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

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Abstract

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.

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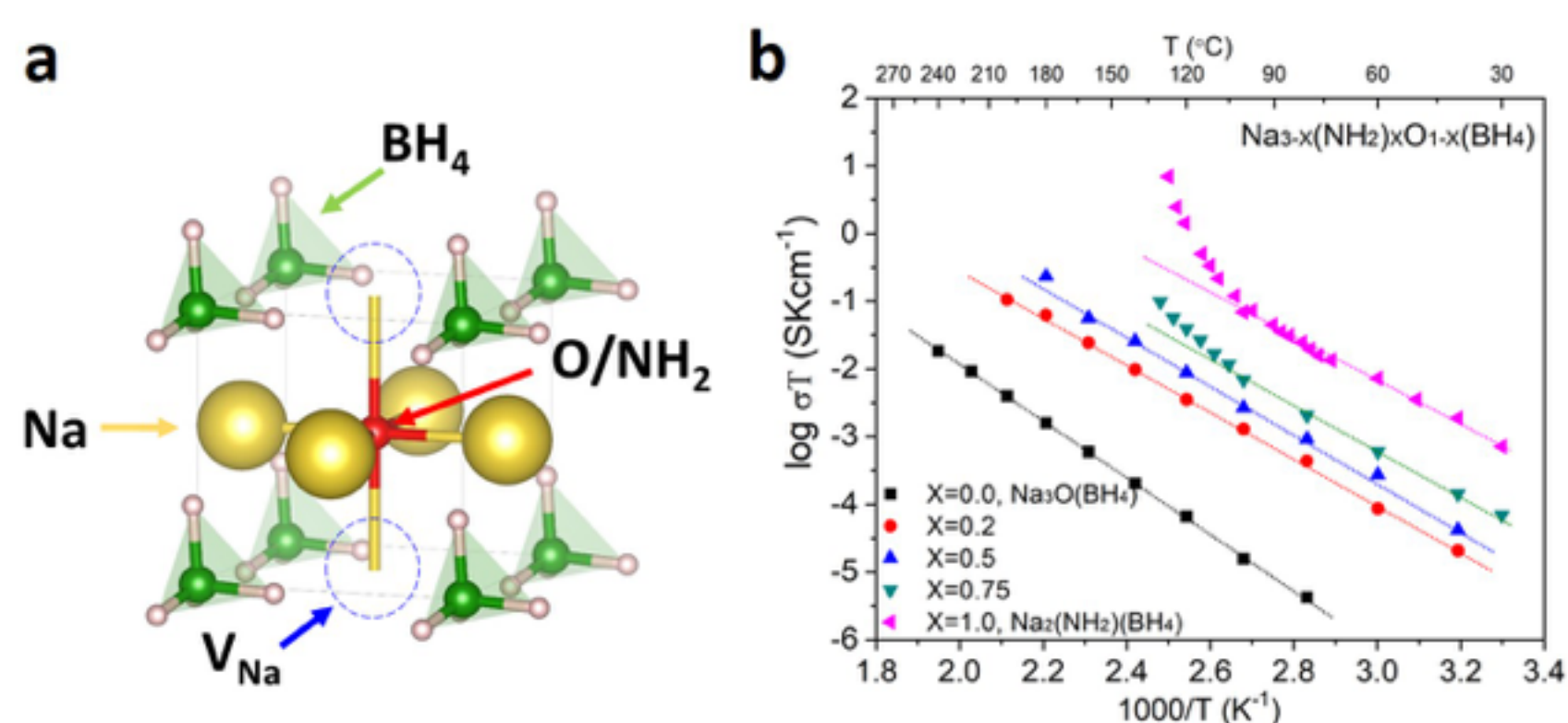
Figure 1. The (a) atomistic model and (b) ionic conductivity of $Na_{3-x}(NH_2)_xO_{1-x}(BH_4)$ cluster-ion APs
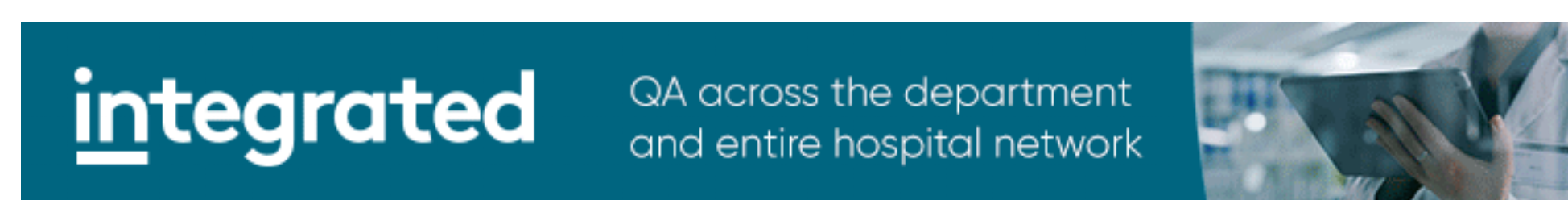
Figure 1

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