Contribution ID: **7** Type: **Invited Speaker Abstract**

Following material synthesis and processing with neutron scattering

Rare-earth alkali halides (REAHs) are promising candidates for solid lithium electrolytes. The library of superionic materials of the form Li3MX6 (where M = Y, La, and X = Cl, Br) continues to increase,[1] having room-temperature lithium ionic conductivity surpassing 1 mS cm-1. In particular, Lithium Indium Chloride adopts a similar structure to the Li3MX6 REAHs and has high conductivity, 1.5 mS cm-1, with the added advantage over other solid electrolytes, such as garnets, with a low synthesis and processing cost.[3] Here, we will describe how Li3InCl6 can be synthesized from a concentrated aqueous solution through controlled dehydration.[3-4] We probed this dehydration/reaction using a multimodal approach that combines in situ neutron diffraction, thermogravimetry, differential scanning calorimetry, and in situ impedance spectroscopy. We expand this study to Li3YCl6 showing how robust the aqueous-based synthesis is, comparing it to a standard mechanochemical synthesis route.

This work was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Division of Materials Science and Engineering. The work on Li3YCl6 was supported by DOE's Office of Energy Efficiency and Renewable Energy for the Vehicle Technologies Office. This research used resources at the Spallation Neutron Source, a DOE Office of Science User Facility operated by the Oak Ridge National Laboratory.

[1] Park, K.-H.; Kaup, K.; Assoud, A.; Zhang, Q.; Wu, X.; Nazar, L. F. High-Voltage Superionic Halide Solid Electrolytes for All-Solid-State Li-Ion Batteries. ACS Energy Lett. 2020, 5, 2, 533–539.

[2] Li, X.; Liang, J.; Luo, J.; Norouzi Banis, M.; Wang, C.; Li, W.; Deng, S.; Yu, C.; Zhao, F.; Hu, Y.; Sham, T.-K.; Zhang, L.; Zhao, S.; Lu, S.; Huang, H.; Li, R.; Adair, K. R.; Sun, X. Air-Stable Li3InCl6 Electrolyte with High Voltage Compatibility for All-Solid-State Batteries. Energy Environ. Sci. 2019, 12, 2665-2671.

[3] Li, W.; Liang, J.; Li, M.; Adair, K. R.; Li, X.; Hu, Y.; Xiao, Q.; Feng, R.; Li, R.; Zhang, L.; Lu, S.; Huang, H.; Zhao, S.; Sham, T.-K.; Sun, X. Unraveling the Origin of Moisture Stability of Halide Solid- State Electrolytes by In Situ and Operando Synchrotron X-Ray Analytical Techniques. Chem. Mater. 2020, 32, 16, 7019–7027.

[4] Sacci, R.L.; Bennett, T.H.; Drews, A.R.; Anandan, V.; Kirkham, M.J.; Daemen, L.L.; Nanda, K. Phase evolution during lithium indium halide superionic conductor dehydration. J. Mater. Chem. A, 2021,9, 990-996.

Topic

Energy Materials

Primary author: SACCI, Robert (ORNL)

Presenter: SACCI, Robert (ORNL)