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Experimental and Modeling Studies of Metal Halide Catholyte and Cathode Materials to Enable Low-temperature Molten Sodium Batteries

Adam M. Maraschky, Rose Y. Lee, Stephen J. Percival, Martha M. Gross, Amanda S. Peretti, Erik D. Spoerke, Leo J. Small
Sandia National Laboratories, Albuquerque, NM USA 87185

Low-cost, long-duration energy storage is critically needed for the resilience of the electric grid powered by renewables like wind and solar. Low-temperature (<130 °C) molten sodium (Na) batteries with NaI-metal halide molten salt catholytes have been developed to address this requirement. This technology avoids the safety concerns caused by metal dendrites and flammable organic solvents found in Li-metal or Li-ion batteries. One of the remaining challenges for molten Na batteries is to achieve high current density performance while cycling at temperatures just above the melting point of Na (98 °C). In particular, catholyte stability under high rates and wide capacity windows presents the greatest hurdle for practical applications. To optimize the catholyte compositions under phase restrictions and conductivity requirements, our group has examined a variety of chemistries, including mixtures of NaI with $AlCl_3$, $AlBr_3$, and $GaCl_3$. To better understand the failure modes within the catholyte, we have performed electrochemical kinetics studies and mathematical modeling of the iodide-triiodide speciation. Results reveal the equilibrium speciation limitations to usable capacity and current densities for the given catholyte compositions. Additional experiments, including cyclic voltammetry and chronoamperometry, probe the influence of the electrode material on electrochemical kinetics and stability during cycling. Insights from these fundamental studies provide guidance for the future design of robust catholyte chemistries and cathode materials.

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