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SNL Energy Storage Technology and Systems – Energy Storage Safety

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Heat Release from Thermal Decomposition of Layered Metal Oxide Cathodes in Lithium-Ion Batteries

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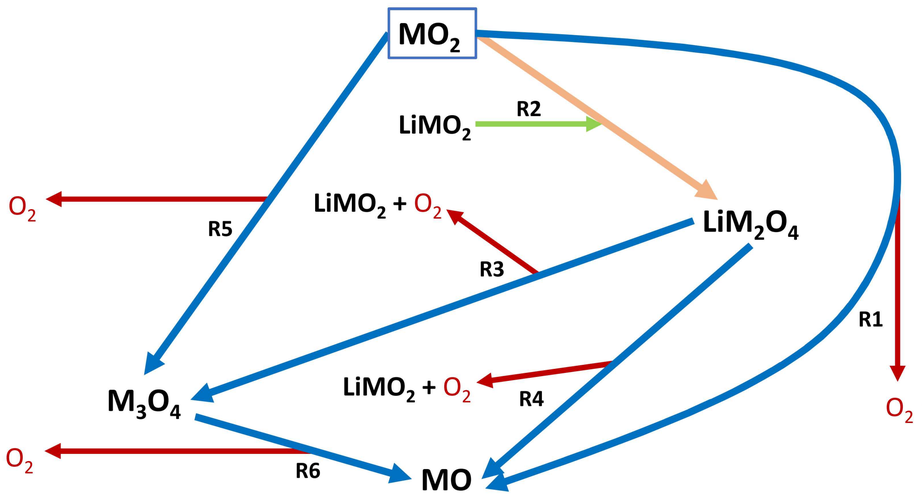
Introduction

- Stationary energy storage systems (ESS) are increasingly deployed to maintain a robust and resilient grid.
- As system size increases, financial and safety issues become important topics.
- Holistic approach: electrochemistry, materials, and whole-cell abuse will fill knowledge gaps.
- Models enable knowledge to be applied different scenarios and larger scales.
- Existing thermal runaway models successful for initial single-cell thermal runaway.
- Model features needed to evaluate safety for large Li-Ion systems include:
  - Applicability to batteries with different form factors, chemistries, SOC.
  - Predictions dependent on material properties.
  - High-temperature chemistry to predict cascading failure.
- Thermodynamics provide a foundation for modeling chemical heat release

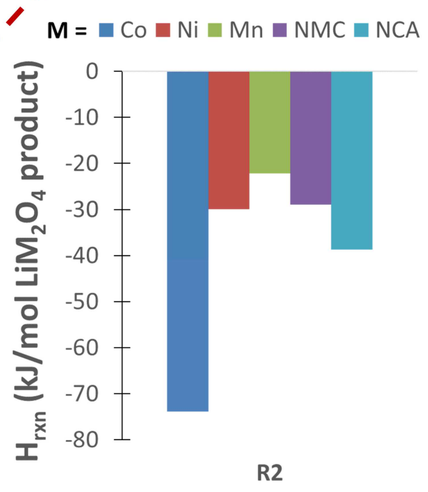
Decomposition of Layered Metal Oxides

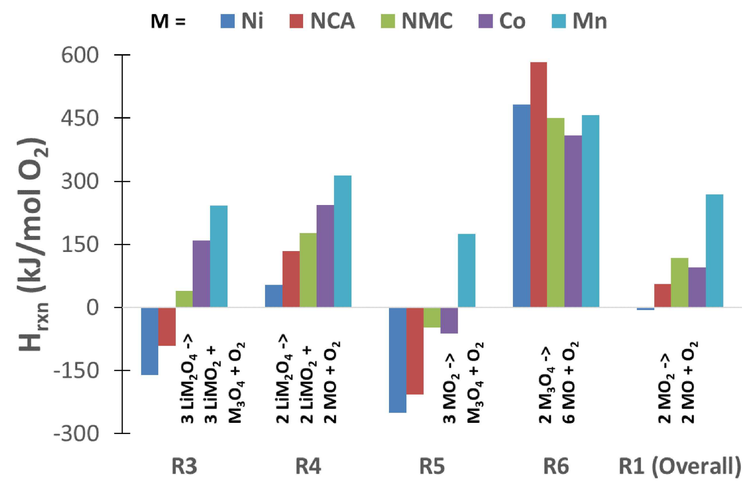
- De-lithiated (high SOC) MO_2 cathodes experience multi-step decomposition
- Most steps produce oxygen except for exothermic formation of LiM_2O_4 spinel



Predicting Cathode Heat Production

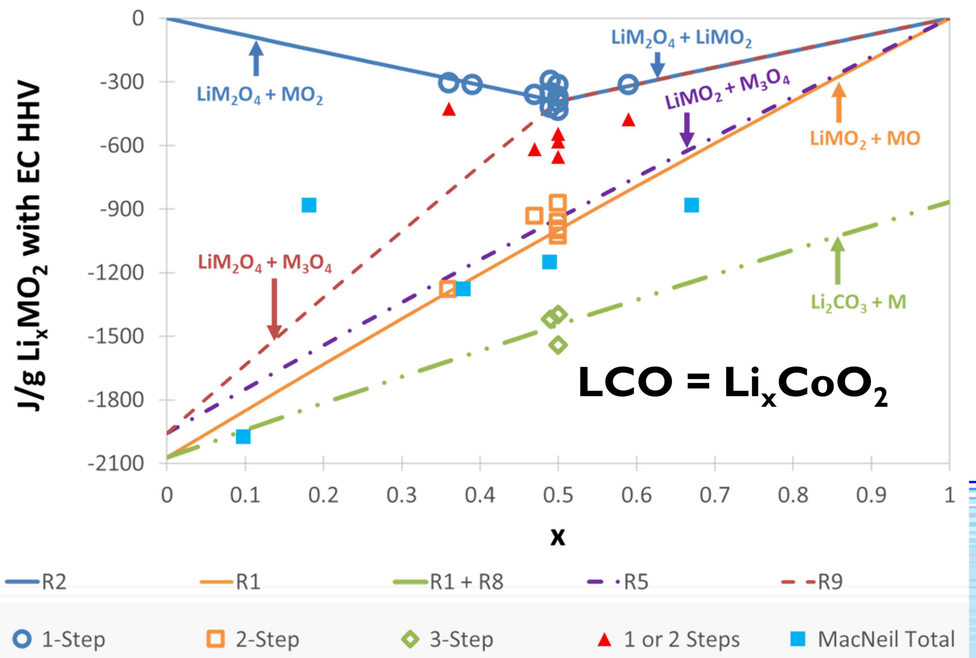
- Heats of reaction can now be calculated for decomposition of **any** Li_xMO_2 with
  - Arbitrary M (single metals or mixtures of Ni, Co, Mn, and Al)
  - Arbitrary x (low x = high SOC)
- Required assembling a new compilation of 32 formation enthalpies from 42 sources
- Electrolyte solvent combustion adds more heat (-472 kJ/mol O_2 for EC)



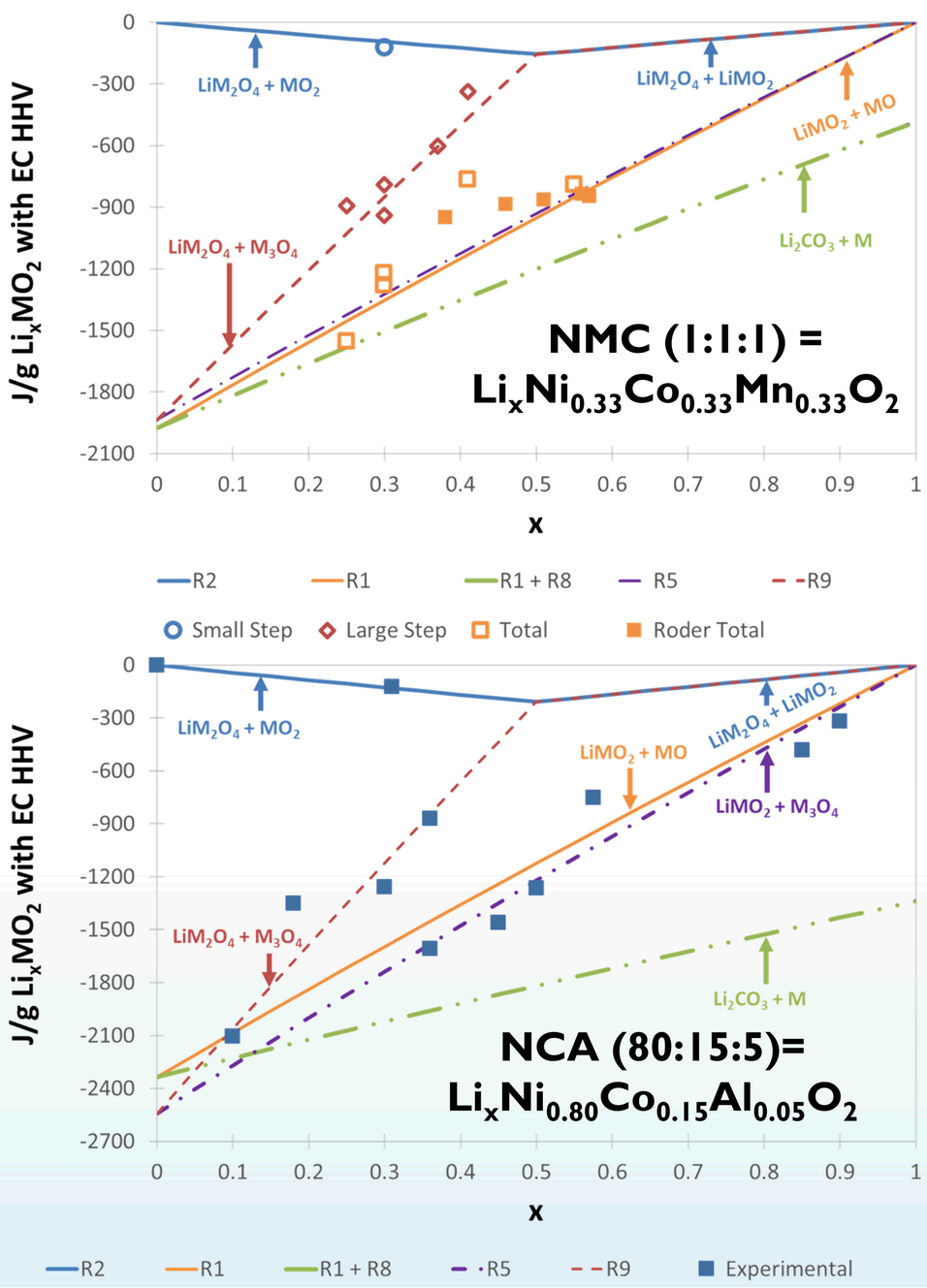


Calorimetry Data Demonstrate Effectiveness of Predictions for Pure and Mixed Metal Oxides

- Calculated heat generation with full combustion of solvent compared to calorimetry data
- Explains trends observed for different states of charge (x) and pure or mixed metal oxides (M)
- 60 calorimetry measurements extracted from 24 sources, scrutinized and processed for comparisons



Predicted and Measured Heat Release Agree for 3 Commercial Cathodes with Varying SOC



Conclusions and Next Steps

- First demonstration of heat release predictions from arbitrary metal oxides with varying SOC
- Allows rapid, *a priori* safety assessments for candidate Li-ion cathode materials
- Facilitates identification of chemical events from thermal data
- Distribution to occur through publication and development of a web-based heat-release calculator
- Cathode thermal runaway models to be developed will utilize these predictions as a sub-model

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