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Cation Transport in Li^+ and Na^+ Rich Antiperovskites JOHN HOWARD, Univ of Nevada - Las Vegas, Los Alamos National Laboratory, LUKE DAEMEN, Los Alamos National Laboratory, YUSHENG ZHAO, Univ of Nevada - Las Vegas, LANL TEAM, UNLV TEAM — A large number of compounds possessing the perovskite crystal structure demonstrate interesting properties such as ferroelectricity, magnetoresistance, and superconductivity. In this study, we present findings on a new class of materials, namely Li^+ and Na^+ rich antiperovskites, with emphasis on cation transport for solid state battery applications. The electrolytes have the general formula A_3BX where A is a Li^+ or Na^+ cation, B is an O^{2-} or S^{2-} anion, and X is a Cl^- or Br^- anion; mixed compositions were also studied. X-ray diffraction techniques were used for phase identification, sample purity, and unit cell refinement. In each case, the materials crystallize in a cubic unit cell with space group $Pm\bar{3}m$. The ionic conductivity was determined for each material as a function of temperature using impedance spectroscopy methods. Activation energies for cation diffusion were determined by fitting the conductivity data to the Arrhenius equation $\sigma = \frac{\sigma_0}{T} e^{-E_a/k_B T}$.

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