

## Supplementary Materials

### Characterization of Lithium-ion Battery Fire Emissions—Part 1: Chemical Composition of Fine Particles (PM<sub>2.5</sub>)

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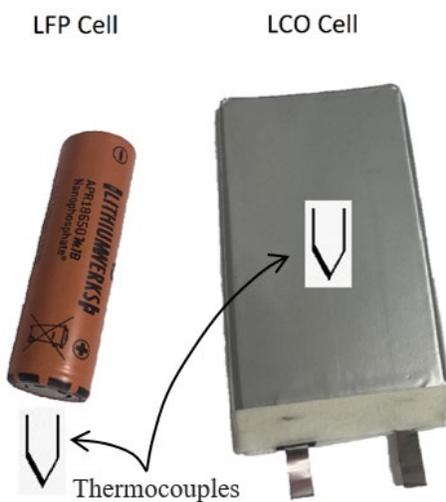


Figure S1. The two LIB types tested: 18650-style lithium iron phosphate (LFP) cells (orange) and a pouch-style lithium cobalt oxide (LCO) cell (grey). The locations of thermocouple placement during cell testing are shown.

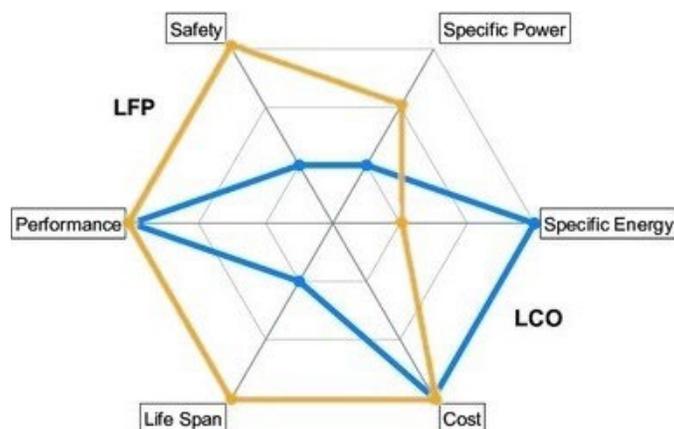


Figure S2. A comparison of LFP and LCO cell characteristics and performance metrics, showing that the LFP cells have better life span, specific power, and safety, while LCO cells have higher specific energy (energy capacity per unit mass) [1].

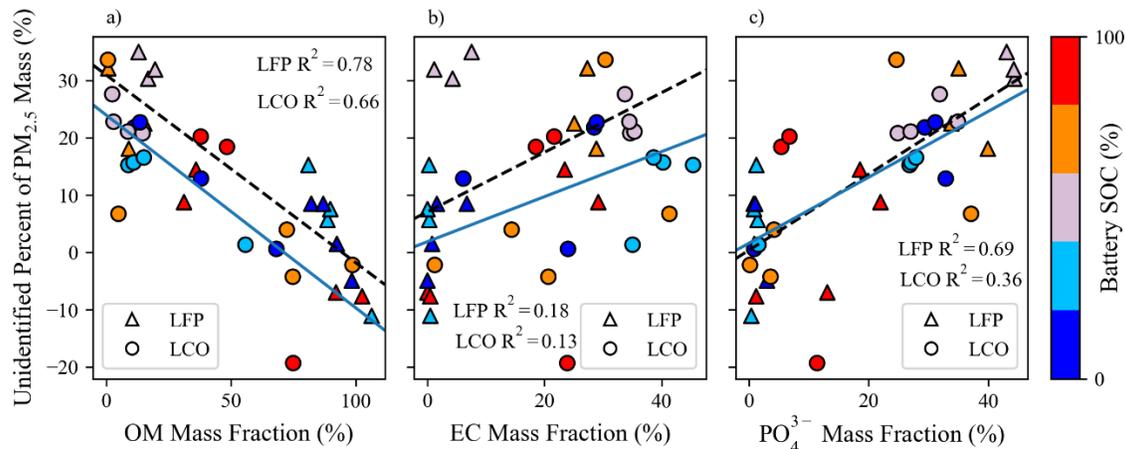


Figure S3. Correlation between the unidentified portion of reconstructed mass and a) organic matter (OM), b) elemental carbon (EC), and c) phosphate ( $\text{PO}_4^{3-}$ ). Both positive and negative unidentified mass fractions exist, meaning that reconstructed mass underestimated and overestimated gravimetric mass, respectively. Looking at the correlation between the unidentified mass fraction and species abundance may help identify what is missing. Panel (a) shows that tests with overestimated reconstructed mass (negative unidentified mass fractions) have high (70–130%) OM mass fractions for both cell types, indicating that OM is a significant contributor to the overestimation of reconstructed mass. This is likely caused by volatile organic gases being adsorbed on the quartz filters but not being accounted for by blank correction [2]. Panels b) and c) show that the unidentified mass fractions increase with EC and  $\text{PO}_4^{3-}$  mass fractions. While EC correlation is low,  $\text{PO}_4^{3-}$  shows a strong trend, indicating that unmeasured phosphorous compounds (e.g., phosphite [ $\text{HPO}_4^{2-}$ ]) may contribute to higher unidentified mass. Refractory carbonates that do not decompose at 840 °C (the maximum temperature during carbon analysis) may also contribute to unidentified mass.

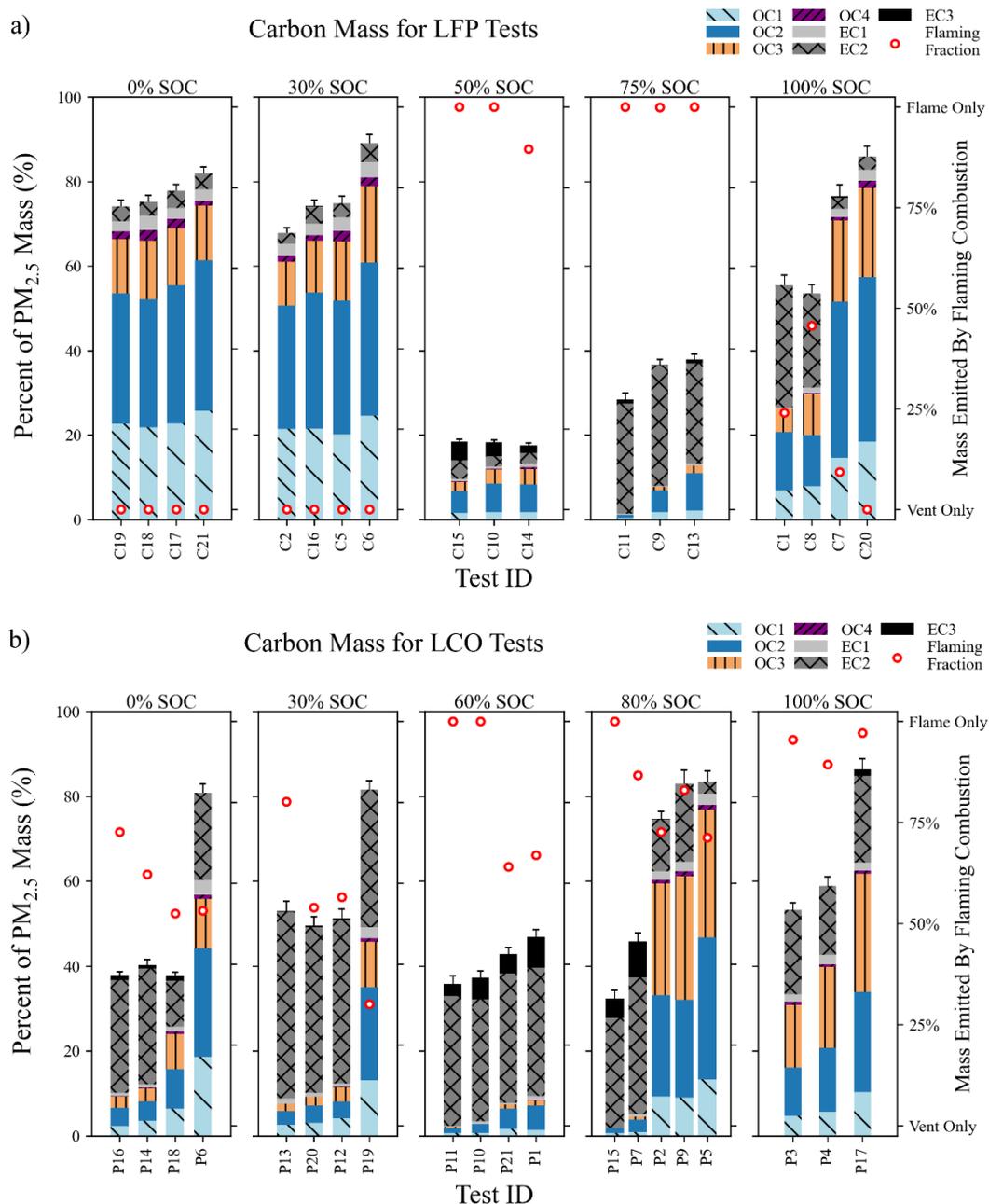


Figure S4. Thermal carbon fractions as a percent of  $PM_{2.5}$  mass for: a) LFP cells and b) LCO cells. Four OC fractions that evolved at different temperatures in a pure helium (He) carrier gas include: OC1 (140 °C), OC2 (280 °C), OC3 (480 °C), and OC4 (580 °C); Three EC fractions that evolved in 98% He/2%  $O_2$  include: EC1 (580 °C), EC2 (740 °C), and EC3 (840 °C) [3]. These fractions are indications of carbon volatility and thermal stability and have been used to distinguish and apportion contributions to  $PM_{2.5}$  from different sources. The percentages of  $PM_{2.5}$  mass emitted in flaming phase are indicated by the red circles (right y-axis). Error bars indicate the combined uncertainty of all mass fractions in each test.

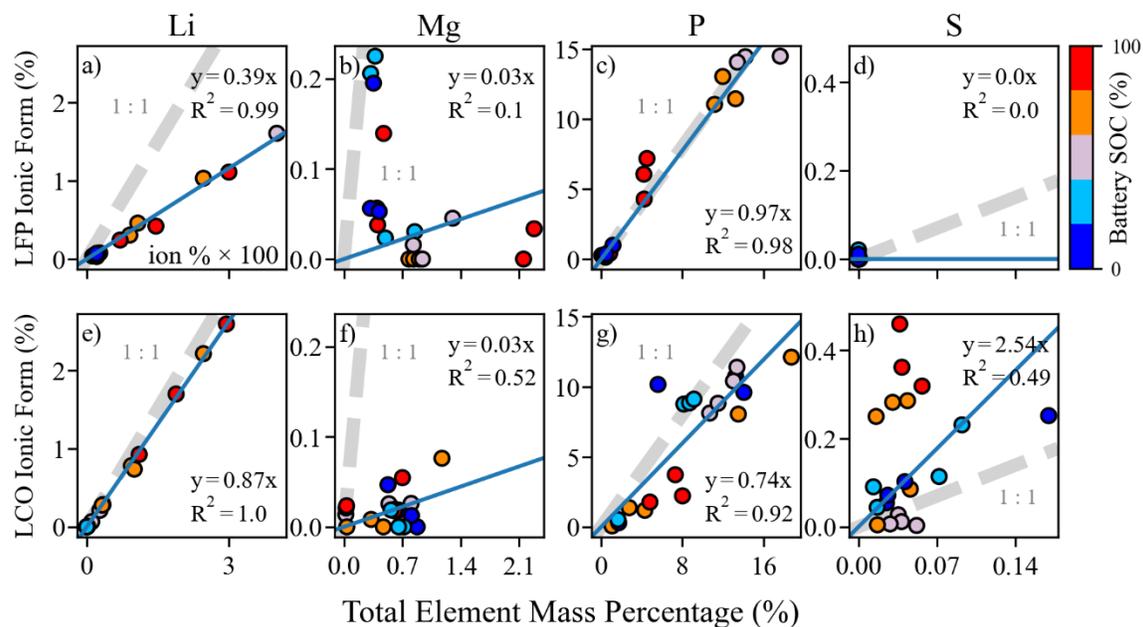


Figure S5. Proportions of total elemental abundance attributed to ionic compounds for LFP (a-d) and LCO (e-h) cells. One outlier has been removed from (a) to better show the dominant relationship. Dot color represents cell SOC for each test.

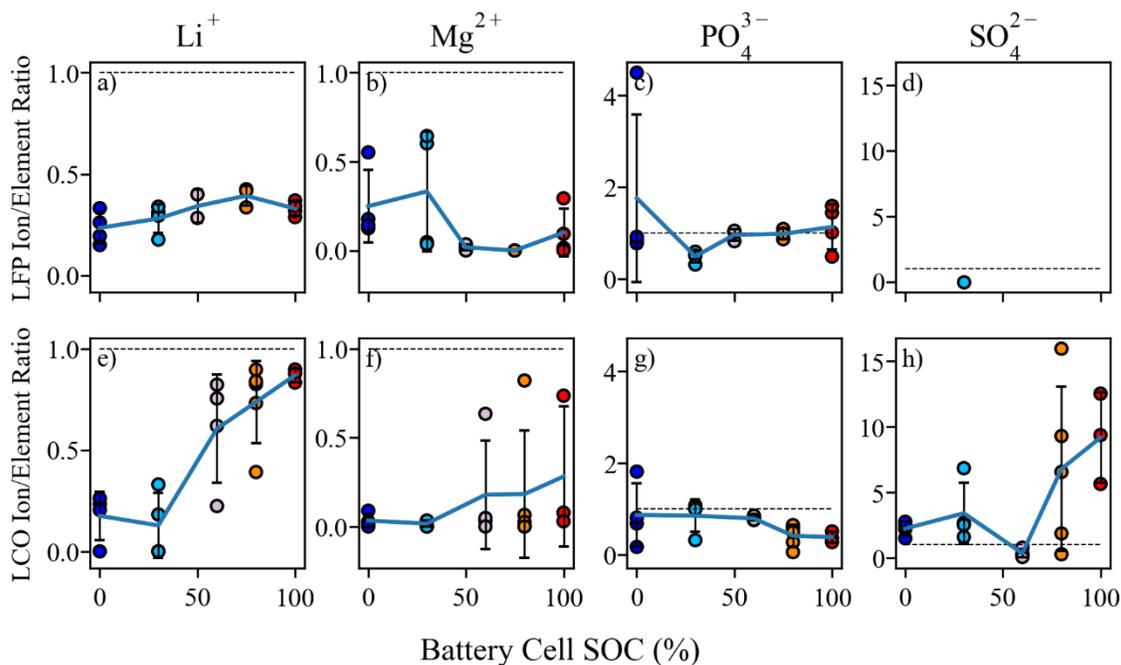


Figure S6. Dependence of ion/element ratios on cell SOC for LFP (a-d) and LCO (e-h) cells. Values over 1.0 suggest measurement error as the components of ionic compounds should all be detected by elemental analysis.

## References:

1. Saldaña, G.; San Martín, J.I.; Zamora, I.; Asensio, F.J.; Oñederra, O. Analysis of the current electric battery models for electric vehicle simulation. *Energies* **2019**, *12*, 2750.
2. Chow, J.C.; Watson, J.G.; Chen, L.-W.A.; Rice, J.; Frank, N.H. Quantification of PM<sub>2.5</sub> organic carbon sampling artifacts in US networks. *Atmospheric Chemistry and Physics* **2010**, *10*, 5223-5239, doi:doi:10.5194/acp-10-5223-2010.
3. Chow, J.C.; Watson, J.G.; Chen, L.-W.A.; Chang, M.C.O.; Robinson, N.F.; Trimble, D.; Kohl, S. The IMPROVE\_A temperature protocol for thermal/optical carbon analysis: maintaining consistency with a long-term database. *Journal of the Air & Waste Management Association* **2007**, *57*, 1014-1023.