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First-principles investigations of ionic conduction in Li and Na borohydrides JOEL VARLEY, TAE-WOOK HEO, KEITH RAY, STANIMIR BONEV, BRANDON WOOD, Lawrence Livermore Natl Lab — Recent experimental studies have identified a family of alkali borohydride materials that exhibit superionic transition temperatures approaching room temperature and ionic conductivities exceeding 0.1 S/cm^{-1}, making them highly promising solid electrolytes for next-generation batteries. Despite the rapid advances in improving the superionic conductivity in these materials, an understanding of the exact mechanisms driving the transport remains unknown. Here we use *ab initio* molecular dynamics calculations to address this issue by characterizing the diffusivity of the Li and Na species in a representative set of closoborane ionic conductors. We investigate both the Na and Li-containing borohydrides with icosahedral ($B_{12}H_{12}$) and double-capped square antiprism ($B_{10}H_{10}$) anion species and discuss the trends in ionic conductivity as a function of stoichiometry and the incorporation of various dopants. Our results support the borohydrides as a subset of a larger family of very promising solid electrolytes and identify strategies to improving the conductivity in these materials. This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

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