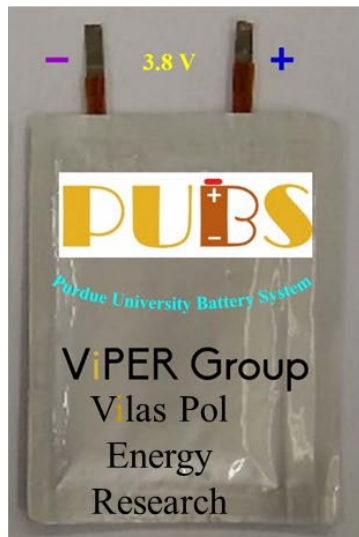
## Lithium-ion

## Sodium ion

## Potassium ion

## Li-S/Solid state

 	 	 	 
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*Interest: Batteries for Renewable Energy Storage and their Safety*



**225 Peer-reviewed publications and 30 US Patents/applications**

# Battery Accidents in News

## Electric scooter emits smoke as it catches fire, watch viral video

Viewed over 2,800 times, the clip begins with immense smoke and fumes erupting from a scooter parked on the side of a road.

By: **Trends Desk** | New Delhi |  
Updated: October 1, 2021 9:56:42 am

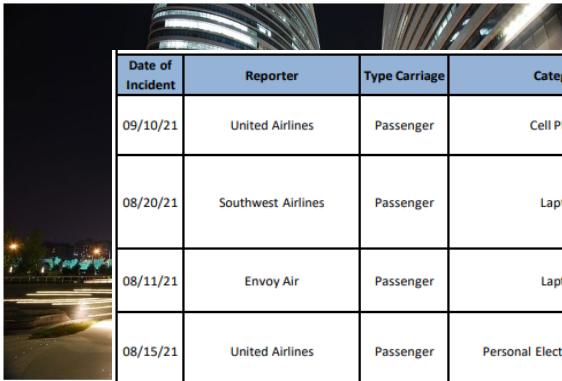


## Two firefighters killed after Beijing battery blaze

An explosion occurred as firefighters were dealing with a fire in a 25 MWh lithium-iron phosphate battery associated with a 1.4 MW rooftop array at a shopping mall in the Chinese capital on Friday.

APRIL 21, 2021 VINCENT SHAW

COMMERCIAL & INDUSTRIAL PV UTILITY SCALE STORAGE CHINA



## An Electric Bus Caught Fire And Set Those Nearby Ablaze

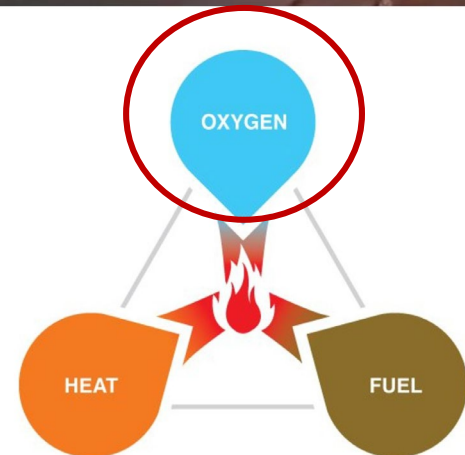
Ev's are the future, but safety is still an issue.

BY ARTUR NOVICHENKO  
PUBLISHED MAY 30, 2021



Date of Incident	Reporter	Type Carriage	Category	Reported Description
09/10/21	United Airlines	Passenger	Cell Phone	A passenger's cell phone battery overheated while the aircraft was on its final approach to Denver, CO. The incident was contained by airline personnel prior to landing. There were no injuries reported.
08/20/21	Southwest Airlines	Passenger	Laptop	A passenger was charging a laptop computer with a small power bank. The power bank started to smoke and spark in a thermal runaway event. The incident was contained by airline personnel. There were no injuries reported.
08/11/21	Envoy Air	Passenger	Laptop	A laptop computer battery began to smoke while onboard a flight that was still at the gate. The laptop was removed from the aircraft prior to takeoff.
08/15/21	United Airlines	Passenger	Personal Electronic Devices	An iPad went into thermal runaway during a flight from Korea to San Francisco International Airport over the Pacific Ocean. The incident was contained by airline personnel. There were no injuries reported.
08/08/21	Alaska Airlines	Passenger	e-Cigarettes/Vape Devices	A passenger's e-Cigarette started overheating. The device was put in a battery containment bag. No injuries were reported.
08/05/21	Alaska Airlines	Passenger	Personal Electronic Devices	A passenger was sleeping with a flashlight around their neck when the battery began to burn. The flashlight was put in a "burn bag" and secured by airline personnel.
08/04/21	Horizon Air	Passenger	e-Cigarettes/Vape Devices	An e-Cigarette device "sizzled and smoked" inflight while headed to Sacramento, CA from Seattle, WA. Airline personnel contained the incident.
08/03/21	Southwest Airlines	Passenger	Battery Packs/Batteries	A piece of luggage containing a Lithium battery powered multi charger device was found smoking while being transferred to another flight. The luggage was removed from circulation by the airline.
07/31/21	United Airlines	Passenger	Cell Phone	A passenger's cell phone battery began to smoke and was contained by airline personnel.

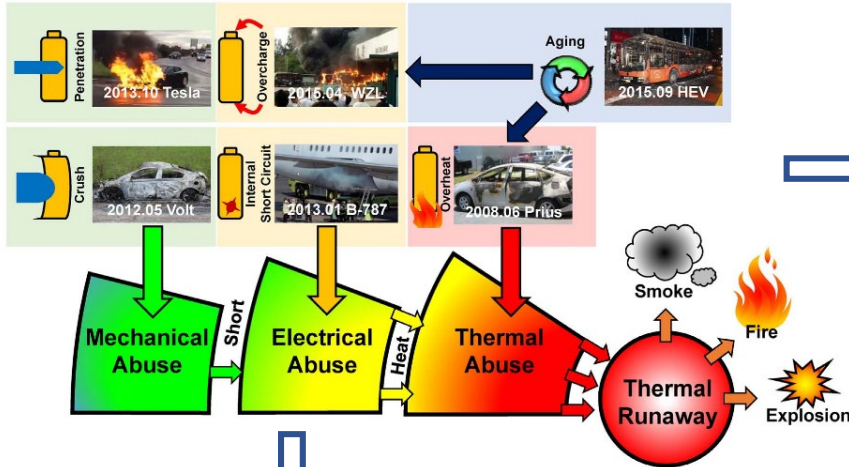
VIPER, Purdue University





# Thermal Runaway

## Causes of Thermal Runaway



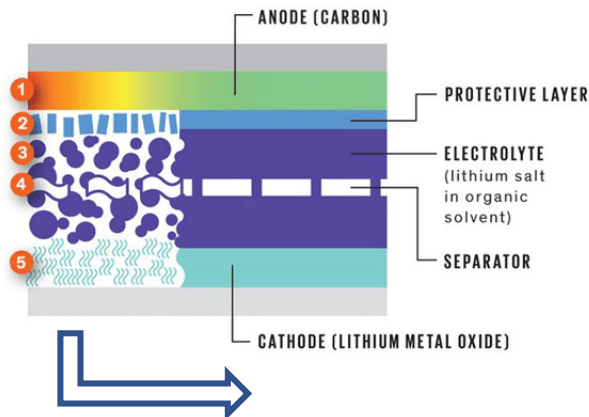
Thermal runaway is self-accelerated process



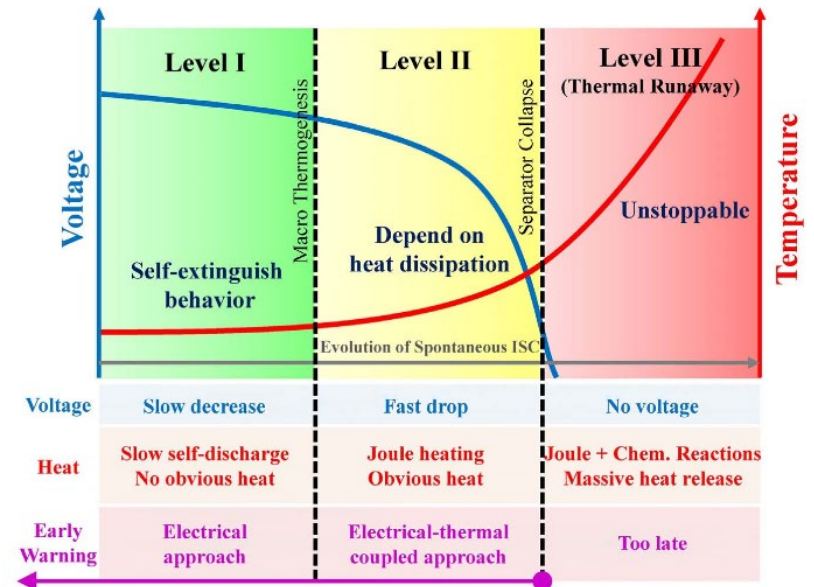
- Heat
- Exothermic Reaction Rate
- Increase in Reaction Rate

## Stages of Thermal Runaway

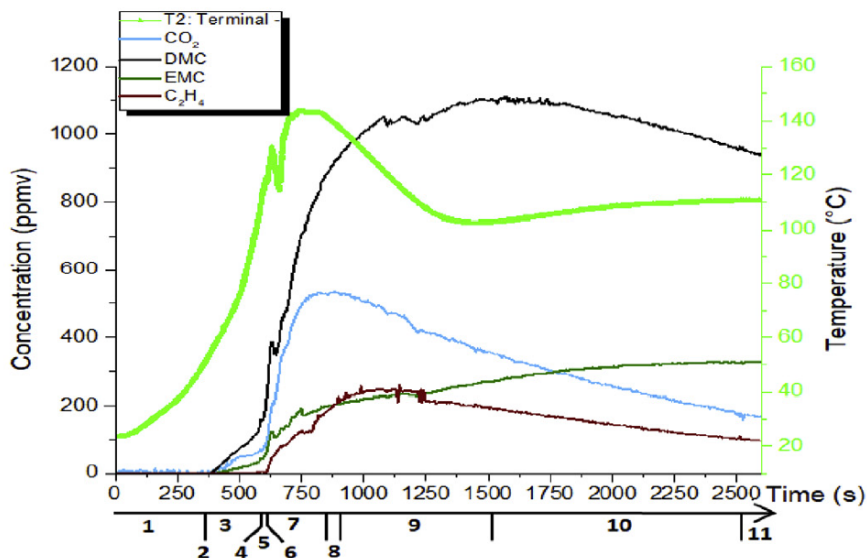
1. Heating starts.
2. Protective layer breaks down.
3. Electrolyte breaks down into flammable gases.
4. Separator melts, possibly causing a short circuit.
5. Cathode breaks down, generating oxygen.



## Level of Internal Short Circuit (ISC)

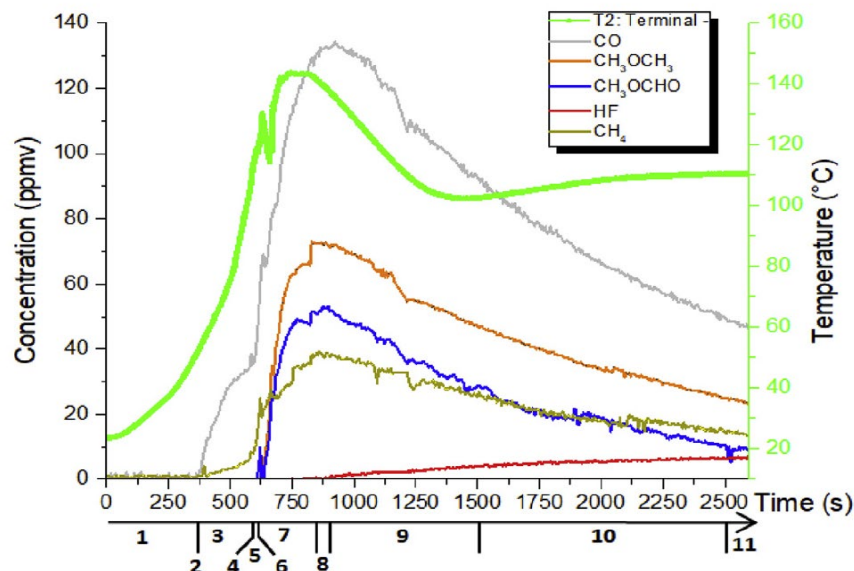


# Gases released from Li-ion Batteries during Thermal Runaway



Gases Released from Batteries:

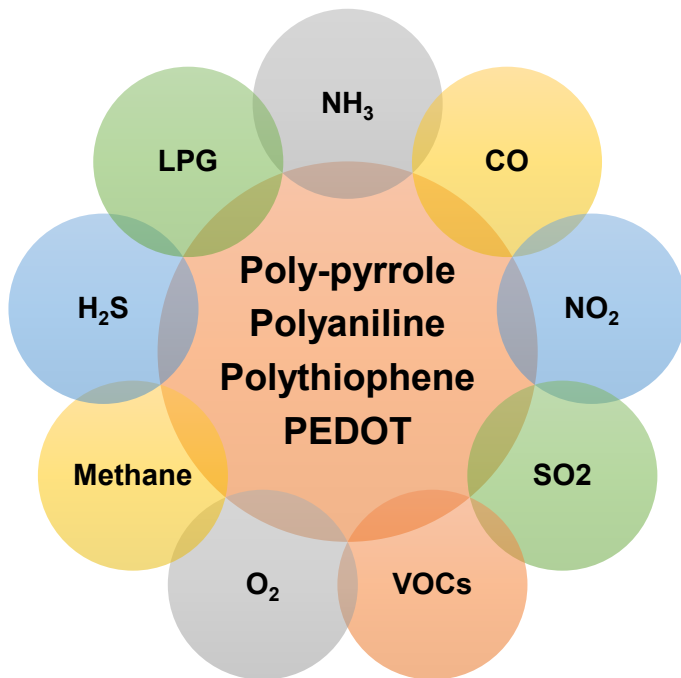
- Carbon Dioxide
- Carbon Monoxide
- Hydro-fluoride



VOCs Released from Batteries:

- Di-methyl Carbonate
- **Ethyl methyl carbonate**
- Ethylene
- Dimethyl ether
- **Methyl formate**

# Conducting Polymer with Impedance Spectroscopy as an Opportunity



## Impedance Spectroscopy

- 2-D or 3-D response
- Impedance is inversely proportional to temperature.
- Non-invasive method.
- Provide in depth information of the electrochemical reactions.
- Interfacial study of the sensor.
- Dielectric effects can be observed.

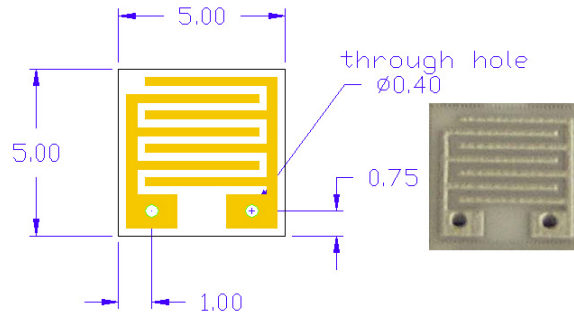
## Advantages of Conducting Polymers:

- Tunability,
- Flexibility,
- Less expensive,
- Operable at Room temperature

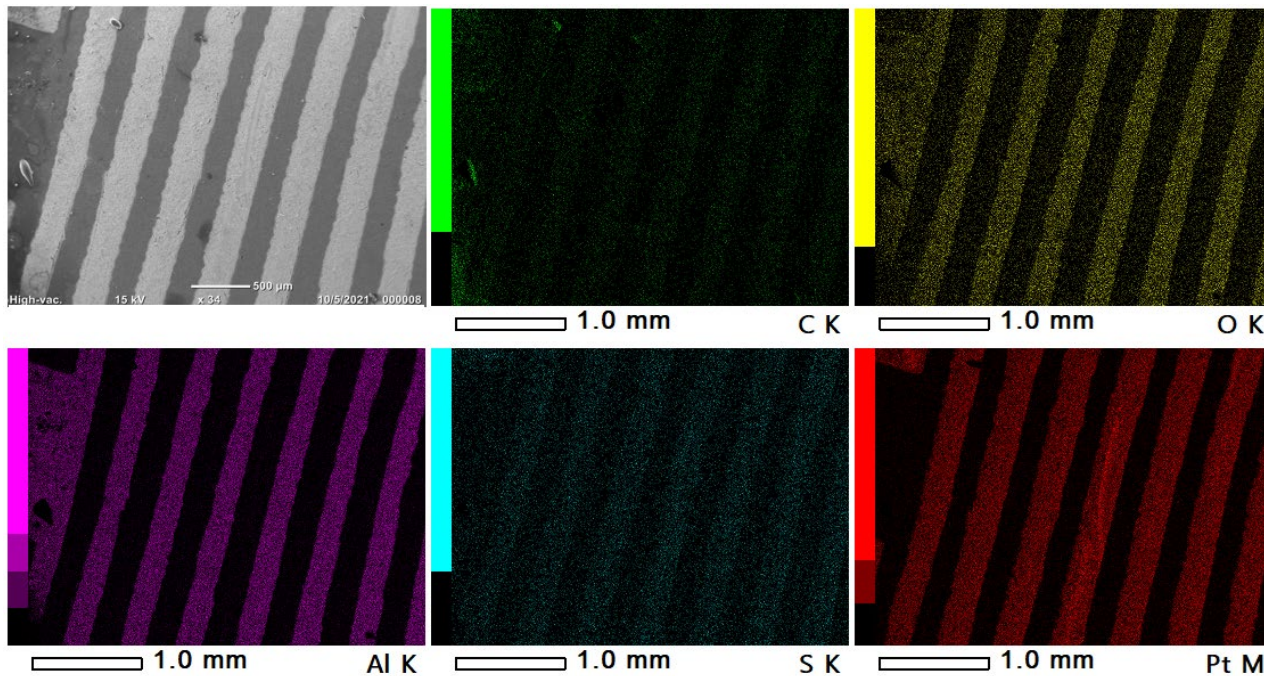
## Disadvantages of Conducting Polymers:

- Non-selectivity

# PEDOT:PSS (poly(3,4-ethylenedioxythiophene polystyrene sulfonate) Sensor



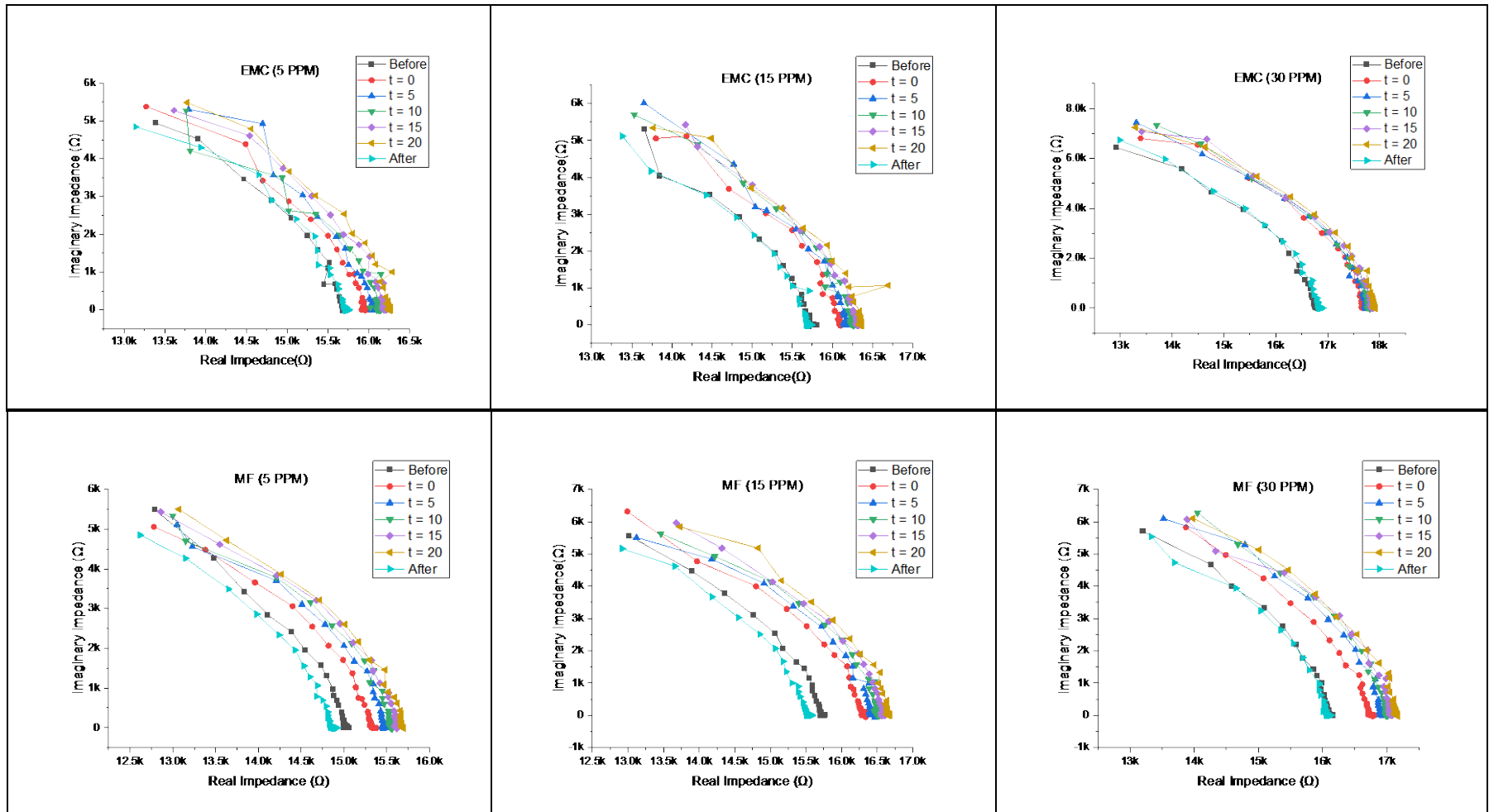
- Interdigitated-Platinum Electrode
- Spin Coated
- Energy dispersive X-ray spectroscopy (EDS)
- Uniform coating of C, S and O indicate presence of PEDOT:PSS





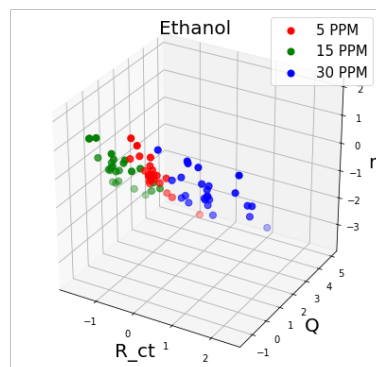
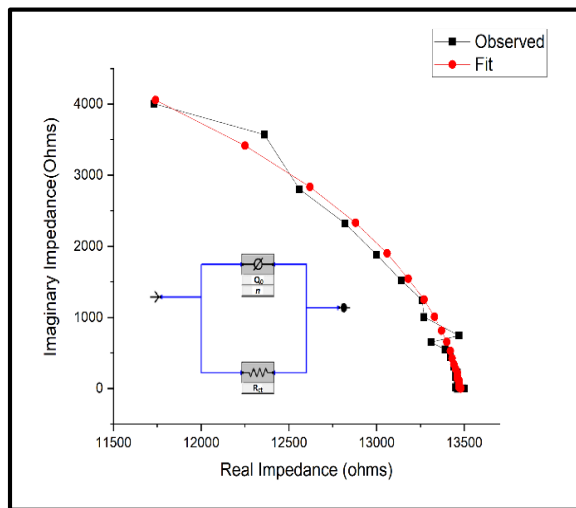
# Impedance response to VOCs released from Batteries

(EMC and MF released as the byproduct of decomposition of Electrolytes)

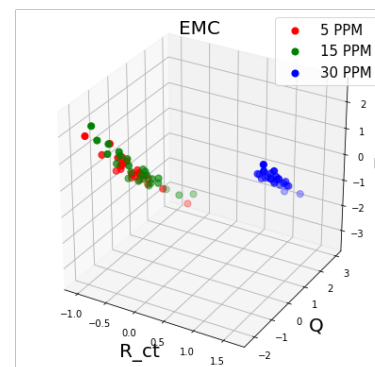




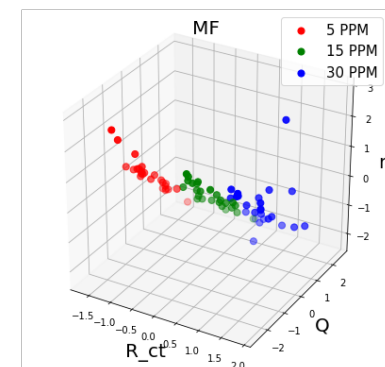
# Equivalent Electrical Parameter



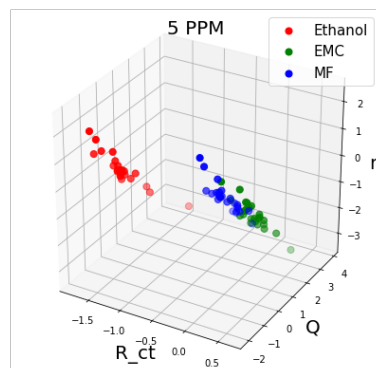
(a)



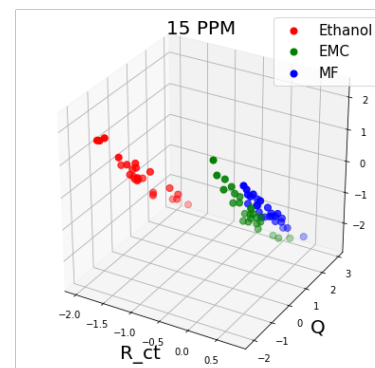
(b)



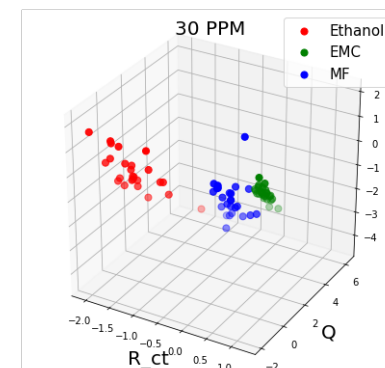
(c)



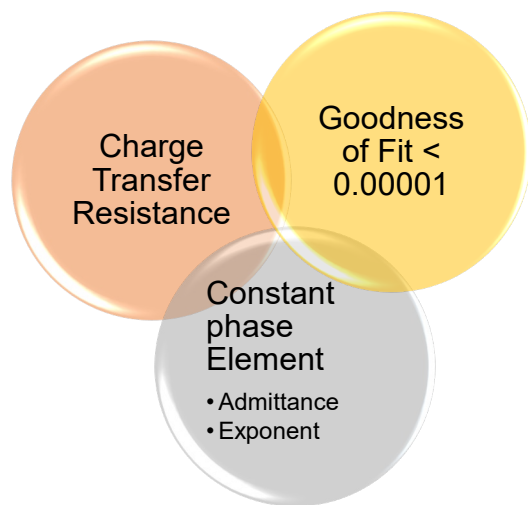
(d)



(e)



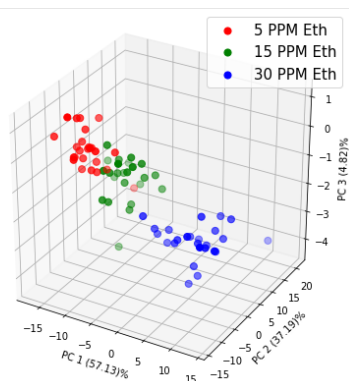
(f)



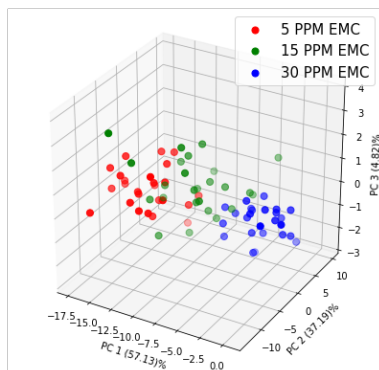
# Principal Component Analysis

PCA:

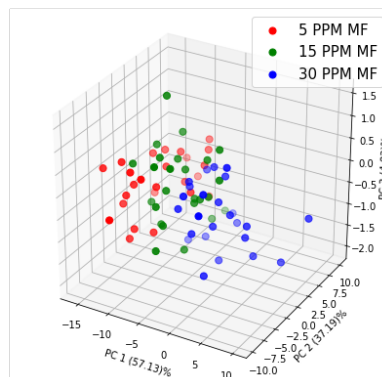
- Dimensionality Reduction Methods (3D/2D)
- PCs defines Data > 95%
- Classify Analytes in Respective groups.



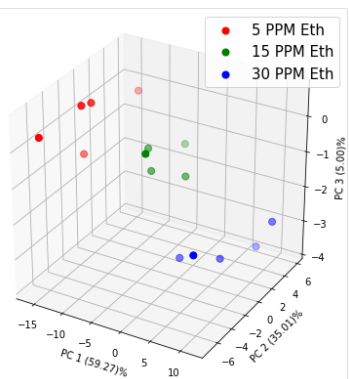
(a)



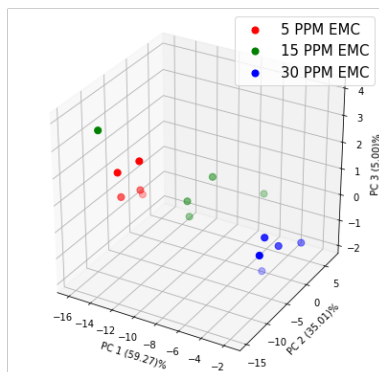
(b)



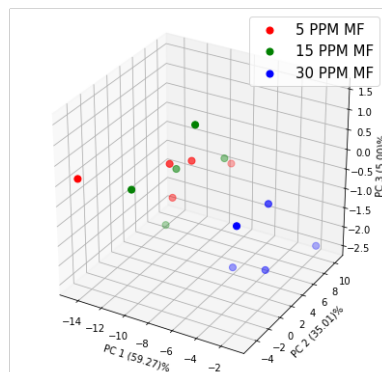
(c)



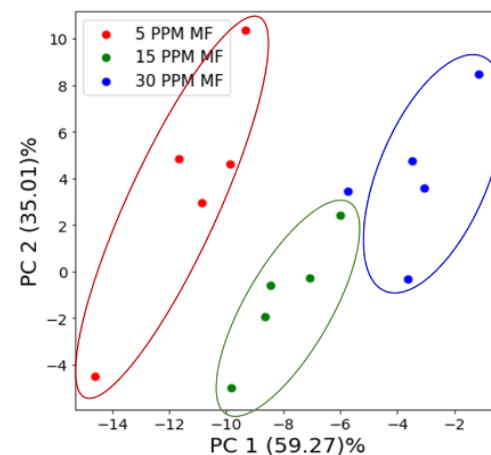
(d)



(e)

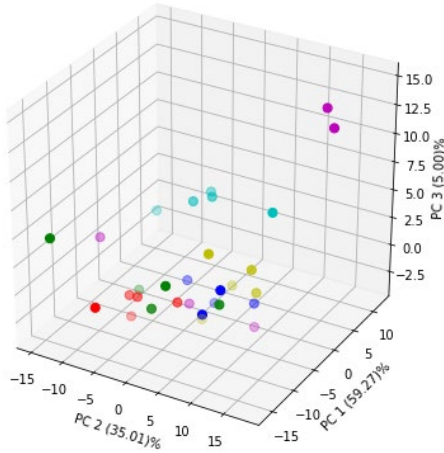


(f)

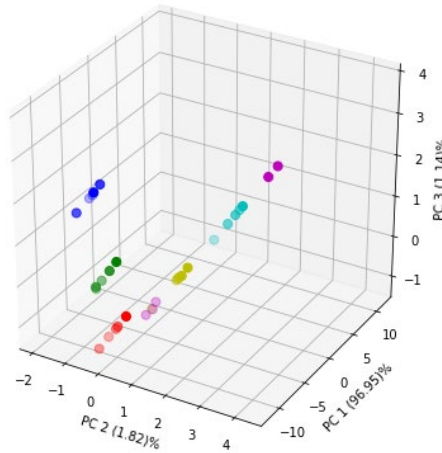


# Principal Component Analysis of different Classes

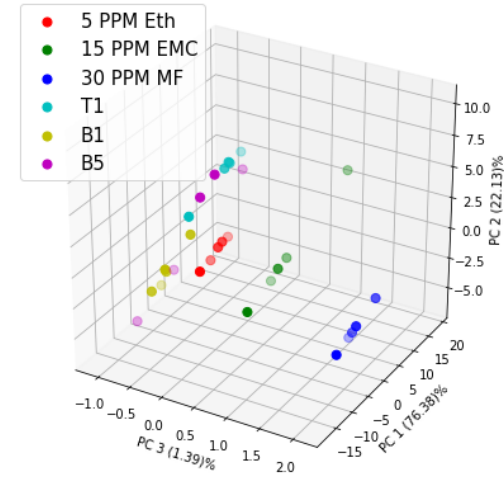
{B1(Eth 5 PPM + MF 30 PPM) + B5 (EMC 15 PPM + MF 30 PPM) + T1 + Single Analyte}



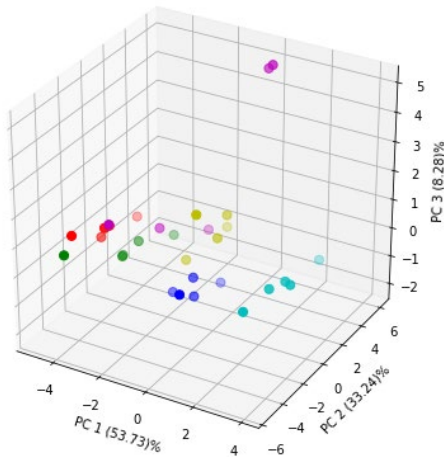
All Data-Set



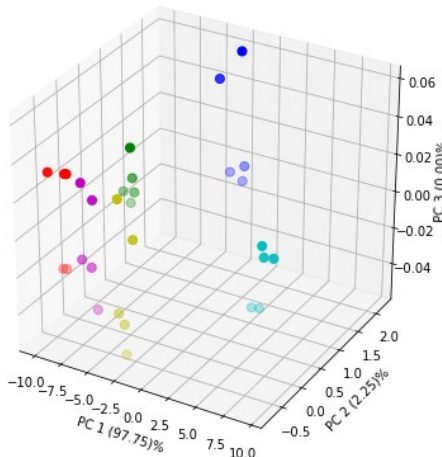
Real Impedance



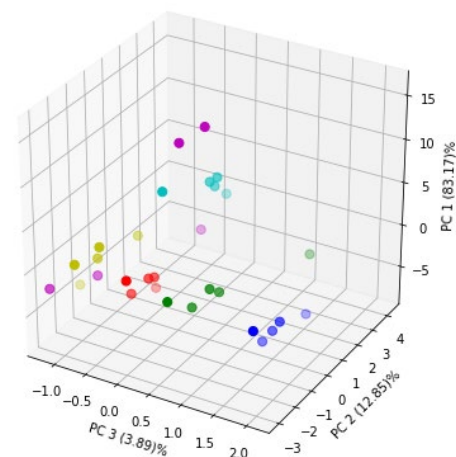
Imaginary Impedance



Decades Frequencies



Real Impedance (Low Freq.)

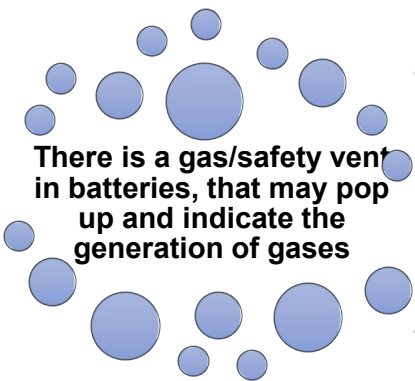


Imaginary Impedance (High Freq.)



# Classification Accuracy using Logistic Regression Algorithm (Machine Learning Algorithm)

	Complete Dataset	Real Impedance	Imaginary Impedance	Real and Imaginary Impedance at Decade frequencies	Real Impedance at low frequencies and Imaginary Impedance at High Frequencies
Set 1	83.33	75	73	76.66	<b>86.66</b>
Set 2	88.33	85	<b>91.66</b>	86.66	88.33
Set 3	<b>86.66</b>	80	85	83.33	83.33
Set 4	<b>90</b>	83.33	70	80	83.33
Set 5	<b>95</b>	91.66	86.66	90	90
5 PPM	<b>96.66</b>	96.66	80	53.33	93.33
15 PPM	<b>90</b>	73.33	70	80	86.66
30 PPM	90	83.33	90	<b>93.33</b>	90
Ternary	94	<b>96</b>	88	88	92
Binary	<b>75.55</b>	72.22	62.22	60	64.44
Single	<b>88.88</b>	81.11	66.66	80	86.66
Classes	<b>83.9</b>	79.13	68.26	73.47	74.78



There might be leakage with very low pressure.

The popping noise could be very low and it will not generate any signal or warning to alert the users.

Gas Sensors



**Thank You!**