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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/ma2020-025966mtgabs

Peer reviewed

Temperature-Dependent Atomistic Dynamics Correlated to Cation Transport in Cluster-Ion Anti-Perovskites

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Citation Ping-Chun Tsai *et al* 2020 Meet. Abstr. MA2020-02 966

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Abstract

As fast-ion conductors, cluster-ion anti-perovskites (APs) are attractive for potential new mechanisms of conduction whereby cation and anion motion is highly correlated [1,2]. Cluster-ion APs, like perovskites, have a framework that accommodates diverse atomic substitutions. Furthermore, the potential for cluster-ion substitution onto one or both anion sites (A and B in X_3AB) provides additional compositional degrees of freedom. To identify model cluster-ion APs for understanding such conduction mechanism, we have synthesized and characterized ~20 cluster-ion APs compositions, from which $Na_{3-x}(NH_2)_xO_{1-x}(BH_4)$ has been identified as an ideal model system for understanding the correlation between cluster-ion rotation and cation transport as shown in Figure 1. Particularly, $Na_2(NH_2)(BH_4)$ exhibits an unusual positive deviation from ideal Arrhenius behavior indicative of a flattening of the energy landscape with increasing temperature. Concurrently, the sodium conductivity increases by 10^4 to 10^5 , which is most likely due to some combination of the effects of Na vacancy introduction and NH_2 and/or BH_4 anion mobility. Herein, synthesis, property, and characterization of the cluster-ion APs, aimed at understanding the temperature-dependent atomistic dynamics and its effects on cation transport, will be discussed in the presentation.

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.

References:

- [1] Hong Fang and Puru Jena. Li-rich antiperovskite superionic conductors based on cluster ions. *Proceedings of the National Academy of Sciences*, 2017, 114, 110461.
- [2] Hong Fang and Puru Jena. Sodium Superionic Conductors Based on Clusters. *ACS Appl. Mater. Interfaces*. 2019, 11, 963-972.

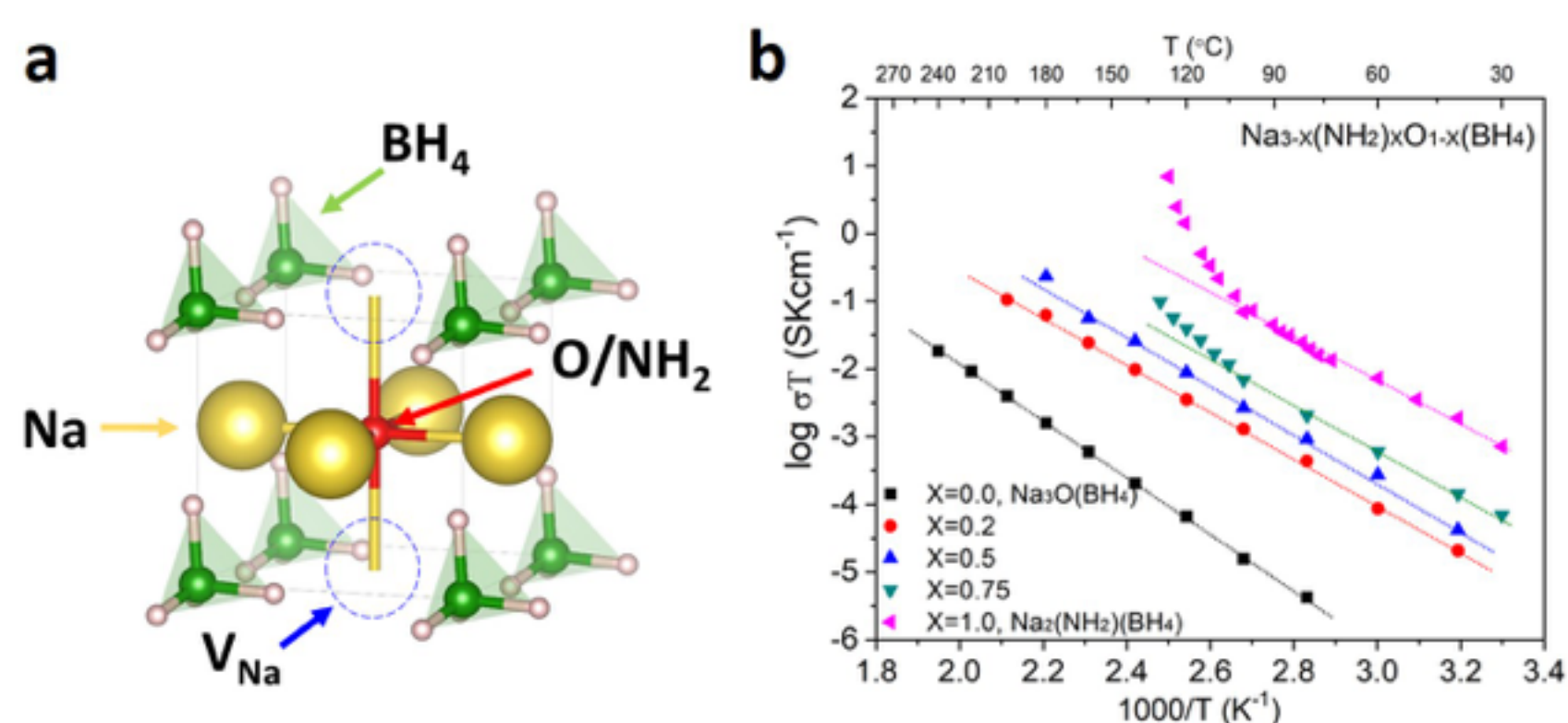


Figure 1. The (a) atomistic model and (b) ionic conductivity of $Na_{3-x}(NH_2)_xO_{1-x}(BH_4)$ cluster-ion APs

Figure 1

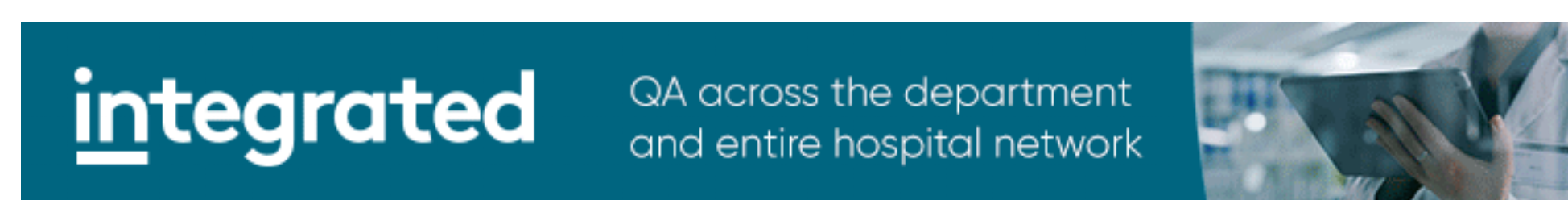
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