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Journal
ECS Meeting Abstracts, MA2020-02(5)

ISSN
2151-2043

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Publication Date
2020-11-23

DOI
10.1149/ma2020-025945mtgabs

Peer reviewed

ECS Meeting Abstracts

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Tuning Ionic Conductivity in Sodium Anti-Perovskite Ionic Conductors

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ECS Meeting Abstracts, Volume MA2020-02, A05: Advances, Challenges, and Development of Solid State Battery Electrochemistry and Materials

Citation Yiliang Li *et al* 2020 *Meet. Abstr.* **MA2020-02** 945

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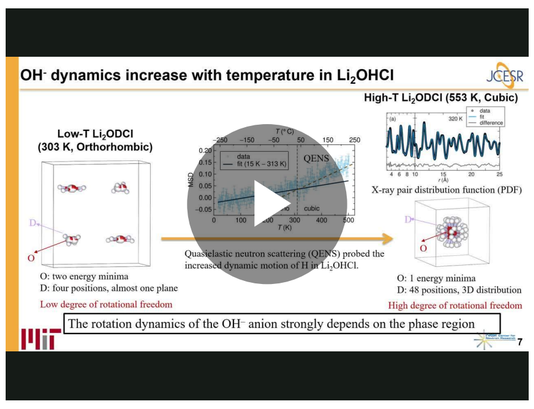
Abstract

Abstract

Anti-perovskite materials have recently attracted great interest as a family of non-flammable solid state electrolytes with high ionic conduction.[1] Typical solid-state electrolyte materials have temperature dependent ionic conductivity following linear Arrhenius behavior over a substantial range of temperature, corresponding to a constant activation energy E_a. However, we have discovered several anti-perovskite materials that have strong positive deviations from Arrhenius behavior, leading to rapidly rising ionic conductivities with increasing temperature.



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Na_3OCl and Na_3OBr are typical anti-perovskite compositions with atomic structure shown in Figure 1a. Strong deviations from Arrhenius (linear) behavior were observed in the temperature dependent conductivity measured by impedance spectroscopy, where $Na_3OCl_{0.5}Br_{0.5}$ reaches the highest ionic conductivity with increasing temperature, as shown in Figure 1b. The structural origins of such behavior, such as change of octahedral tilt systems and order/disorder phase transition, has been investigated using multiple temperature-resolved characterization methods including synchrotron XRD, NMR, dielectric property measurements, and calorimetry, and modeled using AIMD and DFT. This work will give insight to tuning solid state electrolyte with high ionic conductivity.

This work was supported as part of the Joint Center for Energy Storage Research, an Energy Innovation Hub funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences.

Figure : Temperature dependent ionic conductivity and atomic model of Na-based anti-perovskites.

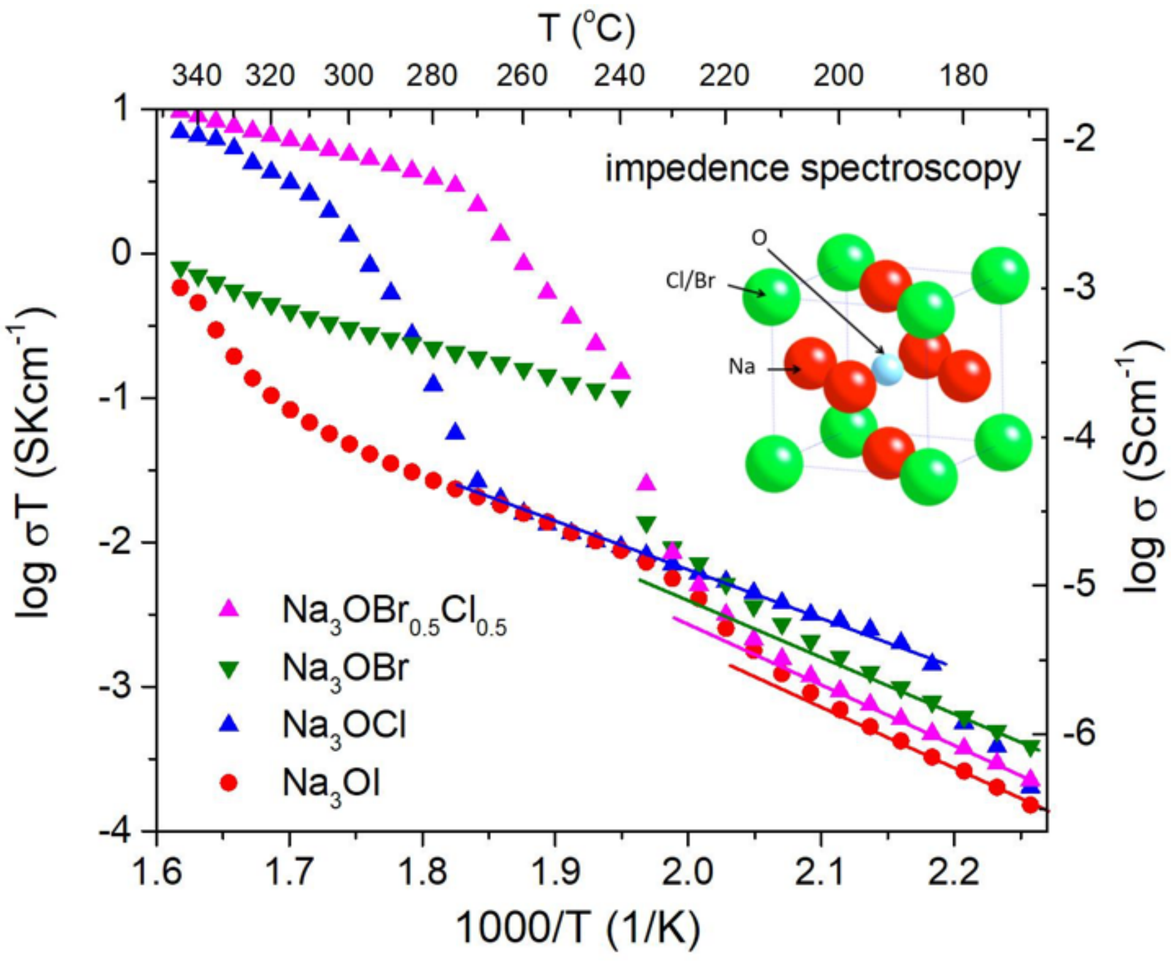

Figure 1

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