Title:

Advancing Secondary Battery Materials with Semi-automated Combinatorial Experiments

Abstract:

Advanced battery materials for next-generation technologies involve complex chemistries (at least pseudo-quaternary). These materials typically lie in systems where only a handful of compositions have been explored. Furthermore, in cases where further substitutions may prove useful, only a few substituents have been considered in traditional battery development. To fully understand the impact of composition and structure upon the battery properties, thousands of samples are required. Herein, a suite of high-throughput (HTP) methods (a maximum total throughput of 892 samples/week) developed and utilized in the McCalla lab is presented. HTP experiments include X-ray diffraction, electrochemistry (to yield important metrics such as energy density, cycling stability, and electrochemical stability window), electrochemical impedance spectroscopy (to determine ionic conductivity and stability against metallic anodes), and DC conductivity measurements. These methods, all in high-throughput, permit the systematic design of cathodes, anodes and solid electrolytes for both Li- and Na-ion batteries.

This presentation will then demonstrate progress made in developing various components of advanced batteries using our HTP experiments, both showing improved performance and highlighting new understanding about these materials. The Li- and Na-ion battery components studied include cathodes and ceramic oxides as solid electrolytes. In each case, HTP screening of substituents (up to 56 dopants tested simultaneously) yields materials with significantly improved properties and advances our fundamental understanding of the complex role of composition in these systems.