

Title: Modeling Chemical Heat Sources in Li-Ion Batteries for a Broader Range of Materials and Conditions

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Abstract:

Calorimetry data have been used over the past two decades to develop models of thermal decomposition of single Li-Ion cells that yield reasonable predictions of the onset of thermal runaway. However, predictions of cascading runaway in systems with many cells require models that capture the total heat release with greater fidelity. This work is targeted at extracting additional information from existing calorimetry and chemical composition data to model electrode decomposition processes occurring at higher temperatures. The updated thermochemical models include more rigorous dependence on materials properties to enable application to customized battery builds with better predictive capability than previous models. Comparisons of the models to experimental data yield insights that are not always obvious from comparisons of data alone.